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conference on the application of computing methods to reactor problems

May 17-19, 1965

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PROCEEDINGS OF THE
CONFERENCE ON THE
APPLICATION OF COMPUTING METHODS
TO REACTOR PROBLEMS

May 17-19, 1965

Margaret Butler
General Chairman

Sponsored by
Argonne National Laboratory
European Nuclear Energy Agency
Mathematics and Computation Division,
American Nuclear Society

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PREFACE

This conference on reactor mathematics and the application of computers to the solution of reactor problems had three sponsors and 242 participants. The conference was originally proposed and planned by the Mathematics and Computation Division of the American Nuclear Society. Argonne National Laboratory served as the host facility, and the European Nuclear Energy Agency handled the European arrangements.

Five years ago, in April 1960, a similar meeting, a "Seminar on Codes for Reactor Computation," was held in Vienna, Austria, sponsored by the International Atomic Energy Agency.

Bengt Carlson of LASL served as Chairman of the Technical Program Committee and was assisted by Charles Kelber, ANL; Tom Olsen, MARTIN; and Johnny Rosen, ENEA. In organizing the program, the Committee's aim was to achieve a balance of reactor physics computation, mathematics, and computer programming technique in the presentations. After reading this volume you can evaluate the success of their efforts.

AEC support has made possible the publication of these proceedings which have been edited by Alvin Glassner, Joyce Kopta, and Ellen Thro, of the Laboratory's Technical Publications Department. Doris Haight of the Applied Mathematics Division transcribed the tape-recorded discussion periods and the Session Secretaries assisted in the editing of this material. Actual publication was efficiently handled by the Argonne Graphic Arts Department.

This first meeting sponsored by the Mathematics and Computation Division is to be followed by a second International Conference, cosponsored by the Mexican AEC, to be held in Mexico City, in the spring of 1967--and, hopefully, many more.

Margaret Butler
General Chairman

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INTRODUCTION

MARGARET BUTLER:

I am very glad to see all of you here. For a while the last few months, especially the last few days, we were worried that maybe we wouldn't make it. To get the meeting underway, I am pleased to introduce Dr. Albert Crewe, Director of Argonne National Laboratory, who will convey to you our official welcome.

DR. CREWE:

It is a pleasure to welcome you on behalf of the Laboratory, and I must say it is a particular pleasure to me to welcome the large contingent from Europe, including even some from my own home country. I am sure you are all aware of the interest of this Laboratory in the subject of your conference, and I won't belabor the point very much more except that I do wish you well in your meeting, and hope that ultimately, in a decade or two, you may completely solve our problems and eliminate the need for our critical facilities and other kinds of experimental data-taking equipment.

I must say that I, as a nonreactor physicist, was quite shocked when I first learned of the inaccuracies involved in the calculations of reactor problems, particularly due, not completely to your problems, but to those of the people measuring cross sections. I must say I was also rather delighted to see that the sense of humor still remains in the naming of reactor codes. I often wonder what fraction of the effort goes into writing the codes and what fraction of the effort goes into choosing a name for the code. I haven't dared investigate this in our own Laboratory. One is always afraid of the answers one might get.

I hope that while you are here you will have some opportunity to look around the Laboratory. If you do, please don't be surprised if you find people who know nothing about reactors. About half of the people in the Laboratory know nothing about reactors and, the other half, of course, do know a little. It is, of course, due to the generosity of some of the nonreactor people that we are meeting in this fine, new auditorium, the existence of which is due to the relative affluence of the high-energy physicists, as opposed to the reactor physicists, a state which doesn't in general last very long, as you well know. Again, I welcome you to the Laboratory; I hope you will have a chance to look around, to enjoy the tours, which take place, I believe, tomorrow or the day after, and I wish you well in your meeting.

MARGARET BUTLER:

Next, I would like to introduce the man who is in no small way responsible for this meeting--Dr. Ira Zartman, Chief of the Reactor Physics Branch of the Division of Reactor Development and Technology, United States Atomic Energy Commission.

DR. ZARTMAN:

I don't know that I can claim too much of the responsibility because the work was not done by me, but by Margaret and her cohorts with the assistance that I am sure she got from the Secretariat of the European Nuclear Energy Agency. I wish to welcome you to this conference on behalf of the Atomic Energy Commission, and also on behalf of the European Nuclear Energy Agency, a group which is playing an important part in the development of the exchanges of information in the fields of nuclear energy between the United States and the European countries comprising the Agency's activities. It is encouraging to see such a large number of people here at this meeting who are actively engaged in the field of reactor development, particularly from the computational standpoint. As Dr. Crewe has mentioned, the ideal is to calculate the reactor and not have to go through the long, laborious, experimental procedures of designing them entailed when one goes through the many critical experiments. I think the easy days of reactor development have long passed by, when you could put a hunk of fissionable material into an environment and play around a little bit to get it critical. Now, it is not that which one is after, nearly as much as to economize on the neutrons that you have available, because if you can't make the best economy with the neutrons that come out of this fissioning process, the business interests and the utilities won't be very much interested in the nuclear energy program. So, I think, the field of computation is going to be a big help in the development of the reactor program.

The AEC encourages the efforts of professional societies to set up conferences, symposia, and seminars of this type. We feel this is one way of proceeding and carrying out our development in the best possible manner. We are not only appreciative, therefore, of the American Nuclear Society's Division of Mathematics and Computation for acting as a cosponsor of this meeting, but we are also interested in the international activities of other countries and, as such, we encourage and spend lots of time, money, and effort to bring about meetings, seminars, and conferences involving our colleagues from other countries. In particular, we are very appreciative of the activities of the European Nuclear Energy Agency.

Two weeks ago, we had a rather profitable seminar at Brookhaven on the evaluation of neutron cross-section data. A five-day session, restricted to evaluators--people who are actually working in this field--was held there, and the organization of that meeting was rather unusual, but extremely beneficial. It took place in the form of discussions without having papers elaborately prepared in advance. The discussions were summarized on the spot, printed during the night, and distributed the next day; by the time the participant went home, he had a stack of reports of the discussions and could even review them on his way home if he were that interested. The conference there was not all work, however, because somehow or other they found time to spend half a day at the World's Fair and help reduce the

deficit. I must say that on the following morning everyone seemed to be in a very good, alert condition, so I think they devoted themselves entirely to seeing the sights of the Fair. I don't know what Argonne has to offer to this Conference in a similar fashion. The Chicago area, of course, is well known for entertainment, and I suppose all of the activities of this Conference will not be devoted exclusively to testing and discussing reactor codes.

I would like to say a few words about the AEC's relationship with the European Nuclear Energy Agency because it may not be widely known; at least I have run across numerous people who are not fully aware of some of these relationships. About, I guess, five or six years ago, these relationships became established largely through the European American Nuclear Data Committee, at first, and then, shortly afterwards, we had a committee called the European American Committee on Reactor Physics. The European Nuclear Energy Agency had recommendations from these groups on various activities that could be exchanged or on which cooperative efforts could be undertaken. I know that Dr. Kowarski came to Washington on several occasions to discuss some of these topics; out of all this have come a number of cooperative efforts in the form of meetings, largely, but more recently, the ENEA has set up a Centre for Neutron Data Compilation at Saclay and, also, a Computer Programme Library at Ispra. To improve the cooperative efforts between the ENEA and the United States we have entered into an agreement with the Agency to exchange information in the nuclear-data field and, also, to exchange programs for nuclear energy computation with these two centers. The exchanges will be centered in the United States--for the neutron data compilations, through the Brookhaven Sigma Center, for the shielding calculations, through the Radiation Shielding Information Center at Oak Ridge, and for the nuclear energy codes, here, with the Argonne Code Center. Now, I will not enter into any discussion about the operation of these centers. One of the items on the agenda of this meeting covers that. However, I would like to mention that the aim is to bring about an exchange of nuclear energy computer programs in this country with the European countries, and to try to have the centers obtain and distribute among the users in their respective countries the computer programs that are developed in these countries. Through these centers we hope to encourage the establishment of certain standards for the contents of these programs and the abstract descriptions of them, and to try to develop common languages to describe them. Through these cooperative efforts we hope to encourage further development of computer codes and, also, to issue publications.

The efforts and the relationships have been excellent, and I look forward to this meeting as being a further example of the good relationship between the two groups--the United States AEC and the ENEA. In particular, I feel that we owe a great deal to Dr. Perret and his cohorts in encouraging this type of a meeting and in going to the great trouble that they do in the ENEA Secretariat to assure these meetings are a success. I hope, that as

you proceed, from now on in the conduct of this meeting that you will find it a pleasant experience to share your information and to enter into fruitful discussions with your colleagues from abroad. Thank you.

SESSION I

NUMERICAL ANALYSIS AND REACTOR MATHEMATICS

Monday, May 17, 1965

CHAIRMAN: Robert Avery
Argonne National Laboratory

CO-CHAIRMAN: James H. Alexander
General Atomic

SCIENTIFIC SECRETARIES: Harold Greenspan
Edwin Pennington
Argonne National Laboratory

RECENT DEVELOPMENTS IN COMPUTERS AND THEIR IMPLICATIONS FOR REACTOR CALCULATIONS*

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University of California
Los Alamos, New Mexico

(Paper presented by W. J. Worlton)

I. INTRODUCTION

The word symbiosis has a Greek origin meaning "to live together" and usually implies that two or more forms of life live together for their mutual benefit. The concept can be generalized to mean any mutually beneficial relationship, including different areas of science. It would be difficult to conceive of physics without mathematics, medicine without chemistry, or engineering without physics. The present high level of development of the sciences could hardly have been achieved without the very effective mutual assistance which they provide each other.

This paper, and indeed this conference, is concerned with the symbiotic relationship between the Nuclear Sciences and the Computer Sciences. Although conceived earlier, both of these sciences were born in the 1940's, and have matured together. The Nuclear Sciences have provided motivation and direction for the Computer Sciences, and the Computer Sciences have provided the means for solving problems in the Nuclear Sciences which could not have been attacked in any other way. The need for scientific computation was felt so strongly by the National Laboratories and other laboratories of the AEC contractors that they pioneered the development of stored-program computers in the early 1950's, e.g., the ORACLE at Oak Ridge National Laboratory, the AVIDAC at Argonne National Laboratory, and the MANIAC-I at Los Alamos Scientific Laboratory. It would be impossible to write a "Who's Who" of the early development of computing without including a large number of nuclear scientists whose influence covered both fields: von Neumann of the Atomic Energy Commission, Householder at Oak Ridge, Ulam and Metropolis at Los Alamos, Flanders at Argonne, and Ehrlich and Hurwitz at Knolls.⁽¹⁾ Although computing now has a much broader base of support than just the Nuclear Sciences, there remains a strong and important relationship between these disciplines.

In this paper we will analyze the effects of recent changes in computing technology on this continuing relationship, including the growing capabilities of computers, the changing price structure of computing, and the requirements imposed on the computing industry by reactor calculations.

*Work performed under the auspices of the U. S. Atomic Energy Commission.

We have confined our attention to the ultra-high-speed computers rather than to the whole range of computers which might possibly be used in such calculations.

2. THE REQUIREMENTS OF REACTOR CALCULATIONS

2.1 Classification of Reactor Calculations

Sangren,⁽¹⁻⁷⁾ following the work of Radkowsky and Brodsky,⁽⁸⁾ has been largely responsible for a unified classification of the wide range of reactor calculations. This conceptual model, shown in Fig. 1, notes the four major areas of reactor calculations and the important approaches in each area. The classification can be carried further to show code types and methods of solutions, but soon loses its conceptual value as it gains completeness. The model is intended to provide only a general insight and is an intentional oversimplification of a very complex and overlapping field.

Fig. 1. Classification of Reactor Calculations

2.2 The Limitations on Reactor Calculations

Problems in the analysis of nuclear systems, together with the problems in the aerospace industry and weather analysis, belong to that difficult class of scientific calculations for which there has never been a computer with enough speed, storage, or adequate input-output equipment to satisfy the demand. This has implied that crude, inexact methods were used rather than the more elegant, but more expensive, methods. It has meant that one-dimensional codes were used when two and three dimensions were really needed to provide complete and accurate information. It has meant that diffusion theory was used where transport theory was needed.

It has meant using a series of time-independent calculations, with hand calculations in between, instead of time-dependent calculations. It has meant running Monte Carlo calculations to low confidence limits. It has meant restricting the number of calculations which have gone into parameter studies for optimization purposes. As the capabilities of computers have increased, some of the restrictions imposed earlier have been removed. But as the computing time for a particular type of calculation is reduced, the calculation is then used as part of a parameter study, thus imposing new quantitative requirements.

The most important restriction, however, has been qualitative in nature. There has always been a class of problems for which the available computers were inadequate--problems which were simply out of the question, either because of excessive storage requirements or excessive running time. Calculations which take a full 8-hr shift to complete border on the impractical, since a very large fraction of the total computing capacity is committed to them, and they thereby exclude other calculations. Thus, both quantitative and qualitative boundary conditions have been imposed on reactor calculations by the speed of the computers available.

Storage capacity has also imposed restrictions on the class of possible reactor calculations. An attempt has been made to bypass the storage restrictions by segmenting problems to allow the use of an external storage medium, usually magnetic tape or disk, as an extension of main storage. The effect of this has been to increase the code preparation and debugging time (since the control algorithms are more complex), increase the probability of error (since no external storage device is as reliable as main storage), and increase the running time (since access to any auxiliary storage device is relatively expensive in time).

2.3 Increase in Computing-capacity Requirements

The increase in computing-capacity requirements over a long period of time in a scientific research center can be gauged quantitatively from Fig. 2. This figure shows the history of the computing capacity, measured in 7090 units, installed at Los Alamos Scientific Laboratory since 1952. The step function shows actual capacity, and the straight line is a "rule of thumb" line showing the growth in requirements. This curve, approximated by $C = 2^{0.5t}$, indicates that there is a long-term increase in computing-capacity requirements of about a factor of two every 2 yr. Selengut⁽⁹⁾ has suggested that the speed of available computers increases by about an order of magnitude (a factor of ten) every 5 yr. This would correspond to an increase of $C = 2^{0.67t}$ rather than $C = 2^{0.5t}$. However, this value was suggested for short-term increases rather than the long-term experience shown in Fig. 2. The curve is not meant literally, of course, but has provided an accurate guide for anticipating computing requirements for many years.

Fig. 2

Growth in Computing-
capacity Requirements

2.4 Some Specific Requirements of Reactor Calculations

Each problem type in Fig. 1 has its own peculiarities and needs. For example, Monte Carlo calculations have only modest storage requirements, but have long running times; diffusion-theory codes have less stringent requirements for running time, but use large blocks of storage; S_n calculations use both large amounts of storage and large amounts of running time. Since the S_n calculations present some of the more difficult problems, these requirements will be examined in detail.

Average running times for S_n calculations of varying dimensionality are shown in Table 1, with the 7030 used as a reference computer. From this table it is possible to gauge the increase in computer speed needed to reduce multidimensional S_n -calculation time so these calculations can be used as part of an optimization study. This is a point that is easily overlooked: the single-calculation time does not provide a correct estimate of the usefulness of a code, since dozens or even hundreds of these calculations are used in the optimization of a nuclear system. Note that each dimensional increase costs about a factor of twenty in running time over the lower dimensions. This includes a factor of two in the number of angular rays to be evaluated, and a factor of about ten for the number of space points used.

Table 1

REPRESENTATIVE RUNNING TIMES FOR S_n CALCULATIONS

Computer Speed X 7030	Execution Time for S_n Calculations		
	1-D, min	2-D, min	3-D, hr
1	10.0	200	67.0
5	2.0	40	13.0
10	1.0	20	6.7
20	0.5	10	3.3
100	0.1	2	0.7

It would require a computer which was twenty times as fast as the 7030 to run two-dimensional problems at the same rate at which we now run one-dimensional problems. This provides us with a guide for estimating the computing power needed for S_n calculations: we gain a dimension when the speed of computers increases by a factor of twenty.

The extremely wide range of running times and storage requirements for S_n calculations is indicated by Table 2. Both absolute and relative numbers of mesh points for which the angular flux must be evaluated are indicated as a function of n , the S_n order, and d , the number of space dimensions. The number of angular rays is given by $M = 2^d n(n+4)/8$; the number of space points is assumed to be 10^{d+1} . Thus the number of mesh points for each energy group is given by

$$P_{n,d} = 10^{d+1} 2^d n(n+4)/8.$$

The calculation time does not increase precisely with the number of mesh points, however, since the additional mesh points increase the convergence rate. The total number of mesh points for which the angular flux must be calculated is given by $GP_{n,d}$, where G is the number of energy groups. For twenty-five energy groups the angular flux array can range in size up to 40,000,000 points! This storage requirement is usually reduced by telescoping the storage, i.e., each new value of the angular flux is stored in the same storage cell as some previous value, so that one of the space variables is estimated and fluxes retained only on the boundaries.

Several conclusions can be drawn from this analysis. First, it is clearly impossible to store the angular flux array in main storage for multi-dimensional S_n problems. This implies that the use of these calculations is solidly tied to efficient auxiliary storage devices with low cost-per-word, fast access time, and high transmission rate. If we were to conjure up such a device, it would have a storage capacity of fifty-million words, an access time of a few milliseconds, a transmission rate approximating the main storage, and a cost of a few cents per word. All of these characteristics have been achieved in separate devices, but not in a single device.

Table 2
 REPRESENTATIVE MESH-POINT REQUIREMENTS
 FOR S_n CALCULATIONS

n	d	M	$P_{n,d}$	$R_{n,d} = P_{n,d}/P_{2,1}$
2	1	3	300	1.00
4	1	8	800	2.67
8	1	24	2,400	8.00
16	1	40	4,000	13.33
2	2	6	6,000	20.00
4	2	16	16,000	53.33
8	2	48	48,000	160.00
16	2	80	80,000	266.67
2	3	12	120,000	400.00
4	3	32	320,000	1066.67
8	3	96	960,000	3200.00
16	3	160	1,600,000	5333.33

A second conclusion from Table 2 is that the general use of three-dimensional S_n calculations awaits the development of a computer which is several hundred times as fast as the computers which are presently available. Although the next generation of computers will reduce the calculation time to where a few three-dimensional calculations of high interest can be done, they will still consume a large fraction of the total computing capacity.

Although the above requirements are sufficiently stringent that they will give job security to computer designers for many years to come, they by no means exhaust the field. Reactor dynamics, for example, present a compounding of the difficulties encountered in criticality calculations. A burnup code is a means of running a controlled series of criticality calculations, with a nuclide-depletion calculation added.

Kinetics calculations have all of the difficulties of criticality calculations, but with the effects of time dependence added. It would seem unlikely that the computing industry could produce a computer in the next 20 yr which would exhaust the requirements of reactor calculations.

3. RECENT DEVELOPMENTS IN COMPUTER DESIGN

3.1 The New Computers

The computers considered here will be those whose first delivery date is scheduled in 1964 through 1967 and whose internal speed is at least equal to the 7030. Nine computers fall into this category. Table 3 summarizes some of the pertinent information about these computers.

Table 3

THE NEW HIGH-SPEED COMPUTERS

Manufacturer	Computer	Approximate Monthly Rental, \$ ^{a)}	Approximate Speed X 7030 ^{b)}	Approximate Delivery (first)
CDC	3800	50,000	1	1/66
CDC	6600	80,000	6	9/64
CDC	6800	85,000	20	7/67
GE	635	55,000	1	11/64
IBM	360/62	58,000	1	9/65
IBM	360/70	80,000	2	9/65
IBM	360/92	142,000	20	9/66
PHILCO	213	78,000	2	9/65
UNIVAC	1108	45,000	2	8/65

^{a)}Rentals vary by a factor of two, depending on configuration. These values are taken from Adams Associates, "Computer Characteristics Quarterly (Mar)."

^{b)}These speeds are taken from LASL tests.

The speeds given in the table are subject to several qualifications: (1) they are based on large scientific calculations; (2) there is considerable variation in relative computer speeds even within this class of calculations; (3) except for the 6600, the values given are manufacturer's estimates; (4) the values given are for single-processor systems, even where multi-processor systems are offered.

The first-delivery dates in Table 3 are also approximate, as some organizations have found the hard way!

Several facts of interest for reactor calculations are immediately apparent from this table. First, computers will soon be available which exceed present computer speeds by a factor of twenty. This is a rather important number in view of the discussion in Section 2.4, since this means that we will gain a dimension in reactor calculations with the delivery of these faster systems. Second, computer rentals and purchase prices have not significantly increased; if anything, they have decreased. Since computer speeds have increased, this means that more problems can be run for the same amount of money that was possible previously, or, put another way, the cost per problem will be considerably lowered by the new computers. Third, IBM is getting a significant amount of competition in the high-speed computer market. Since IBM is not continuing the 7090-series of computers, and the 7030 sales were fairly small, the IBM hold on the high-speed market has been broken. 7094 users are faced with reprogramming, regardless of whether they stay with IBM or go to another manufacturer, so many users are for the first time taking a hard look at other manufacturers. This probably accounts to some extent for the improved price-performance structure being offered to the customers for the new computers.

3.2 The Trend in Computer Speeds

Figure 3 shows computer speeds measured in 7030 units plotted against the first delivery date of the computer. There is a double trend in this development. The lower line shows the general speed trend for the IBM-7090-series, as well as its predecessors and competitors. The upper line is an ultra-high-speed development, started by the 7030, which will apparently cause the termination of the lower line. The cluster of computers at the end of the lower line are all capable of multiprocessing operation; where this option is exercised, these computers fall even closer to the upper line. Since ultra-high speed is crucial to many types of reactor calculations, we can all view this accelerated development of faster computers with a great deal of satisfaction. In fact, the research organizations represented here today probably had a considerable influence on the development.

Fig. 3
Increase in Available
Computing Speed

These trends cannot be projected indefinitely into the future, of course, although it will be interesting to see how far and at what rate the development will go. The length of the transmission lines in computers is already becoming a crucial factor in achieving speeds; after all, nature will send information no faster than about one foot per nanosecond. One way to overcome this limitation is to design smaller computers, so that the signals need not travel so far. Another is the use of parallel circuits, such that many signals are being transmitted at once, i.e., to break the single transmission time into many shorter, parallel transmission times. The

first of these methods is being employed in the microminiaturization-packaging techniques employed in integrated-circuit technology. The second is being employed in multiprocessing designs. The combination of smaller circuits with multiprocessing systems will allow faster computers to be developed for some time.

3.3 The Trend in Computer Costs

Figure 4 shows a 12-yr trend in the cost of running a problem. As a figure of merit for problem cost, we have taken the monthly rental divided by the speed of the computer. Thus, if rentals are equal but one computer is twice as fast as another, twice as many problems can be run for the same amount of money on one computer as compared to the other. This implies that the cost per problem is cut in half. This figure of merit needs to be qualified by a factor which determines the percent of the computing capacity which can be profitably used. The figure of merit used here is most meaningful to users who can saturate the capacity of a computer with useful work. Absolute costs become important for those organizations which can use only a fraction of the time they have available on a computer. For example, a 360/70 has a cost per problem which is about four times the cost per problem for the 360/92; if the capacity of the 360/92 can be fully occupied, then the 360/92 is a much better buy. However, if the 360/70 will satisfy the requirements, the absolute cost becomes dominant, and a factor of two can be saved in problem cost.

Fig. 4
Trend in Problem Cost

Several startling facts are apparent from Fig. 4. The first is that it takes a three-cycle semilog plot to show the decrease in computer costs in a 12-yr period. Let's hope that trend continues! The second is that the year 1965 will see a sharp discontinuity in the trend of computer costs. For whatever reasons, we will suddenly be able to buy computing power in 1965 and 1966 which is cheaper by a factor of ten than it was 2-3 yr ago. We have attempted to discover the reason for this by discussing the new price structure with some leading manufacturers, and they give two main reasons for this dramatic development: competition and integrated circuits. The competition has developed largely because IBM has had to let go of a market of several hundred large-scale users in the 7090-series, and their competitors have done some fine work in producing competitive machines. Integrated-circuit technology could be seen on the horizon as early as 1959, but is just now making its impact felt on the industry. These circuits are cheaper to manufacture by about a factor of four, they are more reliable, and because their manufacturing processes can be automated, they allow more firms to compete for this market. The ease with which a product can be produced strongly influences the competition.

A question which is frequently considered about computer systems concerns the relative merit of several small systems compared to one large, fast system. Figure 5 is a log-log plot of cost per problem versus the speed of the computer, which can be used in the analysis of this question. This plot shows that it is in general true that the faster the computer is, the less it costs to run a problem on it. As with Fig. 4, this needs to be qualified with the assumption of total use. A least-squares fit of this data gives

$$C = 65S^{-0.83},$$

where C is cost per problem in arbitrary units, and S is the speed of the computer in 7030 units. In other words, the cost of running a problem on a computer is inversely proportional to the 0.8 power of the speed of the computer. For example, the 360/92 is about nine times as fast as the 360/70, but the rental is only higher by a factor of two; thus, it would cost about four to five times as much to use nine 360/70's to do the work of the 360/92, if questions other than cost are assumed to be equivalent for the two systems.

Fig. 5
Problem Cost vs.
Computer Speed

The trend to faster computers, then, carries with it the inherent implication of lower cost per problem. It is surprising to find that a problem which cost \$800 to run on the 704 can be run on modern computers for \$8!

3.4 The Trends in Computer Storage Systems

Computer storage systems can be classified in several ways; in Table 4 they are classified by their access mechanism as being (1) random access (e.g., magnetic cores), (2) cyclic access (e.g., magnetic disks), and (3) serial access (e.g., magnetic tape). The figures given in Table 4 are area prices only and do not reflect any particular systems. Classified by their functions, storage systems are used for (1) main storage (which communicates directly with the Central Processing Unit) and (2) auxiliary storage (which serves both as an extension of main storage and for input-output communications).

Table 4
COMPARISON OF STORAGE SYSTEMS

Storage System	Approximate Cost/Word, \$	Approximate Access Time	Approximate Transmission Rate, kc	Reliability	Removable?
Random access					
Fast	20.00	1/2-1 μ sec	10,000	Very high	No
Bulk	2.00	5-10 μ sec	1,000	Very high	No
Cyclic access					
Drum	0.20	5-20 msec	1,000	High	No
Disk	0.02	5-200 msec	1,000	High	No a)
Serial access					
1-in tape	0.00002 b)	5 msec-5 min	200	Medium	Yes
1/2-in. tape	0.00002 b)	5 msec-5 min	100	Low	Yes

a) Some manufacturers have developed removable disk packs.

b) This price does not include the cost of the transport

Main storage, which is the most critical in the computer's hierarchy of storage, has imposed restrictions on reactor calculations largely because the standard capacity has been limited to 32K (K = 1024). This restriction will be lifted considerably by the new computers, which have a standard capacity of 128K, or 131,072 words. The addressing capability of the new computers will allow expansion of directly addressed storage to twice that amount, or 262,144 words, and some computers can address up to two-million words. However, the cost of computer storage systems is inversely proportional to their access time, and million-word main storages are not yet practical, even if they are possible: at \$20 per word, a million-word main storage would not normally pay for itself.

Since the delivery of the first 704, in January 1956, the cycle time of computer main storage has decreased by a factor of 50--from 12 μ sec in the 704 to 250 msec in the 6800. The effective access time of storage

systems has decreased even further, however, since all modern main-storage systems consist of many independent boxes which have interlaced addresses, so that the probability of a conflict in access requests is considerably decreased. The 6800, for example, has 32 independent boxes of storage, so the probability of random requests going to the same box is rather small.

For many years there has been a technology gap between the devices used for main storage and those used for auxiliary storage--a gap of three orders of magnitude in access time and a similar, but inverse, gap in cost. This gap is now being filled by the introduction of a type of random-access storage which has speed and cost which are lower by a factor of ten than the main storage. This is usually referred to as "bulk storage." The advantage of bulk storage is that it can be addressed as an extension of main storage; the disadvantages include its cost (100 times the cost of disk) and its limited capacity compared to disk (defined both by its cost and the addressing limitation). For very large storage requirements, bulk storage at \$1 or \$2 per word is clearly too expensive to pay its way. Its usefulness will depend on those applications which require an intermediate-size storage, say 500,000 words, for which the access time rather than the transmission rate is crucial. This is a specialized requirement, and the applications of bulk storage are not yet well developed.

One of the most far-reaching developments in storage systems is the design of high-performance, low-cost disks. Whereas tapes have been used previously for auxiliary storage, they are rapidly being replaced by disks, both in software and in applications. Disks have several advantages over tapes: (1) they are much more reliable, (2) they have larger storage capacity, (3) they have higher transmission rates, and (4) they have lower positioning times. These advantages have led to entirely new concepts in operating systems as well as the ability to handle efficiently very large data arrays in scientific applications. There is a world of difference between a computer with 32K of main storage using tapes for auxiliary storage, and a computer with 128K of main storage using disks for auxiliary storage. This combination will allow large multidimensional reactor calculations to be programmed with very little more difficulty than was previously attached to one-dimensional calculations.

Associative storage, also called "content addressable storage," is a new approach to the addressing problem. Whereas the traditional method of referring to the contents of main storage is by an explicit address, associative storage is referred to by its contents. The reference quantity, called a key, is simultaneously compared with the contents of every cell in the storage, and the cell which matches the key is then read out. In the most general case, the key can refer to any part of the storage word. The most obvious application for associative storage is for applications which depend on "table look-up" procedures. An identifier is stored with the

data, and it is then not necessary to search for the data, since readout is instantaneous upon presenting the identifier to the storage. Tables of the form $[\theta, f(\theta)]$ could be stored, and instantaneous access could be obtained from $f(\theta)$ upon presenting the argument θ . This could have important applications in Monte Carlo codes which require functions of random numbers. Associative stores are several times as expensive as directly addressed stores, and the need for the associative store is specialized, so very large capacities of this type will probably not be used. However, a few thousand words of associative storage for tables would be useful in many reactor calculations.

3.5 Trends in Computer Organization

Demands for increased speed and reliability in computers have led to several forms of parallel computer designs, called "multiprocessing." The term multiprocessing implies that more than one computer unit is active at any given instant in time. We will use the term explicit multiprocessing to refer to those designs in which the Central Processing Unit (CPU), the Storage Units, and the Input-output Control Units are separable--physically, logically, and electronically. Figure 6 illustrates this design. In these designs, there may be several CPU's, several completely independent Storage Units, several Input-output Control Units, and more of each can be added to meet computing, storage, and input-output requirements. The advantages of the explicit multiprocessing designs lie in their modularity and reliability. The computing, storage, and input-output capacity of the machine can be tailored to fit the needs very precisely, and if the needs increase, more units can be added. Computers of this design almost never go off the air completely, since all units are duplicated. The GE-600 series computers, the Philco 213, and the Univac 1108 are examples of computers using this design.

Fig. 6. Explicit Multiprocessing Design

Multiprocessing is used in another form in the CDC-6000 series and the IBM-360/92 (see Figs. 7 and 8); we will refer to this form as implicit multiprocessing. In these designs there is only a single CPU, but there are many independent logical units within the CPU which operate concurrently. Instead of a single arithmetic unit, for example, there are many independent arithmetic units within the CPU. Instead of a single instruction stack, there may be an instruction stack for floating-point, another for fixed-point, and another for branching instructions, and another for store instructions--and each of these may have their own operand registers. It appears to be easier to obtain high speeds with implicit multiprocessing than with explicit multiprocessing; accompanying the higher speeds is an inherent lower cost per problem.

Fig. 7. Implicit Multiprocessing Design

Fig. 8. Block Diagram of 6600

The logical extension of multiprocessing is found in highly parallel designs, such as the Westinghouse Solomon-II. Instead of having just two or three CPU's, this design offers up to 1024 CPU's, each with their own storage and arithmetic unit. The arithmetic units are relatively simple, and individually are not particularly fast, but when 1000 add-instructions are executed simultaneously, the effective instruction time is lowered by three orders of magnitude! The difficulty in this design lies in the programming. In order to obtain high performance with this design, it is necessary to keep a large number of the CPU's busy, and not every mathematical method is amenable to simultaneous operations on all mesh points. For those methods which can take advantage of the design, the gain is very great; the particle-in-cell method in hydrodynamics and elliptic partial differential equations in general are the most immediate areas of application. This design, however, falls into the category of special-purpose computers, and is unlikely to replace conventional designs.

3.6 Trends in Computer Software

Any discussion of software which pretends to be at least partially complete must divide software into two general categories: 1) programming languages, and 2) operating systems.

Programming languages are designed to make life easier for the programmer--at least in theory. There can be little question that great strides have been made in this area since the early days of internally stored-programmed computers when programmers worked in octal machine codes stored in absolute locations. The next development was relative and regional assembly programs which allowed operation mnemonics and symbolic data references. It is difficult to imagine the immense amount of manpower which would be required to program the entirety of today's volume of problem codes by such techniques.

The advent of FORTRAN and other automatic-coding languages provided a breakthrough in allowing the problem proposer to develop his own problem codes without requiring the services of an expert. In terms of computer efficiency, however, this is not an unmixed blessing. An appreciable amount of machine time is used in compiling, retrying incorrect codes, and simple misuse of the language itself. Often the language is not capable of permitting efficiency even though the programmer is aware of shortcuts and other methods of obtaining efficiency. For this reason, some compilers allow supplemental use of "longhand" coding. There are drawbacks to this technique, however, if one wishes to run his code on an incompatible computer. Longhand coding still is the only efficient coding technique if one is interested in maximum computing speed and flexibility. The question is one of programmer efficiency versus computer efficiency.

Continuing efforts are being made to improve the efficiency and flexibility of programming languages. It is somewhat surprising, however, that there are only a few small, scattered efforts being made in developing languages which are more convenient for the programmer. There are only trivial technical obstacles which prevent such refinements as superscripts, subscripts, "displayed" division, and mathematical function symbolism being used without artificial, cumbersome, and "unnatural" notational devices.

At present there seems to be a philosophical contest between one general all-encompassing language and numerous more-or-less specialized languages. In the latter case we have, for example, FORTRAN, ALGOL, and others for scientific users; COBOL, COMTRAN, and others for business users; and APT for industrial users. It is not clear how this contest will end, but it appears that computer manufacturers are making every effort to reduce the number of languages to one, if possible.

IBM has for some time been developing NPL, New Programming Language, as a possible future successor to FORTRAN. Many programmers are questioning the desirability of such a replacement in the immediate future. It would appear that the final answer to this question will depend in large measure upon the compiling speed and object code efficiency achievable with NPL. There are some who doubt this will ever be possible. Many do not expect this to occur within the next three to five years. The reaction to an administrative decision to discontinue FORTRAN within the near future would likely be most interesting to witness!

The development of elegant(?) debugging techniques over the last decade has not kept pace with the relatively elegant development of the programming languages. The feasibility of remote consoles and multi-programmed operating systems will doubtless accelerate developmental efforts in more convenient, faster response-time debugging methods. To some degree, the success of such methods will depend upon the user's ability not to waste excessive amounts of computer time.

Programming languages for use with multiprocessor computers would not need to be significantly different from uniprocessor languages. If, however, one program used more than one processor, it would be necessary to augment the language for control purposes. The maximum output of a multiprocessor system would normally be obtained if each problem run limited itself to one computer module.

Parallel processors of the SOLOMON type would pose difficulties in problem formulation in many cases due to boundary conditions, activating and de-activating various processors, conditional branching, and so forth. Such difficulties would give rise to special language statements. For many types of problems, new mathematical formulations would, in addition, be required.

With regard to operating systems there appears to be a definite trend towards multiprogramming (or multitasking) supervisors. In a multiprogramming system, one computation may be interrupted in order to give the computer another calculation while input-output is being performed for the first problem or because the second problem is of higher priority or because an allotted amount of time has expired which is cyclically given to a set of problems. Improved computer efficiency should therefore result unless the "overhead" is too high. Another advantage is that the computer is available to more problems "simultaneously"--some of which might be debugging runs which would otherwise have to wait for problems to be completed.

A trend which has been apparent for some time and which greatly improves "turnaround" time is that of parallel execution of input-output on-line. At the present time a single 1100-line-per-minute printer attached to our 7030 usually has a problem's output available within 5 min (rarely as long as 15 min) after a problem's completion. Before the acquisition of this printer, output was written on a tape to be printed on a 1401, and the total delay would usually be from 1-2 hr. It is anticipated that our next computer will have three printers--two of which will be used in this fashion. Parallel input methods also reduce turnaround time.

The problem of higher volumes of output from future faster computers is a question of no little concern. The assistance of the programmer will be required to reduce the amount of output per unit of computation if reasonable and practical amounts are to be generated. One technique which would appear feasible would be for the user to store detailed results on a large storage device and request only "summary" type results to be printed. If, then, within 24-48 hr (or ?), the user needs some of this stored information, it could be provided. Following that, the stored information could be destroyed or transferred to tape or removable disk. The aim would be to print only that information which would actually be used.

It also appears that there is a trend towards greater use of graphical and plotting devices. The information content per page with such devices can often be extremely high. A variety of such graphical devices, as well as film viewers and printers, are currently available.

Software trends, in general, would tend to indicate greater convenience in the area of programming languages. On the other hand, it would appear that some amount of inconvenience may be imposed on the programmer because of more complicated operating systems which attempt to maximize computer efficiency. This, however, should result in improved service and turnaround time.

4. CONCLUSION

To understand any rapidly developing technology it is important to analyze trends rather than current status. This is especially true for those who are responsible for influencing the selection and design of computing equipment. The trends toward higher speeds, lower costs, parallel organization, and larger capacity memories are all beneficial to the scientific users of computing equipment. There is a parallel trend, however, which should be viewed with some concern: The combining of commercial and scientific computing requirements into a single design. This could be beneficial since it might contribute to lower overall costs for the manufacturers and users. The scientific user must beware, however, that scientific requirements do not get diluted in the mixture, such that his needs are overlooked. Scientific users should analyze and document their requirements, and then transmit these to the manufacturers in order to influence the design of future computers. It may be of sufficient importance for the Reactor Mathematics and Computation Division to establish a committee on computer design, whose purpose would be to summarize the continuing requirements of reactor calculations and present these to the manufacturers.

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THE CALCULATION OF THERMAL-NEUTRON SPECTRA-- GENERALIZED FREE-GAS THEORY

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ABSTRACT

The direct solution of the complete Boltzmann equation for thermal neutron spectra in reactor lattice cells, by the multigroup collision probability method, for example, is undesirable for two reasons. Firstly, since the spectrum is insensitive to nearly all of the detail of the scattering law, the essential physics is hidden, making physical insight nearly impossible. Secondly, as a corollary, the calculations are excessively wasteful of machine time and storage capacity. A second-order differential thermalization operator is derived from the Boltzmann equation and designated the Generalized Free Gas operator. A similar operator has been used by Cadilhac *et al.* It contains all the important physics to sufficient accuracy, avoids massive compilations, and gives rise to band matrix equations which are easy to solve. When applied along with a judicious combination of collision probability and diffusion theory, spectra can be calculated about one hundred times faster. Examples of the application of the NEUROSES code are given, including the spatial variation within a cell of the temperature coefficient of reactivity.

INTRODUCTION

1. Methods Based on Boltzmann Equation

Suppose a reactor physicist has just begun a study of thermal-neutron spectra in lattice cells and wishes to calculate cell parameters, such as ηf and its temperature coefficients. He would find that there is an exact equation governing the neutron flux, the Boltzmann transport equation, specified in terms of the neutron-scattering law $\Sigma_s(E', E, \cos \theta)$. The scattering cross section, from an initial neutron energy E' to a final energy E through an angle θ , is determined experimentally, and he would discover that today it is known with sufficient accuracy for most reactor materials. He would soon come upon the fact that the Boltzmann equation exists in two forms, an integrodifferential form and the Peierls' integral form. The former is solved by some variation of the SN method and is not very useful in

engineering practice, because it can be applied only to very simple fuel elements; so he chooses the integral form. He notes in the literature⁽¹⁾ that the spectrum is approximated accurately by assuming the scattering law isotropic in θ in the laboratory system of co-ordinates. Finally, he writes down the equation he must solve for the spectrum $\phi(\underline{r}, E)$;

$$\Sigma_T(\underline{r}, E) \phi(\underline{r}, E) = \int_{\text{cell}} d\underline{r}' P(\underline{r}', \underline{r}, E) \left[\int_0^\infty \Sigma_s(\underline{r}', E', E) \phi(\underline{r}', E') dE' + S(\underline{r}', E) \right]. \quad (1)$$

Here $P d\underline{r}$ is the probability that a neutron of energy E leaving point $\underline{r}'$ isotropically will make its next collision in $d\underline{r}$ at $\underline{r}$, Σ_T is the total cross section, and S is the neutron source strength per unit volume.

Our physicist is forced by the complexity of the equation to turn to numerical methods of solution and realizes that a large modern computer is a necessity. He adopts the simple idea of collision probabilities and divides his cell into L volumes A_ℓ , whose dimensions are no larger than approximately a mean free path, within each of which the physical properties, flux, and source may be taken as constant. He also divides the energy or velocity range into J groups and arrives at a finite difference approximation to (1). For example, in terms of neutron density $N(V)$, velocity $V = \sqrt{E/kT_0}$, and equal velocity intervals ΔV ,

$$\Sigma_{T\ell j} A_\ell V_j N_{\ell j} = \sum_{k=1}^L P_{k\ell j} A_k \left[\sum_{i=1}^J (\Sigma_{s k i j} V_i N_{k i} \Delta V) + S_{k j} \right], \quad (2)$$

with the collision probabilities P given by

$$P_{k\ell j} = \frac{\Sigma_{T\ell j}}{A_k} \int_{A_k} d\underline{r}' \int_{A_\ell} d\underline{r} \frac{e^{-n_{k\ell j}(\underline{r}', \underline{r})}}{4\pi|\underline{r}' - \underline{r}|^2}. \quad (3)$$

Here n is the number of mean free paths between $\underline{r}$ and $\underline{r}'$. About half of the machine time is spent in calculating (3), and the remainder using the large tables of $P_{k\ell j}$ and $\Sigma_{s k i j}$ to solve (2) by a sophisticated over-relaxation iterative method. The production of the $\Sigma_{s k i j}$ from experimental or assumed phonon spectra also needs a complicated program.

This direct method became possible with the advent of the IBM-704, and has been used successfully by Honeck^(2,3) and others, who describe all the relevant techniques. Surely with the increased speed and capacity of the computers of today nothing more need be added to this straightforward approach. Our reactor physicist need not explore further.

2. Objections - The Case for a Simpler Method

The authors believe that there are two important reasons against the general use of the direct method. The foremost objection is that physical insight has been sacrificed to the computer god, a not uncommon happening today. The role of mathematics in science should be first of all to find the thread running through the confused mass of experimental data, the thread which gives them meaning and interest, and then be the slave in producing numerical solutions. This thread usually generates new physical ideas, and these are "pearls of great price," which give wide service in guiding theory and experiment, in providing physical intuition, and in protecting against the misuse of theory or computer code.

In the present case, Eq. (2) is the delight of the numerical analyst, but unlike the theoretical physicist, he doesn't realize that he is hiding the needle of the basic physics in a haystack of detail and thereby wasting most of his efforts. It has been shown by Schaefer and Allsopp,⁽⁴⁾ and by Cadilhac et al.,^(5,6) (hereafter called I and II) that the neutron spectrum is insensitive to most of the enormous mass of detail in the scattering law. A simple second-order differential transport equation will be derived below, called the Generalized Free Gas equation, which contains the essential thread of the physics of the problem, and which shows that only the first two energy moments of the scattering law play any important part in the formation of the spectrum. This knowledge provides a broad base for physical insight and interest.

The second objection is a corollary to the first; the direct method makes excessive demands on computer time and memory capacity, due to the size and complexity of the complete scattering law. It might be thought that this point is invalid for today's computers. However, consider a typical case of 80 energy groups ($J = 80$) and 10 space points ($L = 10$), giving 800 mesh points (see Part II). Based on Honeck's⁽²⁾ experience, this would need some 15 min on a machine like the IBM-7090 to obtain fluxes to the required accuracy of 1 part of 10^8 . This time is still not negligible in burnup codes, especially when applied to a whole reactor and over its working temperature range. In the simple Generalized Free Gas theory proposed in this paper, the matrix equations take band form and may be inverted directly, making the solution some 60 times faster than the iteration of (2). This still leaves the few minutes needed for calculating the $\frac{1}{2} L(L+1) J$ independent values of $P_{k\ell j}$. As discussed in Part I below, this time may be virtually eliminated in most applications by the judicious use of transport-corrected diffusion theory together with the important fuel collision probabilities. The latter may be calculated quite accurately, even for complex fuel elements, by a simple procedure given by Schaefer⁽⁷⁾ and extended by Jonsson and Leslie.⁽⁸⁾ The net effect is that a method is available that contains the essential physics with sufficient accuracy and is about one hundred times faster than the direct method (see Part II), a typical case needing only some 10 sec on a modern computer.

The increased speed of the next generation of computers will partially reduce the effectiveness of this second argument. However, because a large library is needed for the tabulation of Σ_{skij} , $\frac{1}{2} J(J+1) L$ in number, at several different temperatures, the direct method suffers from slow read-in times and limited direct-access memory capacity. In fact, the 800-mesh-point case cannot be accommodated in the standard 32K-word memory. These machine parameters are not likely to improve greatly in the next generation of computers. On the other hand, the Generalized Free Gas theory uses only a twentieth of the scattering-law data, and gives an overall reduction by a factor of ten in read-in times and storage requirements (see Table 1 below).

Historically, the authors⁽⁹⁾ developed the simple model in 1959 because of its physical insight and because of the small demand it makes on the computer. A code NEUROSES⁽⁹⁾ (neutron spectrum in energy and space) was completed in 1960, for use on the English Electric DEUCE computer, a machine only slightly bigger than the IBM-650! During the past five years NEUROSES has been used many times, often on a 1000-point mesh, for the calculation of ηf and the spatial variation of its temperature coefficient within a lattice cell. It has been tested against experiment, primarily for gas-cooled reactors, with good agreement obtained.

The authors feel that the two reasons given above are cogent. It is hoped that the simpler theories will hold their ground.

Such a theory will be presented below, which contains all the essential physics, which avoids massive compilations, and which gives rise to matrix equations which can be solved quickly.

3. Simpler Theories

Some very simple theories are in use and successful in certain calculations. For example, the SPECTROX method,⁽¹⁰⁾ first demonstrated by the authors, uses the Generalized Heavy Free Gas equation⁽⁴⁾ and only two space values, the mean fluxes in fuel and moderator. The method uses diffusion theory in the moderator and collision probabilities in the fuel. It is probably the simplest realistic theory. It has been quite successful in predicting reactivities and moderator temperature coefficients in Calder Hall-type reactors.

However, these simpler models are generally too limited in applicability. Thus, SPECTROX gives little information on the spatial variation of temperature coefficients in a cell, important to heat transient studies, and is too inaccurate in the vicinity of absorption resonances, such as those of Pu²⁴⁰.

The theory presented below is intermediate between SPECTROX and the full Boltzmann equation.

In Part I the Generalized Free Gas equation is derived by a new method, and the complete cell-flux equations are specified. In Part II these equations are written in finite-difference form, and a method of solution is given. Part III illustrates briefly some of the many applications.

PART I--THEORY

1. The Generalized Free Gas Equation

The main barrier to a simple theory is the complex integral operator of Eq. (1). This operator may be rewritten formally in terms of $q(E)$, the net number of neutrons slowing down past energy E . In what follows we shall use the dimensionless variable $X = E/kT$. Now q is related to the flux by

$$q = \int_0^x dy \int_x^\infty dz [\Sigma_s(z, y) M(z) \psi(z) - \Sigma_s(y, z) M(y) \psi(y)], \quad (4)$$

where $M(x) = xe^{-x}$ and $\phi(x) = M(x) \psi(x)$. From this it follows that the integral scattering operator in (1) is given in terms of q by

$$\int_0^\infty \Sigma_s(y, x) \phi(y) dy = \Sigma_s(x) \phi(x) + \frac{dq}{dx}. \quad (5)$$

Thus the complication is shifted to q .

The essential idea in this paper is that $q(x)$ is slowly varying, so that the first few derivatives of q should contain all the important effects. We derive a differential equation as follows.

Let $\psi(x^1)$ in (4) be expanded as

$$\psi(x^1) = \sum_{n=0}^{\infty} \frac{1}{n!} (x^1 - x)^n \psi^{(n)}(x). \quad (6)$$

This will be valid except possibly near sharply varying absorption resonances or strong sources, where Placzek-function discontinuities may reduce its usefulness. However, for $A = 1$ (hydrogen gas), this objection does not apply, and for large- A moderators the "ripples" are confined to short intervals of energy of little importance. This leads us to expect that (6) will be useful for all A . Substitution in (4) gives⁽⁴⁾

$$q(x) = \sum_{n=1}^{\infty} \frac{1}{n!} F_n(x) \psi^{(n)}(x), \quad (7)$$

where the F_n are given by the recurrence equation

$$F_n^{(1)}(x) + nF_{n-1}(x) = M(x) M_n(x), \quad (8)$$

and are defined therefore entirely in terms of the energy moments of the scattering law

$$M_n(x) = \int_0^\infty \Sigma_s(x, y)(y - x)^n dy. \quad (9)$$

A general differential equation for q may be found by successive differentiation of (7), with elimination of the $\psi^{(n)}$, $n \geq 2$. Because of the detailed balance condition, the kernel of (4) is symmetric, making the integral equation for q self-adjoint. This will be true also for the inverse equation for ψ . We shall require therefore that the general differential equation for q , which replaces this inverse operator, shall be self-adjoint. Finally, our desired equation has the form

$$\psi^{(1)}(x) = j(x) q(x) - \frac{d}{dx} k(x) \frac{d}{dx} q(x) + \dots \quad (10)$$

(the nomenclature of II is used). It is instructive to rewrite (10) in the form

$$q(x) = \frac{\xi \Sigma_s(\infty)}{G(x)} \left(x \frac{d}{dx} + x - 1 \right) \left[\phi(x) + \frac{H(x)}{\xi \Sigma_s(\infty)} \frac{dq}{dx} + \dots \right], \quad (11)$$

with

$$G(x) = \xi \Sigma_s(\infty) x j(x) M(x), \quad H(x) = \xi \Sigma_s(\infty) k(x) M(x), \dots \quad (12)$$

The G , H , etc., may be considered as arbitrary, except that $G(x) \rightarrow 1$ as $x \rightarrow \infty$, so that the asymptotic slowing-down density is given correctly. They may be arbitrary since the differential bracket in (11) ensures that the flux is Maxwellian as leakage and absorption tend to zero, that is, as q , dq/dx , ..., tend to zero. It is also clear how to add higher derivatives.

When H , ..., are zero, (11) reduces to the Generalized Heavy Free Gas (GHFG) equation.⁽⁴⁾ When G and H only are retained, the equation will be called the Generalized Free Gas (GFG) equation. It is but an obvious extension of the former. Equations of higher order are of little importance, for the second-order equation already contains the important physics sufficiently accurate as will be shown below.

The $j(x)$, $k(x)$, ..., can all be found from the scattering law by substituting (10) into (7). If only two terms are retained, j and k will be given approximately as j_A and k_A . We find from the coefficients of $\psi^{(1)}$ and $\psi^{(2)}$ that

$$j_A = \frac{1}{F_1} \left(1 + \frac{d}{dx} F_1^{(1)} k \right); \quad (13)$$

$$k_A = \frac{\frac{1}{2} \int_0^x F_2 dy}{F_1^2 \left(1 + \frac{d}{dx} \frac{F_2}{2F_1} \right)}. \quad (14)$$

As expected, the coefficients of the $\psi^{(n)}$, $n > 2$, are not zero in general when (13) and (14) are substituted. However, there are two cases when they are zero, so that j_A and k_A are exact. The first is for free hydrogen gas ($A = 1$), showing that (10) is the exact inverse of the integral Eq. (4). Then (10) becomes the well-known Wigner-Wilkins equation. The second case is for a free gas with $A \rightarrow \infty$, since then the coefficients are of order A^{-2} for $n > 2$, and so zero in the limit. In this case k_A is also zero, and j_A is constant, so that (11) becomes the well-known Wilkins (HFG) equation. Both of these limiting cases are for free gases; hence the new name, Generalized Free Gas equation.

Equation (10) was derived first by Cadilhac et al.,^(5,6) but the new derivation above is simpler and clearer.

From (13), $G_A(\infty)$ may be found. It differs very little from unity for all practical moderators, being worst for D_2O with a value of 0.989. This small error is one indication of the excellent accuracy of the GFG theory. In practice the normalized $\bar{G}_A(x) = G_A(x)/G_A(\infty)$ will be used.

The physical insight of the GFG approach is provided by the transparency of the GFG differential equation relative to the original integral equation. It is clear that only the first two moments of the scattering law are important. From the shapes of $G(x)$ and $H(x)$ compared to those of a free gas, many of the effects of atomic binding can be forecast.⁽⁴⁾ An example of $H(x)$ for graphite at 600°K is given in Fig. 1. It is based on a Debye model with $\theta_D = 2.7T$. It differs considerably from the corresponding function in II. H is also shown for UO_2 gas. Many properties of G and H may be found in I and II.

2. Cell Equations in the GFG Theory

(i) Collision-probability Approximation

The cell equation in the GFG theory can be written immediately by using (1), (3), (5), and (11) in the collision-probability approximation. There are two coupled equations: the "neutron conservation equation,"

$$\Sigma_{T\ell}(x) \phi_{\ell}(x) A_{\ell} = \sum_{k=1}^L P_{k\ell}(x) A_k \left[\Sigma_{sk}(x) \phi_k(x) + \frac{dq_k(x)}{dx} + S_k(x) \right], \quad (15)$$

and the "detailed balance equation,"

$$q_k(x) = \frac{\xi_k \Sigma_{sk}(\infty)}{\bar{G}_{Ak}(x)} \left(x \frac{d}{dx} + x - 1 \right) \left[\phi_k(x) + \frac{H_{Ak}(x)}{\xi_k \Sigma_{sk}(\infty)} \frac{dq_k(x)}{dx} \right] \quad (16)$$

Fig. 1. $H(x)$ as a Function of Energy for Graphite and $UO_2(g)$

The boundary conditions in energy are:

$$q_k(0) = 0; \quad q_k(x_f) = f_k, \quad (17)$$

where x_f is the cut-off energy; generally between 2 and 4 eV, f_k is the number slowing down past x_f , and may be assumed flat in space, or better, may be estimated from a one-group solution of (15) at x_f .

The boundary condition at the cell outer wall may be of two types: (a) zero net current, in which case specular reflection in the $P_{k\ell}$ integrals is correct, or (b) an in-current may be present, which is taken care of by setting the S_k equal to the first flight collision densities. If the

cell boundary is circularized at the radius r_b , conserving volume, a prescription more accurate than specular reflection has been developed by Honeck.⁽¹⁾ This is to reflect neutrons off the circular boundary isotropically, which may be done explicitly, or more easily by adding an outer annulus one or two mean free paths thick (radius r'_b) of large scattering mass and zero absorption, with the zero-current condition applied to r'_b . Quite small pitches may be approximated quite accurately in this way.

In this approximation the input parameters are the constants ξ_k , A_k , and T_k , and the energy-dependent quantities Σ_{sk} , Σ_{ak} , $P_{k\ell}$, $\bar{G}_{Ak}(T_k)$, and $H_{Ak}(T_k)$.

In the above complete specification the thermalization effects have been simplified as much as is feasible. The two functions G_k and H_k replace the entire scattering law Σ_{skij} . As a consequence, most of the effort in the GFG theory is directed to the difficult calculation of the $\frac{1}{2} L(L+1)J$ independent values of $P_{k\ell}(x)$.

(ii) Diffusion Approximation

Fortunately, this transport kernel can be greatly simplified in most cells, with no important loss in accuracy, by using transport-corrected diffusion theory in the bulk moderator. Usually the cell is divided by a circular "channel wall," of radius r_c , into an inner and outer zone. The inner contains the fuel element, coolant, and possibly supporting or dividing annuli. This central zone will be divided into L collision-probability regions, for which the flux equations are (15) and (16). The outer zone is the main moderating region, and it will be assumed to be one-dimensional, by circularizing the outer boundary, for example. This is justified if Honeck's fictitious bounding annulus is used, and as long as the fuel zone does not depart radically from radial symmetry. The outer zone will be divided into N annuli, within each of which $\Sigma_{sn}(x)$, $\Sigma_{an}(x)$, $D_n(x)$, $\bar{G}_{An}(x)$, and $H_{An}(x)$ are constant. The diffusion theory will generally provide a good approximation if transport corrections are used at r_c . The $H(r_c)$ function of Carlvik and Pershagen⁽¹¹⁾ is suitable for this purpose.

The two zones can be connected by finding the number $N_\ell(x)$ of neutrons per second making their first collision in A_ℓ , having just come inwards through the "channel wall." It is known from several sources [for example, Stuart and Woodruff⁽¹²⁾] that N is insensitive to whether the incoming angular distribution is proportional to $\cos \theta$ or $\cos^2 \theta$. The actual distribution lies somewhere between these limits, and the former will be assumed. Then

$$N_\ell(x) = 4J_{in}(x) \Sigma_T \ell(x) A_\ell P_{\ell m}(x), \quad (18)$$

with

$$4J_{in} = \phi(r_c, x) + 3H(r_c) D(r_c, x) \frac{\partial \phi(r_c, x)}{\partial r}, \quad (19)$$

where $P_{\ell m}$ is the collision probability connecting region ℓ to the whole outer zone, and is given accurately enough in most cases by $1 - \sum_{k=1}^L P_{\ell k}$.

The complete set of flux equations can be written now. There are three types of "neutron conservation equations:" (a) the inner-zone equations are given by (15) with $N_\ell(x)$ added to the right-hand side, (b) the connecting equations at r_c ,

$$\sum_{k=1}^L A_k \left[\Sigma_{ak}(x) - \frac{dq_k(x)}{dx} - S_k(x) \right] = 2\pi r_c D(r_c, x) \frac{\partial \phi(r_c, x)}{\partial r}, \quad (20)$$

and (c) the diffusion equations of annulus n ,

$$\left[\Sigma_{an}(x) - \frac{1}{r} \frac{\partial}{\partial r} D_n(x) \frac{\partial}{\partial r} \right] \phi_n(r, x) = \frac{\partial q_n(r, x)}{\partial x} + S_n(r, x). \quad (21)$$

The "detailed balance equation" (16) is valid for each volume k or n .

The boundary conditions on energy are, as before, given by Eq. (17). The radial boundary condition for no net current is

$$\frac{\partial \phi(r'_b, x)}{\partial r} = 0, \quad (22)$$

whereas in-currents of various types may be allowed for by the general condition

$$\alpha(x) \frac{\partial \phi(r_b, x)}{\partial r} + \beta(x) \phi(r_b, x) = 0. \quad (23)$$

The input parameters are the constants ξ_k , A_k , r_c , r_n , r_b , r'_b , and T_k , and the energy-dependent quantities Σ_{sk} , Σ_{ak} , D_n , $\bar{G}_{An}$, H_{An} , as well as the $\frac{1}{2} L(L+1)J$ values of $P_{k\ell}(x)$.

3. Calculation of Collision Probabilities

Very little will be said in general about this very large subject, in which a host of techniques exist. If there is radial symmetry, the use of the S_N method is better than direct calculation of $P_{k\ell}$. However, if only inner-zone $P_{k\ell}$ are needed, relatively simple theories are well developed. Collision probabilities for gas-cooled fuel clusters can be obtained easily through the work of Schaefer,⁽⁷⁾ recently extended to ring-to-ring probabilities in clusters by Jonsson and Leslie,⁽⁸⁾ and needing only fractions of a second on a modern computer. Good progress on a simple model for liquid-cooled clusters has been made in unpublished work by Hill of English Electric Co. and Leslie of the A.E.A.

4. Comparison of Methods

The three main theories: the GFG with and without the diffusion approximation, and the exact Boltzmann, have been completely outlined now. It would be of interest to compare them with regard to the amount and type of independent input parameters, other than the common Σ_{sk} and Σ_{ak} . Two cases are illustrated in Table 1, each having 10 space (k) regions (1 in fuel and 9 in moderator) and 80 energy (j) groups, for a total of 800 mesh points. In case A, typically represented by a simple Calder Hall cell, there are only two zones with different physical properties, the fuel and the moderator, the latter having constant D. In case B, all regions have different properties, and all entries are energy dependent.

Table 1

		Case A			Case B		
		Diffusion GFG	Coll. Prob. GFG	Exact	Diffusion GFG	Coll. Prob. GFG	Exact
Transport Kernel, No T	$P_{k\ell j}$	80	4,400	4,400	80	4,400	4,400
	D_{nj}	1	0	0	720	0	0
	Total	81	4,400	4,400	800	4,400	4,400
Scattering Law, T Dependent	$\bar{G}_{Akj}$	160	160	0	800	800	0
	H_{Akj}	160	160	0	800	800	0
	Σ_{skij}	0	0	6,320	0	0	31,600
	Total	320	320	6,320	1,600	1,600	31,600
Grand Total		401	4,720	10,720	2,400	6,000	36,000

It can be seen from Table 1 that 95% of the scattering-law data is redundant in all cases. Without using the GFG theory the general case cannot be fitted into the standard 32K-word memory unit. Also apparent

is the enormous saving in calculating $P_{k\ell}$ when the diffusion approximation is used, and generally the remaining 80 $P_{k\ell}$ can be evaluated with ease in this case. The amount of storage required is significantly reduced by using the GFG theory, often by a factor of ten.

PART II--METHOD OF SOLUTION

1. Finite-difference Equations

These have been outlined in detail in Ref. 9, and in any case are relatively straightforward and tedious. It has been found very convenient and accurate to use a velocity mesh V_j with equal intervals $\Delta V = 0.1$. This covers the Maxwellian region, Pu^{239} resonance, and Pu^{240} resonance with comparable number of mesh points. It is necessary to extend the mesh up to at least 2 eV because of the important thermalizing effects in the Pu^{240} resonance.

One point should be stressed. The finite-difference forms for the "neutron conservation equations" must conserve neutrons to high accuracy. Terms like dq/dV should be integrated exactly over the mesh interval. All other terms have been approximated by

$$\int_{V_j-(1/2)}^{V_j+(1/2)} F(V) dV \doteq F(V_j) \Delta V. \quad (24)$$

One difficulty occurs over the dq/dV term in the "detailed balance Eq." (16). In order to conserve neutrons, this term must be found by solving the finite-difference form of the "conservation equations" for dq/dV in terms of the unknown fluxes (or densities). This means inverting equations like (15) to find the form

$$S_\ell + \frac{dq_\ell}{dx} = \sum_{k=1}^L a_{\ell k}(x) \phi_k(x), \quad (25)$$

which produces a matrix with half-band width $2L - 1$ in general. This procedure nearly doubles the amount of work in solving the equations. The inversion is much more economic than doubling the number of finite-difference equations by solving for ϕ and q . This trouble is nearly eliminated in the diffusion approximation.

The above method for the coupling coefficients has been written into the machine code NEUROSES.

2. Method of Solution

The enormous advantage of the GFG theory is that the matrix equations assume band form. The half-band width in the general collision probability form is $2L - 1$, but reduces to $N + 2$ in the simple diffusion case A above.

When the code was first used in 1959, several iterative methods were tried. The GFG equations are not of the form in which the central coefficient is always larger than the sum of the off-diagonal ones, but the difference depends on energy. Thus there are no simple convergence criteria. Over-relaxation has always diverged, but line Liebmann works slowly with a highest convergence eigenvalue of about 0.995, of no use in practice.

Next, a "forward step" method was used, starting from the lowest velocity line. This always diverged just beyond the Maxwellian peak.

The direct triangularization and back substitution always works and is very fast. Flux residuals are approximately 10^{-8} , and neutrons are conserved to about $\frac{1}{2}$ in 10^4 on a standard 800-point mesh. This kind of accuracy is required for studies of temperature coefficients.

3. Comparative Times for Solution

The number of operations required to solve (2) by iteration is $(LJ)^2 I$, where I is the number of iterations; the corresponding number for Gauss elimination of a band matrix of half-band r is $2(LJ) r^2$. For the full GFG case, $r = 2L - 1$; for the simple diffusion case, $r = N + 2$. These three cases are in the ratio 200:3:1 for the standard mesh. (From Honeck's results⁽²⁾ it is estimated that I is about 60 for 10^{-8} accuracy in flux.) This shows clearly the great speed of the GFG theory, literally turning minutes into seconds.

PART III--APPLICATIONS

1. Importance of H Term

To find the sensitivity of the spectrum to the H term, that is, to find the difference between the predictions of the GHFG and GFG theories, a SPECTROX spectrum was calculated for a typical advanced gas-cooled reactor (AGR) cell at the fairly high irradiation of 20,000 MWD/T. The values of $H(x)$ used in the calculation are shown in Fig. 1. The fuel cluster consisted of two rings of UO_2 rods, the inner containing 6 pins, the outer 12, held at a temperature of 1,200°K. A graphite support sleeve was also present. The extent and disposition of various regions may be learned from Fig. 3. The results are plotted in Fig. 2 in the region of the Pu^{240} resonance,

where the discrepancies are largest. The NEUROSSES result for $H = 0$ is also plotted, its mean moderator flux not being distinguishable from the corresponding SPECTROX flux.

Fig. 2
 $\bar{N}$ for Pu^{240} Resonance Region

H produces a deeper narrower depression in the fuel spectrum, similar to that found in II for a homogeneous medium, increasing the resonance escape probability. The effect in the moderator is quite different. But on the whole the effects are not large, considering the strong absorption. This is best seen by comparing the Pu^{240} reaction rate in the three spectra, for one neutron slowing down at 2 eV. These are: NEUROSSES ($H = 0$), 0.1046; SPECTROX ($H = 0$), 0.0983; SPECTROX ($H \neq 0$), 0.0955. The effect of H is only 3%, justifying the omission of the higher-order q derivatives in (10). The S_N value⁽¹³⁾ is approximately 0.1014, some 3% below NEUROSSES ($H = 0$), as expected. We can conclude that SPECTROX will not be improved by adding an H term, which is unfortunate. This 3% effect is 0.3% in reactivity, and this is appreciable. The corrected SPECTROX flux was 1.5% higher than SPECTROX ($H = 0$) flux at the Maxwellian peak.

2. Temperature Coefficients

The temperature coefficient of any region has been found by running NEUROSSES twice with the temperature of the desired region altered by 100°K. An example of the spatial variation of the temperature coefficient is shown in Fig. 3 for two irradiations. The coefficients are roughly proportional to the $\xi_k \Sigma_{sk} A_k$ of the region concerned, and the plotted results

are divided by this factor. It is of interest to note the change of sign at zero irradiation, the expected increase in the coefficient as the fuel is approached, and the appreciable positive prompt fuel coefficient deriving from the O_2 moderation.

Fig. 3. Spatial Variation of Temperature Coefficient for an AGR Cell

It is regretted that space does not permit any more to be said in Part III. These effects will be reported at length elsewhere.

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Discussion of Paper
Presented by Mr. Schaefer

MR. GRIGGS (Reactor Development Laboratory, Windscale): The approach about which Dr. Schaefer is talking is now very much in use in the United Kingdom in the design calculations of the AGR's. This approach is contained in the ARGOSY program, which uses the differential operator rather than an integral operator.

MR. SCHAEFER: We have used the simplified generalized heavy free gas equation for some time but not the higher terms in the expansions. I think you are referring to the use of the SPECTROX approximation, which is even simpler than that I have derived here, and your own work has shown that it is not accurate enough in the Pu^{240} resonance region. It needs the extra term as well.

MR. GRIGGS: My own work has shown that you can jazz it up in the case of the Pu^{240} resonance without coming to too much trouble.

MR. SCHAEFER: I would raise a serious objection to jazzing things up in that you have the enormous computer god on one side and the fudging on the other. I have been trying to present a case half-way between, which contains essential physics and which is easy to use on a computer.

MR. JARVIS (Atomic Energy of Canada): I do not agree that carbon is an in-between moderator. I think it is heavy, and when you come to deal with D_2O I would want to see it proved that you can get away with two moments. If you can't, you may have moved some work from the ordinary procedure, but you will throw a lot of work into calculating the moments. Again, this depends on your mathematical model, of course. I think it is painting the picture a little black in the normal type of calculations to say the matrix is full, because it is not. It is heavy down the middle, then it gets gray, and then certainly wiped out toward the edges because the elements get so small that they are of no use and, in fact, dangerous to use. I would ask if D_2O is heavy, or light, or in-between.

MR. SCHAEFER: The matrix isn't completely full; it is a hundred times fuller though. Secondly, D_2O is the worst possible case. There are several clues, however. We haven't compared yet any full-scale direct method runs with the simpler theory, but certainly towards the higher energy end the discrepancy is worst. The worst discrepancy seems to be about 1.1%, as indicated in the paper. D_2O is essentially heavy because of the oxygen. I still believe, without proof, that this theory will handle D_2O with all the accuracy required because of the detailed balance laws.

MR. NEILL (General Atomic): I was curious about the elimination of the scattering anisotropy. How well does it handle very heavily absorbing resonances--very strong resonances--more than you might encounter in regular lattices? And, with the elimination of anisotropies of scattering, how well did it do in the vicinity of control rods?

MR. SCHAEFER: I must refer the anisotropy question to Honeck or someone who worked on this a fair amount. I am basing my remarks on his and a few other people's work. As for strong resonances, I have taken the case of Pu^{240} level and you can't imagine a stronger resonance than this. I chose an enriched system. However, if the resonance is above about 1 eV, like in the Pu^{240} case, then this series does go over to the Greuling-Geortzel formulation. Therefore, it will take care of resonances just as much as that theory will. As for the Pu^{239} , again this is a fairly strong resonance. The calculation isn't so badly different from that for Pu^{240} as you saw from my flux curve; the tips connected with the Pu^{239} are not much, because of moderating effects, I think, compared to the Pu^{240} . Influence of the H term is not so important there. It amounts to only 5 or 10%. I think we picked most of it up. The flux changed by only about 1-2% when we put the H term in. It is a very heavily absorbing case in the Pu^{239} region.

THE CALCULATION OF NEUTRON SPECTRA IN THE DOPPLER REGION

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(Paper presented by R. J. Brissenden)

1. Introduction

The completely numerical attack on the problem of Doppler coefficients in reactors presented in this paper is based on the existence of very large computers capable of handling immense quantities of data quickly and efficiently. Given this capability it is possible to use a sophisticated model both for the description of the compound-nucleus formation and decay, in the generation of neutron reaction cross sections, and for the distribution of neutrons over energy resulting from these reactions with simple geometric configurations, in the generation of neutron fluxes for slowing-down situations. In this way we are able to take account of all the effects which are of some unknown importance but which are very difficult to handle in any other manner. While it is difficult to estimate the relative importance of such secondary effects as interference levels, shadowing between nuclides and between trains of levels of different J-states and of such primary effects as resonance overlapping, resonance scattering, resonance blockading, and spatial flux-shaping it is possible to argue the case for a completely numerical attack which makes it attractive even where alternative analytic approaches provide sufficiently good answers.

The problem may be divided into two parts: the nucleonics calculation and the neutronics calculation. In a purely numerical attack these will not interact; in other words, no a priori knowledge of the neutronics calculation required will be built into the cross-section data. Thus we have to produce cross sections as a function of energy in great detail. While this is a time-consuming job, even for a large computer, it only has to be done once and then the tabular cross sections stored on magnetic tape become available for neutronics calculations which are much faster. In fact, for relatively complex situations, they are faster than any corresponding analytic calculation which approximates all the primary effects.

To tabulate any cross section through the Doppler region (≤ 20 keV) requires $\sim 120,000$ energy points unless the energy mesh is cunningly chosen to fit the pattern of resonances. The complexity involved in using a mesh which varies for different nuclides does not justify such parsimony; therefore the mesh has been chosen adequately for all nuclides of interest in the range of temperatures of interest. Naturally, in so doing it over-specifies the cross sections of any particular nucleus (by a factor of two for U^{238} , for instance).

The calculation of cross sections is performed by three programs: RESP, GENEX, and RESINT. These correspond to three very natural subdivisions of the calculation, and each is briefly described in the following sections of this paper. The program RESP uses all available data on the resonance structure of the nucleus under consideration to construct a chain of resonances in the order of decreasing energy, starting from about 21 keV and using a random number generator to sample from the distribution laws for widths and spacings. The resolved resonances are brought in where available and included in the chain in the appropriate place. Less precise information about fluctuations in strength functions and α -values, which are usually available over narrow energy bands just above the resolved region, is utilized by means of a forced sampling procedure. In order to deal comprehensively with the Doppler region it is necessary to allow exit channels from the compound nucleus for photons, binary fission fragments, and neutrons in three scattering processes corresponding to two excited states of the bombarded nucleus. The data required to generate partial widths for these processes relies heavily on theoretical interpretation and models, and it is important to correlate on established experimental measurements. Even so there remains a considerable reservoir of uncertainty which is due to the poor accuracy of measurements in the regions of interest and the anomalous position of the theoretical basis of the fission process.⁽¹⁾

The second half of the calculation is done by the code GENEX, which generates cross sections from the level parameters, including Doppler broadening to various temperatures as required. The cross sections are formed from an approximate multilevel formulation which neglects terms at least of second order in the widths for processes. The Doppler broadening is performed analytically by use of a good fit to the broadening function.

The cross sections which come from GENEX require corrections to allow for the effects of distant levels which are temperature dependent. This correction takes the form of an additional $1/v$ cross section designed to make the total area under the curve up to the theoretical total given by the resonance parameters. The correction is of the order of a few per cent and is put in by the code RESINT.

The solution of the neutron-flux equations is obtained in the Doppler region starting from the integral equation for the neutron density in the case of isotropic scatter. Assuming a flat source for each of a number of regions of constant composition, the integral equation can be written as a series of linked first-order differential equations. The linkage involves the calculation of collision probabilities, which is not described in this paper. The differential equations are solved in a manner which preserves neutron balance, in the program SDR, and the fluxes are output to tape. The flux tapes can be edited and photographed in a variety of ways by the program SDRED which completes the series.

To demonstrate the working of the system, a hypothetical problem has been chosen, consisting of a mixture of U^{235} and U^{238} in hydrogen, the atomic mass of the fuel being taken as infinite. This then provides a problem with an exact analytic solution, but which also illustrates one important characteristic of the Doppler region, that is, the shielding of the U^{235} resonances by the U^{238} resonances, and vice versa. The results are analyzed in terms of escape probabilities, and it is shown that the probability of escape from a U^{238}/U^{235} mix is greater than the product of the escape probabilities for the U^{238} alone and the U^{235} alone. The size of the shielding interaction effect is calculated by a simple model and shown to be comparable with that obtained from the SDR code.

2. The Generation of Energy Levels in the RESP Code

The energy range of interest is the Doppler region where the effects of temperature on reaction rates is significant. Above this region lies another in which the Doppler effects are no longer significant, although it is not necessarily true that resonance structure is unimportant. However, the purpose of this paper is to deal with the Doppler region, which is taken to be from 3 eV to 20 keV. The Doppler region extends far into the so-called unresolved region in which individual resonances have not been observed. We are therefore driven to a statistical description of cross sections, and the data actually derived are a sample from the distributions describing the resonance behavior.

2.1 Spacings

Wigner⁽²⁾ has given a qualitative argument which suggests that the distribution of spacings is given by

$$P(s) ds = \frac{1}{2} \pi S / \langle S \rangle^2 \exp \left(-\frac{1}{4} \pi S^2 / \langle S \rangle^2 \right) ds, \quad (2.1.1)$$

where $\langle S \rangle$ is the mean spacing. This distribution comes approximately from the assertion that the level spacing is the same as the spacing of eigenvalues of a real symmetric matrix with random elements. The distance S between the eigenvalues of a (2×2) matrix is given by

$$S^2 = \xi_1^2 + \xi_2^2, \quad (2.1.2)$$

where ξ_1 is the difference of the diagonal elements and ξ_2 is the sum of the off-diagonal elements. Then,

$$S ds d\phi = d\xi_1 d\xi_2, \quad \text{where } \phi = \tan^{-1} (\xi_1/\xi_2), \quad (2.1.3)$$

that is to say, the probability of finding a level distance S from a given level is proportional to S . It is clear that this is only a plausibility

argument, but better results have been obtained.⁽³⁾ If $q(s)ds$ is this probability in general, then it is related to the spacing law $P(s)ds$ by the equation

$$P(s+ds) = \frac{P(s)}{q(s)} [1 - q(s) ds] q(s+ds). \quad (2.1.4)$$

Solving this, we get

$$P(s) = Aq(s) \exp - \int_0^s q(s) ds. \quad (2.1.5)$$

If we use our approximate value of $q(s)$, this becomes

$$P(s) ds = ks \exp\left(-\frac{1}{2}ks^2\right) ds.$$

By introducing the mean spacing

$$\langle s \rangle = \int_0^\infty sP(s) ds = \sqrt{\pi/2k},$$

we get Wigner's spacing law.

2.2 Widths

Porter and Thomas⁽⁴⁾ have studied the distribution of widths for neutron emission from the compound nucleus by the statistical procedure of maximum likelihood to choose between two distributions which look plausible. They concluded that the experimental evidence supports strongly that the neutron width fluctuates according to a chi-squared distribution with one degree of freedom. This implies that the reduced width amplitude is distributed on a Gaussian.

They advanced a qualitative argument which supports this view for heavy nuclei. Starting from the extreme complexity of the wave functions on the surface of the compound nucleus, the argument involves the central limit theorem in a loose manner to produce Gaussian distributions. They put forward as a hypothesis that all reduced width amplitudes are distributed on Gaussians and that many of the distributions are independent. Strong support for this is obtained by examination of known resonances,⁽³⁾ since it leads immediately to a Porter-Thomas distribution for the observed widths, the Porter-Thomas distribution being defined as the usual chi-squared distribution function renormalized by dividing the variate by the number of degrees of freedom.

Accordingly we sample from

$$P(x, \rho) dx = \frac{(\rho x)^{\rho-1}}{\Gamma(\rho)} e^{-\rho x} dx \quad (2.2.1)$$

where

$2\rho = \nu$, the number of degrees of freedom;

$x = \Gamma / \langle \Gamma \rangle$, the actual width over the mean width.

The choice of the two parameters ν and $\langle \Gamma \rangle$ is usually decided by an analysis of the resolved region together with plausible extensions to higher orbital angular momenta. In the case of fission it is also necessary to reproduce the observed α -value and fission cross section in a somewhat empirical manner.⁽⁵⁾

2.3 Sampling Technique

Starting from a uniform distribution in the range (0-1) which is obtained from a multiplicative type of random-number generator, we first of all form a Gaussian. If ξ_1 and ξ_2 are samples from a uniform distribution, then

$$\begin{aligned} x_1 &= (-2 \log \xi_1)^{1/2} \sin 2\pi \xi_2; \\ x_2 &= (-2 \log \xi_1)^{1/2} \cos 2\pi \xi_2; \end{aligned} \quad (2.3.1)$$

gives two variates on Gaussians. By inverting the relations we find,

$$\frac{\partial(\xi_1, \xi_2)}{\partial(x_1, x_2)} = \frac{1}{2\pi} \exp \left[-\frac{1}{2} (x^2 + y^2) \right].$$

Hence,

$$d\xi_1 d\xi_2 = \left[\frac{1}{\sqrt{2\pi}} \exp \left(-\frac{1}{2} x_1^2 \right) dx_1 \right] \left[\frac{1}{\sqrt{2\pi}} \exp \left(-\frac{1}{2} x_2^2 \right) dx_2 \right],$$

which are the required Gaussians. The chi-squared distribution is now obtained in the usual way as the sum of squares of samples from independent Gaussians. At the same time the samples renormalized to have unit length (considered as a vector) provide the direction cosines needed for the interference effects by means of the Vogt⁽⁶⁾ nomenclature.

If x is taken from a Porter-Thomas distribution with two degrees of freedom, then

$$P(x, 1) dx = e^{-x} dx.$$

$$\text{Let } y = \sqrt{4x/\pi}.$$

Then

$$P(x, 1) dx = (\pi/2) y \exp\left(-\frac{1}{4} \pi y^2\right) dy, \quad (2.3.2)$$

which is the Wigner spacing distribution.

2.4 Forced Sampling

The random levels generated by sampling freely from the distributions described in the last three sections are not necessarily going to be consistent with low-resolution measurements in the region just above the resolved energy band. To take advantage of this additional information a forced sampling procedure can be used. Instead of sampling freely, we sample only from the subspace of samples of given size with given mean value. The procedure will be described in terms of a variate x belonging to a distribution $f(x)$, $0 \leq x < \infty$. If we wish to sample N times to produce a sample $\{x_i\}$ with the additional property that $\sum x_i = \lambda$, then an unbiased sample is obtained by selecting x_i from $\phi_i(x)$, where,

$$\begin{aligned} \phi_i(x) &= f(x) / \int^{\lambda - \lambda_i} f(x) dx; \quad 0 \leq x \leq \lambda - \lambda_i \\ &= 0; \quad \lambda - \lambda_i < x < \infty \end{aligned} \quad (2.4.1)$$

and where

$$\lambda_i = \sum_{j=1}^{i-1} X_j; \quad i = 1, 2, 3, \dots, N-1; \quad \lambda_1 = 0.$$

and

$$X_N = \lambda - \lambda_{N-1}.$$

The proof follows by induction on $\phi_i(x)$; $i \leq k$.

If the order of the sample is relevant, then it must be randomly shuffled, because the ordering of the variates in the sample is clearly going to place the more probable variates first. In fact, when resonances are generated in the order of decreasing energy, the sample must be randomly

shuffled. The method of generating the distributions ϕ_i is by rejection from $f(x)$ and this leads to difficulties. If the value of λ is improbably small, the rejection rate towards the end of the sample can become astronomical. To overcome this, the sampling is terminated, and the remaining members of the sample are given the most probable values consistent with the whole sample having the correct mean.

3. The Calculation of Cross Sections in the GENEX and RESINT Codes

The R-matrix formation is much too complex in its full form to be used in this type of program, which is attempting to generate hundreds of thousands of cross sections. An approximation is used which was ascribed to Bethe by Lane and Thomas⁽⁷⁾ and which is, in fact, a well-known algebraic device for the approximate inversion of a matrix. The total cross section and the cross section for a process x can be written as

$$\begin{aligned}\sigma_t &= (\pi/k^2) \sum_{\ell, \Gamma, J} 2g_J \operatorname{Re} \left\{ 1 - \exp(2i\phi_\ell) \left[1 + i \sum_{\lambda \lambda'}^c (\Gamma_{\lambda c} \Gamma_{\lambda' c})^{1/2} A_{\lambda \lambda'} \right] \right\}; \\ \sigma_x &= (\pi/k^2) \sum_{\ell, \Gamma, J} g_J \left| \sum_{\lambda \lambda'} (\Gamma_{\lambda n} \Gamma_{\lambda' x})^{1/2} A_{\lambda \lambda'} \right|^2.\end{aligned}\tag{3.1.1}$$

The level matrix A is given in terms of its inverse:

$$(A^{-1})_{\lambda \lambda'} = (E_\lambda - E) \delta_{\lambda \lambda'} - \frac{1}{2} i \sum^c (\Gamma_{\lambda c})^{1/2} (\Gamma_{\lambda' c})^{1/2},$$

when

- J is the spin of the compound nucleus;
- ℓ is the orbital angular momentum of the incident neutron;
- λ is the energy index of the levels;
- Γ is the parity symbol;
- c is the channel-designating index;
- $\delta_{\lambda \lambda'}$ is Kronecker's delta;
- k is the wave number.

The approximate inversion is done by putting

$$A^{-1} = D + \Sigma$$

where D is the diagonal of A^{-1} . Then,

$$A = (D + \Sigma)^{-1} = D^{-1}(1 + \Sigma D^{-1})^{-1} \approx D^{-1} - D^{-1}\Sigma D^{-1},$$

neglecting terms of order Σ^2 . So the approximation for A is given by

$$A_{\lambda\lambda'} = \frac{\delta_{\lambda\lambda'}}{(E_{\lambda} - E) - \frac{1}{2}i\Gamma_{\lambda}} + \frac{1}{2}i \frac{E_{\lambda\lambda}\Gamma_{\lambda\lambda'}}{\left[(E_{\lambda} - E) - \frac{1}{2}i\Gamma_{\lambda}\right] \left[(E_{\lambda'} - E) - \frac{1}{2}i\Gamma_{\lambda'}\right]}, \quad (3.1.2)$$

where

$$E_{\lambda\lambda'} = 1 - \delta_{\lambda\lambda'};$$

$$\Gamma_{\lambda\lambda'} = \Sigma^c(\Gamma_{\lambda c})^{1/2}(\Gamma_{\lambda' c})^{1/2};$$

$$\Gamma_{\lambda} = \Gamma_{\lambda\lambda'} \text{ is the total width for the level } \lambda.$$

There are no other significant approximations for heavy nuclides. The error introduced is most significant between levels when there is a set of closely packed broad levels. The Pu^{241} nucleus exhibits this type of structure; Fig. 1 shows a comparison of the GENEX approximate treatment with the exact treatment described by Vogt.⁽⁶⁾ The cross sections produced are quite clearly sufficiently accurate for reactor physics purposes.

The infinite matrix A is truncated to the neighborhood of the energy point E at which cross sections are required. The summations indicated in 3.1.1 can then be performed to produce unbroadened cross sections. There are two points connected with this procedure which are worth mentioning at this stage, but which will be enlarged upon in later sections. Firstly, the truncation of the matrix A means that every level of A has its "tails" excluded from the cross-section calculation. This effect is by no means negligible if A is to be kept to manageable proportions. Moreover, the "tails" will be Doppler broadened, and therefore the error in cross sections will be temperature dependent and of the same order of magnitude as some Doppler coefficients. It is fatal, therefore, to neglect them in Doppler-coefficient calculations! Fortunately, the neglected part of the cross section will be smoothly varying (consisting, in fact, of a slight undulation between resonance peaks and slowly rising in a $1/\sqrt{E}$ shape with decreasing energy), and it is possible to correct for this in an accurate way by working out a theoretical cross-sectional area from the resonance parameters; this is then used to correct the approximate area obtained from GENEX by means of an additional $1/v$ component. This job is the function of the RESINT code.

Secondly, the unbroadened resonance shape is not a particularly useful function because of its extreme energy variation, which is maintained throughout the Doppler region. The storage of such a cross-section shape

Fig. 1. Pu^{241} Cross Section for Fission; Comparison of GENEX Treatment with Exact Treatment of Vogt

throughout the Doppler region in tabular form is quite out of the question, requiring at least 2×10^6 mesh points for adequate representation. Consideration of a numerical broadening technique is therefore ruled out and we are driven to analytical broadening. With Doppler broadening, about 120,000 mesh points are required for adequate representation. The Doppler width Δ is given by

$$\Delta = \sqrt{4kTE_n/A},$$

where

A is the atomic mass of the nucleus,

T is the absolute temperature,

k is the Boltzmann constant,

E_n is the incident energy of the neutrons.

With $A \approx 230$ we can construct the following table at 300°K. By means of this table an energy mesh can be constructed which will be roughly logarithmic and which will place something like twenty points in each resonance at high energies, increasing to around one hundred points at lower energies, where the peaks are sharper. The resulting mesh is given in Fig. 2.

E_n (eV)	Δ (eV)
20,000	2.95
10,000	2.08
5,000	1.47
1,000	0.66
100	0.21
10	0.07

Block	Upper Energy, eV	Mesh, eV	Block	Upper Energy, eV	Mesh, eV	Block	Upper Energy, eV	Mesh, eV
1	20633	0.5	17	5273	0.25	33	873	0.03125
2	19353	0.5	18	4633	0.25	34	793	0.03125
3	18073	0.5	19	3993	0.125	35	713	0.03125
4	16793	0.5	20	3673	0.125	36	633	0.03125
5	15513	0.5	21	3353	0.125	37	553	0.03125
6	14233	0.5	22	3033	0.125	38	473	0.03125
7	12953	0.5	23	2713	0.125	39	393	0.03125
8	11673	0.5	24	2393	0.125	40	313	0.03125
9	10393	0.25	25	2073	0.0625	41	233	0.03125
10	9753	0.25	26	1913	0.0625	42	193	0.015625
11	9113	0.25	27	1753	0.0625	43	153	0.015625
12	8473	0.25	28	1593	0.0625	44	113	0.015625
13	7833	0.25	29	1433	0.0625	45	73	0.015625
14	7193	0.25	30	1273	0.0625	46	33	0.01171875
15	6553	0.25	31	1113	0.0625	47	3	0.001953125
16	5913	0.25	32	953	0.03125			

Fig. 2. Energy Mesh Used to Tabulate Cross Sections

The extent to which the term $D^{-1}\Sigma D^{-1}$ needs to be brought into the calculation is dependent on the energy E . It is possible to show that the interference terms, which this represents, vanishes in the mean, so that at sufficiently high energies it should have no effect. The code is therefore arranged so that this term may be brought in, in a progressive manner,

starting at some highest point which is specified. Care must be taken to maintain the positive definite form of the cross sections, but there is very worthwhile saving in computer time as a result. The value of the p-wave contribution to the cross section decreases with decreasing energy, so this also may be progressively reduced to save computer time.

When the approximate form of A given in 3.1.2 is inserted into 3.1.1 we get the unbroadened cross-section shape which has been broadened by the methods developed by Buckler and Pull,⁽⁸⁾ but with a revised calculation of the basic broadening function. The cross section for process x is conveniently divided into three parts by this treatment:

$$\sigma_x = \sigma_x^s + \sigma_x^p + \sigma_x^{\text{int}},$$

the s-wave, p-wave and interference contributions, respectively. The basic broadening function is

$$F(w) = \int_0^\infty \frac{ze^{-z^2}}{z^2 + w^2} dz, \quad (3.1.4)$$

where w is complex. By defining

$$w_1 = \sqrt{\frac{A}{2kT}} \left[Q + i(P - U) \right]; \quad w_2 = \sqrt{\frac{A}{2kT}} \left[Q + i(P + U) \right],$$

where

$$P + iQ = \sqrt{\frac{2}{m} \left(E_\lambda + \frac{1}{2} i \Gamma_\lambda \right)},$$

m being the mass of the neutron and U being the neutron velocity, the broadened cross sections can be written as

$$\sigma_x^s = \mu_T \sum_{\lambda \Sigma S} g_\lambda^s \Gamma_{\lambda n}^{os} \Gamma_{\lambda x}^s \left\{ \text{Re} \left[F(w_1) - F(w_2) \right] \right\} / \Gamma_\lambda^s; \quad (3.1.5)$$

$$\mu_T = 4\sqrt{\pi} (a/\rho)^2 \sqrt{A/4kT}; \quad \rho = 0.002197a \sqrt{E},$$

where

E = neutron incident energy, eV

a = nuclear radius in units of 10^{-12} cm,

If we put

$$\alpha_{\lambda}^P = [\operatorname{Re}\{F(w_1) - F(w_2)\}] + \frac{\Gamma_{\lambda}^P}{2E_{\lambda}^P} \operatorname{Im}\{F(w_1) - F(w_2)\}, \quad (3.1.6)$$

then

$$\sigma_{\mathbf{x}}^P = \mu_T \sum_{\lambda \in \Sigma_P} g_{\lambda}^P \frac{\Gamma_{\lambda n}^{op} \Gamma_{\lambda x}^P}{\Gamma_{\lambda}^P} E_{\lambda}^P \alpha_{\lambda}^P \left(\frac{\rho^2/E}{1 + \rho^2} \right).$$

Finally, defining

$$D^1_{\lambda\lambda'} = D^3_{\lambda\lambda'} = [D(\lambda\lambda')]^{-1} \frac{1}{4} \Gamma_{\lambda} \Gamma_{\lambda'} (\Gamma_{\lambda} + \Gamma_{\lambda'}) \left[(E_{\lambda} - E_{\lambda'})^2 + \frac{1}{4} (\Gamma_{\lambda} - \Gamma_{\lambda'})^2 \right];$$

$$D^2_{\lambda\lambda'} = [D(\lambda\lambda')]^{-1} \frac{1}{2} (E_{\lambda} - E_{\lambda'}) \Gamma_{\lambda} \Gamma_{\lambda'} \left[(E_{\lambda} - E_{\lambda'})^2 + \frac{1}{4} (\Gamma_{\lambda} - \Gamma_{\lambda'})^2 \right],$$

where

$$D(\lambda\lambda') = (E_{\lambda} - E_{\lambda'})^4 + 2(E_{\lambda} - E_{\lambda'})^2 \left[\left(\frac{1}{2} \Gamma_{\lambda} \right)^2 + \left(\frac{1}{2} \Gamma_{\lambda'} \right)^2 \right] - \left[\left(\frac{1}{2} \Gamma_{\lambda} \right)^2 - \left(\frac{1}{2} \Gamma_{\lambda'} \right)^2 \right]^2,$$

we may broaden the interference terms:

$$\begin{aligned} \sigma_{\mathbf{x}}^{\text{int}} = 2\mu_T \sum_{\lambda, \lambda' \in \Sigma_S} \beta_{\lambda\lambda'} & \left[D^1_{\lambda\lambda'} \operatorname{Re} \left\{ F(w_1^{\lambda}) - F(w_2^{\lambda}) \right\} + D^3_{\lambda\lambda'} \operatorname{Re} \left\{ F(w_1^{\lambda'}) - F(w_2^{\lambda'}) \right\} \right. \\ & \left. + D^2_{\lambda\lambda'} \operatorname{Im} \left\{ F(w_1^{\lambda}) - F(w_2^{\lambda}) - F(w_1^{\lambda'}) + F(w_2^{\lambda'}) \right\} \right], \end{aligned} \quad (3.1.7)$$

where

$$\beta_{\lambda\lambda'} = \frac{\cos \theta_{\lambda\lambda'}^{\mathbf{x}s} g_{\lambda}^s \sqrt{\Gamma_{\lambda n}^{os} \Gamma_{\lambda n}^{os} \Gamma_{\lambda x}^s \Gamma_{\lambda' x}^s}}{\Gamma_{\lambda}^s \Gamma_{\lambda'}^s} S_{\lambda\lambda'}$$

and where

$$\begin{aligned} S_{\lambda\lambda'} &= 1 \quad \text{if } g_{\lambda} = g_{\lambda'} \\ &= 0 \quad \text{if } g_{\lambda} \neq g_{\lambda'} \end{aligned}$$

Here $\theta_{\lambda\lambda'}^{\mathbf{x}s}$ is the angle between $\Gamma_{\lambda x}$ and $\Gamma_{\lambda' x}$.

With the use of the same notation the following formulae for the total cross section are obtained:

$$\sigma_t^s = \mu_T \sum_{\lambda \Sigma S} g_{\lambda}^s \Gamma_{\lambda n}^{os} \operatorname{Re}\{F(w_1) - F(w_2)\};$$

$$\sigma_t^p = \mu_T \sum_{\lambda \Sigma p} g_{\lambda}^p \Gamma_{\lambda n}^{op} E_{\lambda}^p \alpha_{\lambda}^p \left(\frac{\rho^2/E}{1 + \rho^2} \right); \quad (3.1.8)$$

$$\sigma_t^{\text{int}} = 4\pi a^2 f(U\sqrt{\alpha}) + 2a \sqrt{E} \mu_T \sum_{\lambda \Sigma S} g_{\lambda}^s \Gamma_{\lambda n}^{os} \operatorname{Im}\{F(w_1) - F(w_2)\} + \sum_x \sigma_x^{\text{int}}$$

for energies in the Doppler region $f(U\sqrt{\alpha}) = 1$.

For energies above the Doppler region, the approximations to the phase shift factors built into these expressions are wrong, and the potential scattering falls off.

3.2 The Doppler Broadening Function $F(w)$

The function $F(w)$ is required to be calculated 10^7 times in a typical cross-section generation from 20 keV, and a very fast routine is required for its computation. It is a very difficult function to calculate inside the circle $|w| = 5$. Outside this circle the asymptotic formula is fast and accurate. The method developed utilized this fact and also the differential equation satisfied by $F(w)$ on any complex arc:

$$-\frac{dF}{dw} + 2wF = \sqrt{\pi}. \quad (3.2.1)$$

It can be seen that the derivatives of F are related to F by a second-order recurrence relationship; thus, given the value of F at some point w_0 , the values in the immediate neighborhood can be constructed from a Taylor expansion. The square circumscribing $|w| = 5$ was used to define a tabular domain. Noting that

$$F(w) = -F(-w); \quad F(\bar{w}) = \overline{F(w)}, \quad (3.2.2)$$

it is clear that only the first quadrant of this square is required. The square with corners 0, 5i, 5i + 5, 5 was therefore divided into 2,500 equal squares by a 50 x 50 uniform mesh parallel to the axes. The values of $F(w)$ on this mesh were then recorded. To find a value of $F(w)$, w is first transformed to the first quadrant using 3.2.2 and the nearest corner of the small square containing w is located; finally, a Taylor expansion gives the value required.

Differentiating 3.2.1 n times we get

$$-F^{n+1} + 2wF^n + 2nF^{n-1} = 0,$$

so that

$$F^{n+1} = 2 \left[wF^n + nF^{n-1} \right]; \quad n = 1, 2, 3, \dots \quad (3.2.3)$$

The required Taylor expansion is then

$$F(w) = F(w_0) + \delta w F'(w_0) + \frac{\delta w^2}{2!} F''(w_0) + \dots, \quad (3.2.5)$$

where $\delta w = (w - w_0)$ and F^n is obtained recursively from 3.2.3, the tabular value $F(w_0)$, and Eq. (3.2.1).

The terms of the Taylor series converge like

$$\sum \frac{(2w)^n}{n!} \delta w^n = \sum \frac{(2w\delta w)^n}{n!}.$$

In the worst case, $w = 5$, and $\delta w = 0.05\sqrt{2}$. Thus eight terms give an accuracy of 10^{-7} . At the average point of the domain,

$$w = (2/3)(0.5); \quad \delta w = 0.025\sqrt{2},$$

and only six terms are required.

Beyond the circle $|w| = 5$,

$$F(w) = \frac{\sqrt{\pi}}{2w} \left[1 - \frac{1}{2w^2} + \frac{(1)(3)}{(2w^2)^2} - \frac{(1)(3)(5)}{(2w^2)^3} \pm \dots \right], \quad (3.2.6)$$

and this has an accuracy of at least 0.3×10^{-8} . In fact, only six terms need be taken to get ample accuracy for the broadening process, the maximum error being 3×10^{-6} .

4. The Calculation of Neutron Flux in the SDR Code

The cross sections which have been generated over a piecewise constant mesh are used to calculate fluxes in a variety of geometries, including, of course, the infinite medium. The main effects of interest in the Doppler region are resonance shielding and heterogeneity, with leakage only of marginal interest. The broad strategy is to obtain neutron fluxes in a fairly idealized geometry, consisting of a few regions and to use the fluxes to produce group constants for use in more elaborate transport codes and

diffusion codes. The code has been used extensively to compile sets of group constants which can be interpolated, by simpler models, to compute whole series of reactor types. It has been found that a very few pivotal sets of group constants enable a very wide spectrum of reactors to be studied.

The method of calculation employed stems from the integral equation

$$\Sigma_t(\underline{r}, E) \phi(\underline{r}, E) = \int K(\underline{r}' \rightarrow \underline{r}, E' \rightarrow E) \phi(\underline{r}', E') dE' dV + Q(\underline{r}, E) \quad (4.1.1)$$

which exists when the scattering is isotropic.

Integrating over a volume V_j of constant composition,

$$\Sigma_{tj} \phi_j V_j = \sum_{i,k} P_{i \rightarrow j} S_{ik} V_i + Q_j V_j, \quad (4.1.2)$$

where $P_{i \rightarrow j}$ is the probability that a neutron born in region i has its next collision in region j ; S_{ik} is the scattering source in region i from nucleus k ; Q_j is the total extraneous source in region j ; Σ_{tj} is the total cross-section of region j . Then if we assume that the scattering source in each region is flat, the reciprocity theorem gives

$$P_{i \rightarrow j} \Sigma_{ti} V_i = P_{j \rightarrow i} \Sigma_{tj} V_j. \quad (4.1.3)$$

The scattering sources can be written as

$$S_{ik} = \int_E^{E/\alpha_k} \phi_i(E') \Sigma_{sik}(E') \frac{dE'}{E'(1-\alpha_k)}, \quad (4.1.4)$$

where $\alpha_k = (A_k - 1/A_k + 1)^2$ and A_k is the atomic mass of the k^{th} scatterer, and Σ_{sik} is the scattering cross section of the k^{th} scatterer in region i . Differentiating 4.1.4, we find,

$$\frac{dS_{ik}}{dE} = \frac{1}{E(1-\alpha_k)} \{ \phi_i(E/\alpha_k) \Sigma_{sik}(E/\alpha_k) - \phi_i(E) \Sigma_{sik}(E) \}. \quad (4.1.5)$$

The solution of the Eq. (4.1.5) linked by the flux Eq. (4.1.2) can be solved in a chainlike manner with decreasing energy. The two boundary condition options allowed are:

$$(i) \phi_i = 0 \text{ for all } i, \text{ for } E \geq E_{\text{initial}},$$

where E_{initial} is some starting energy; and in this case an extraneous source $Q_i(E)$ must be supplied to get a flux response below the initial energy;

(ii) $\phi_i = 1/E$ for all i above the starting energy E_{initial} .

In this case there is no need for an extraneous source $Q_i(E)$, and the flux response comes from neutrons scattered from the $1/E$ flux above cutoff.

The overall neutron balance of the system must be maintained throughout the slowing-down process; that is to say, the number of neutrons captured plus the number scattering out of the lower end of the energy band considered must always equal the neutrons fed in at the top of the energy band. In order to have this condition satisfied we must specify the quadrature formula belonging to the Eq. (4.1.5) and use it to deduce the correct interpolation formula for $\Sigma_s(E/\alpha) \phi(E/\alpha)$ which occurs in 4.1.5.

Consider a small energy band Δ_n located at E_n with its upper energy lying on E_n . Then the source into this energy band from above and outside is

$$\int_E^{E_n/\alpha} \frac{\Sigma_s(E') \phi(E')}{E'(1-\alpha)} f_n(E') dE', \quad (4.1.6)$$

where

$$f_n(E') = \min\{(E_n - \alpha E'), \Delta_n\},$$

and the indices i , j , and k have been dropped for convenience. With a simple-slab quadrature formula this becomes

$$S_n = \sum_{j=m}^n \frac{\Sigma_{sj} \phi_j \Delta_j}{E_j(1-\alpha)} \delta_n^j, \quad (4.1.7)$$

where

$$\begin{aligned} \delta_n^j &= \min\{(E_n - \alpha E_j), \Delta_n\}, & E_n - \alpha E_j &\geq 0 \\ &= 0; & \text{otherwise,} \end{aligned}$$

and E_m has been assigned as the first mesh energy falling below E_n/α . If we include the self-scatters of this interval,

$$S_n^T = S_n + \frac{\Sigma_{sn}\phi_n\Delta_n^2}{E_n(1-\alpha)}. \quad (4.1.8)$$

From 4.1.8,

$$\frac{S_{n+1}^T}{\Delta_{n+1}} - \frac{S_n^T}{\Delta_n} = \sum_{j=m}^{j=n} \frac{\Sigma_{sj}\phi_j\Delta_j}{E_j(1-\alpha)} \left(\frac{\delta_{n+1}^j}{\Delta_{n+1}} - \frac{\delta_n^j}{\Delta_n} \right) + \frac{\Sigma_{sn+1}\phi_{n+1}\Delta_{n+1}}{E_{n+1}(1-\alpha)}. \quad (4.1.9)$$

An examination of the mesh shown in Fig. 2 reveals that between E_m and E_n the mesh interval can be halved but not quartered provided $\alpha \geq 0.5$. We therefore make this restriction and use it to simplify 4.1.9. The exception is hydrogen, where $\alpha = 0$, and 4.1.9 simplifies immediately to

$$\frac{S_{n+1}^T}{\Delta_{n+1}} - \frac{S_n^T}{\Delta_n} = \frac{\Sigma_{sn+1}\phi_{n+1}}{E_{n+1}} \Delta_{n+1}. \quad (4.1.10)$$

Lemma:

For $\alpha > 0.5$, it is found that αE_k , αE_{k+1} , and αE_{k+2} cannot all lie in Δ_n . The proof is as follows: since $\alpha < 1$, it follows that $\alpha E_k < E_k$. Thus, if αE_k is in Δ_n , then $E_k > E_n$. Since $\alpha > 0.5$, then $\Delta_n = \Delta_k$ or $\frac{1}{2}\Delta_k$. It follows that

$$\alpha(E_k - E_{k+2}) > 0.5(\Delta_k + \Delta_{k+1}) \geq \Delta_k \geq \Delta_n.$$

Hence the result follows.

By use of this lemma it follows that

$$\delta_n^{m+2} = \delta_n^{m+3} = \dots = \delta_n^n = \Delta_n, \quad (4.1.11)$$

because αE_m either falls in Δ_n or Δ_{n+1} . In the latter event 4.1.11 follows by definition; in the former event it follows from the lemma, since now only αE_{m+1} can also fall in Δ_n . Since, anyway, αE_{m+2} must either fall in Δ_{n+1} or Δ_{n+2} , it follows by exactly the same reasoning that

$$\delta_{n+1}^{m+4} = \delta_{n+1}^{m+5} = \dots = \delta_{n+1}^{n+1} = \Delta_{n+1}. \quad (4.1.12)$$

Insertion of these results in 4.1.9 gives

$$\frac{S_{n+1}^T}{\Delta_{n+1}} - \frac{S_n^T}{\Delta_n} = \sum_{j=m}^{j=m+3} \frac{\Sigma_{sj}\Delta_j}{E_j(1-\alpha)} \left(\frac{\delta_{n+1}^j}{\Delta_{n+1}} - \frac{\delta_n^j}{\Delta_n} \right) \phi_j + \frac{\Sigma_{sn+1}\phi_{n+1}\Delta_{n+1}}{E_{n+1}(1-\alpha)}. \quad (4.1.13)$$

The first sum in 4.1.13 is the required interpolation formula for the expression

$$\Sigma_s(E_n/\alpha) \phi(E_n/\alpha)$$

which occurs in 4.1.5. It is a linear combination of four fluxes adjoining the interval in which E_n/α falls.

In order to locate E_m the position where it was found last time is recorded and the search is started from there. Because the mesh is constant in large blocks, it is possible to compute it once the correct block has been located. Clearly m moves slowly over blocks, so that the search is extremely efficient; normally there is immediate success.

It will be seen from 4.1.13 that ϕ_{n+1} comes into the calculation S_{n+1}^T ; this is unfortunate, but inevitable, if we wish to have a neutron balance. The method of solution is to take $\phi_{n+1} = \phi_n$ as a first estimate and to correct iteratively from S_{n+1}^T . This is very much faster than a direct solution, which in a multiregion problem involves the inversion of a sizeable matrix. It is quite clear that $\phi_{n+1} = \phi_n$ is a very good estimate on a fine mesh and that therefore the indirect approach should be most advantageous.

5. An Example of the Use of SDR

The topic selected to illustrate the power of the numerical attack developed in this paper concerns the interaction of resonances of two different nuclides. To this end U^{238} was enriched to 3% with U^{235} and diluted with hydrogen. The enriched uranium was then given infinite mass so that an analytic solution is possible. The analysis is done in terms of the resonance escape probability. Let F be the collision density excluding heavy scatter, and ϕ the flux. Let Σ_a be the absorption cross section of the mixture and Σ_s the scattering cross section of hydrogen in the mix. Then

$$F = \phi(\Sigma_s + \Sigma_a) = \int_E^\infty \frac{\Sigma_s \phi}{E'} dE', \quad (5.1.1)$$

so that

$$F' = - \frac{\Sigma_s}{\Sigma_s + \Sigma_a} \frac{F}{E}. \quad (5.1.2)$$

Now let q be the slowing-down density; then

$$q = E \int_E^\infty \Sigma_s \phi \frac{dE'}{E'} = EF \quad (\text{from 5.1.1}) \quad (5.1.3)$$

By definition, if p is the escape probability down to energy E ,

$$p/p_0 = q/q_0, \quad (5.1.4)$$

where p_0 and q_0 are the values at E_0 , some initial energy.

Differentiating 5.1.4 and using 5.1.3,

$$\frac{p'}{p} = \frac{q'}{q} = \frac{F + EF}{EF} = \frac{1}{E} + \frac{F'}{F}.$$

Therefore, integrating,

$$\log(p/p_0) = - \int_E^{E_0} \frac{dE'}{E'} \frac{\Sigma_a}{\Sigma_s + \Sigma_a}.$$

With the use of $p_0 = 1$ for a normalization,

$$p = \exp \left(- \int_E^{E_0} \frac{dE'}{E'} \frac{\Sigma_a}{\Sigma_s + \Sigma_a} \right). \quad (5.1.5)$$

Three cases of SDR were run, first of all with U^{235} in hydrogen with the U^{238} missing, secondly with the U^{238} in hydrogen with the U^{235} missing, and thirdly with U^{235} and U^{238} in hydrogen. In each case the escape probability was computed. Using the result 5.1.5, and taking Σ_{a5} and Σ_{a8} as the partial absorption cross sections in the mix of U^{235} and U^{238} , respectively, we see that the three escape probabilities should be given by

$$\begin{aligned} P_5 &= \exp \left(- \int_{E_1}^{E_0} \frac{dE'}{E'} \frac{\Sigma_{a5}}{\Sigma_s + \Sigma_{a5}} \right); \\ P_8 &= \exp \left(- \int_{E_1}^{E_0} \frac{dE'}{E'} \frac{\Sigma_{a8}}{\Sigma_s + \Sigma_{a8}} \right); \\ P_{\text{mix}} &= \exp \left(- \int_{E_1}^{E_0} \frac{dE'}{E'} \frac{\Sigma_{a5} + \Sigma_{a8}}{\Sigma_s + \Sigma_{a5} + \Sigma_{a8}} \right); \end{aligned} \quad (5.1.6)$$

Now

$$\begin{aligned} P_5 P_8 &= \exp \left[- \int_{E_1}^{E_0} \frac{dE'}{E'} \left(\frac{\Sigma_{a5}}{\Sigma_s + \Sigma_{a5}} + \frac{\Sigma_{a8}}{\Sigma_s + \Sigma_{a8}} \right) \right] \\ &= \exp \left[- \int_{E_1}^{E_0} \frac{dE'}{E'} \left(\frac{\Sigma_{a5} + \Sigma_{a8} + 2x}{\Sigma_{a5} + \Sigma_{a8} + \Sigma_s + x} \right) \right], \end{aligned}$$

where $x = \Sigma_{a5}\Sigma_{a8}/\Sigma_s$. Now if $x = 0$, clearly $P_5P_8 = P_{\text{mix}}$; but if $x > 0$, then $P_5P_8 < P_{\text{mix}}$. Thus x gives the interaction effect. Clearly, if no U^{235} resonance overlaps a U^{238} resonance, then $x \approx 0$ and there is no interaction effect.

5.2 Results

The graphs shown in Fig. 3 give the fluxes produced in each of the three runs in an energy band from 3 to 33 eV. One can see that there should be a considerable interaction effect since each U^{238} resonance overlaps two U^{235} resonances, even in this small sample. The shape of

Fig. 3. Fluxes Produced by SDR for Three Related Slowing-down Situations

the flux in the U^{238} resonances does not seem influenced very much by the presence of the U^{235} , but the overall level of the flux in the mixture case is lower because of the extra capture by the U^{235} between U^{238} resonances. In a more realistic calculation in which the assumption of infinite mass is dropped, there would also be considerable humps beyond the U^{238} resonances caused by resonance scattering. These would, of course, be eroded by U^{235} resonances suitably placed, thus enhancing considerably the U^{235} captures. The interaction effect is confirmed in the figures given in the following table:

	<u>Number Density</u>		
U^{235}	0.002743	<u>Range</u> 9.118 keV - 3 eV	
U^{238}	0.008774		
H	0.06692		
	<u>Mixture</u>	<u>U^{238} Alone</u>	<u>U^{235} Alone</u>
Source	0.229676, -4	0.232102, -4	0.239673, -4
Captures	0.124856, -4	0.121760, -4	0.394839, -5
Fissions	0.030231, -4	-	0.441123, -5
Escape probability	0.324785, 0	0.475404, 0	0.6512073, 0

$$P_5 P_8 = 0.309586 < P_{\text{mix}}.$$

In order to analyze this further, we may assume that the U^{235} resonances are randomly distributed among the U^{238} resonances and say that the U^{238} captures are reduced by the presence of an effective U^{235} cross section, which is constant. Clearly in this case we could take

$$\overline{\Sigma_{a5}} = \frac{(\Sigma_s/\tau) \log(1/P_5)}{1 - (1/\tau) \log(1/P_5)}; \quad \tau = \log(E_0/E_1), \quad (5.2.1)$$

for if we insert this into 5.1.5 we get $P = P_5$, so that this is the constant cross section which has the same absorption rate as the U^{235} in the absence of U^{238} .

In a similar way we can take

$$\overline{\Sigma_{a8}} = \frac{(\Sigma_s/\tau) \log(1/P_8)}{1 - (1/\tau) \log(1/P_8)}. \quad (5.2.2)$$

Now if we assert that the resonance integral of U^{235} is independent of small changes in the background scattering while the U^{238} resonance integral varies as the square root of the background scattering, we are in a position to compute effective values for P_5 and P_8 , each accounting to some extent for the presence of the other.

Let,

$$I_8 = \int_{E_1}^{E_0} \frac{\sigma_{a8}\sigma_s}{\sigma_{a8} + \sigma_s} \frac{dE'}{E'}, \quad (5.2.3)$$

where σ_{a8} is the microscopic U^{238} cross section and σ_s is the hydrogen scattering cross section per U^{238} atom. Then from 5.1.6,

$$P_8 = \exp(-I_8/\sigma_s). \quad (5.2.4)$$

We are now going to make a small change in σ_s by an amount $\overline{\Sigma_{a5}}/\rho_8$ where ρ_8 is the number density of U^{238} . Consequently,

$$\frac{\delta P_8}{P_8} = -\frac{\delta I_8}{\sigma_s} + \frac{1}{\sigma_s^2} I_8 \delta \sigma_s.$$

Now if I_8 is proportional to $\sqrt{\sigma_s}$, then

$$\delta I_8 = \frac{1}{2\sigma_s} I_8 \delta \sigma_s,$$

So that

$$\frac{\delta P_8}{P_8} = \frac{1}{2} \frac{I_8}{\sigma_s} \left(\frac{\delta \sigma_s}{\sigma_s} \right) = \frac{1}{2} \log \left(\frac{1}{P_8} \right) \frac{\delta \sigma_s}{\sigma_s}.$$

so finally,

$$\frac{\delta P_8}{P_8} = \frac{1}{2} \log \left(\frac{1}{P_8} \right) \left(\frac{\overline{\Sigma_{a5}}}{\Sigma_s} \right). \quad (5.2.5)$$

Clearly we will have entirely analogous to this

$$\frac{\delta P_5}{P_5} = \log \left(\frac{1}{P_5} \right) \left(\frac{\overline{\Sigma_{a8}}}{\Sigma_s} \right). \quad (5.2.6)$$

The half is missing on the right-hand side of 5.2.6 because I_5 does not vary much with σ_s in the more dilute range of back-scattering that applies to U^{235} ($\sigma_s = 5000$). Inserting the known values of τ , P_5 , and P_8 into 5.2.1 and 5.2.2, we get

$$\left. \begin{array}{l} \overline{\Sigma_{a8}}/\Sigma_s = 0.102205 \\ \overline{\Sigma_{a5}}/\Sigma_s = 0.056510 \end{array} \right\} \begin{array}{l} \tau = 8.019 \\ \Sigma_s = 1.37186 \end{array}$$

Then doing similarly in 5.2.5, we get

$$\frac{\delta P_8}{P_8} = 0.02101,$$

i.e., two per cent of neutrons are lost to the U^{238} by virtue of the U^{235} . Similarly in 5.2.6 we get

$$\frac{\delta P_5}{P_5} = 0.043838,$$

i.e., four per cent of the neutrons escape the U^{235} resonances by virtue of the U^{238} . Also

$$\frac{\delta(P_5 P_8)}{P_5 P_8} = \frac{\delta P_5}{P_5} + \frac{\delta P_8}{P_8} = 0.064848.$$

The observed change in captures is,

$$\frac{P_{\text{mix}} - P_5 P_8}{P_5 P_8} = 0.04919.$$

Now clearly the $\overline{\Sigma_{a5}}$ is influenced by the U^{238} and the $\overline{\Sigma_{a8}}$ is influenced by the U^{235} . Since the changes observed are rather large we ought to treat them simultaneously; if we do this rather more complicated calculation, then

$$\frac{\delta P_5}{P_5} = 0.042619; \quad \frac{\overline{\Sigma_{a5}}}{\Sigma_s} = 0.051181;$$

$$\frac{\delta P_8}{P_8} = 0.019029; \quad \frac{\overline{\Sigma_{a8}}}{\Sigma_s} = 0.099361,$$

where now the mean U^{235} cross section gives the same captures as occur in the mixture and likewise the U^{238} . Now,

$$\frac{\delta(P_5 P_8)}{P_5 P_8} = 0.0616,$$

a small improvement, which probably cannot be bettered with a simple model, because a quite reasonable chance coincidence of large U^{235} levels with U^{238} levels at low energy could cause a swing in $\delta(P_5 P_8)/P_5 P_8$ by 0.01. Therefore, in order to get a real improvement one would need to investigate rather closely the actual distribution of U^{235} levels among the U^{238} levels at low energy, as indeed the SDR code does! The final estimate of P_{mix} is then

$$P_{\text{mix}} = 0.3286.$$

The more realistic problems, in which the fuel atoms have finite mass and there is perhaps some heterogeneity, bring in further difficulties which are not easy to allow for approximately. A comprehensive study of these effects has been undertaken at Winfrith, through use of the SDR code and approximate models, to obtain a system of interpolation of group constants which will satisfactorily account for a very large range of reactors.

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Discussion of Paper
Presented by Mr. Brissenden

MR. JOANOU (General Atomic): As I understand it, you carry this procedure out up to about 20 kV. In the unresolved region, it seems to me that you must have some sort of iterative process between group constants and initial generation of cross sections. If you just generate a cross-section tape from statistical considerations and use this tape to compute average cross sections, this will only be one of many possible sets of average cross sections you could get. It seems to me you have to iterate around the loop in this region.

MR. BRISSENDEN: If we had to iterate, there would be no point in doing the iteration, because there is no black magic in statistics. Either this unresolved region is of no consequence, or it is. If it is of consequence, then it has to be resolved. We cannot iterate. This is one sample from the unresolved region, and if one sample is not good enough, then neither will another one be.

MR. JOANOU: I am not sure whether one sample is good enough, but it seemed to me that the natural process would be to iterate to see if one sample is good enough.

MR. BRISSENDEN: Yes. That is the only information you can glean, whether one sample is good enough. If you took another sample and computed the group constants, did a reactor calculation, and found a significant difference, then there is nothing whatever you can do about it, except go back to the experimenters and say, "Look, I need more resonances."

MR. JOANOU: No, that's not really true. There is a distribution and you could converge. It seems to me you should be able to converge on the cross sections going through once; doing it again will give you another set. These can then be averaged together.

MR. BRISSENDEN: If you average them together you just get another set; which is the best one?

MR. JOANOU: No, you have to keep generating this set over and over again.

MR. BRISSENDEN: This is false. There is an actual set of resonances and it is not the average.

MR. JOANOU: I am talking about the unresolved resonances.

MR. BRISSENDEN: Even for the unresolved resonances, it is not the average. It may be way off. Who knows? The only thing you can say is that it has got to be unimportant.

MR. OKRENT (Argonne National Laboratory): Have you done the process twice in one case and compared?

MR. BRISSENDEN: No. I think that in the case of U^{238} we are reasonably happy that at 2 kV we have enough resolved information and that this unresolved region is really adequately represented by any statistical sample for reactor physics purposes. In the case of U^{235} I am not so sure. One can hope, but this is the reason we have put into this resonance sampling a forcing procedure. Because, just above the resolved region, which ends at about 39 eV, one does have partial information. Some resonances are seen, fluctuations in alpha are seen, and so on. This is sort of half-resolved information, and the only way that we can use this, it seems to me anyway, is to try to get our samples of resonances to have this same pattern of fluctuations, and this we do.

USE OF DISCRETE-ORDINATES METHODS FOR SOLUTION OF PHOTON TRANSPORT PROBLEMS*

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Introduction

Although both neutron and photon distributions are described by the same Boltzmann transport equation, the numerical methods commonly used to solve this equation differ, depending upon which particle distribution is sought. When neutron fluxes are computed, spherical harmonics or discrete-ordinates methods are employed, whereas when photon distributions are calculated, Monte Carlo or moments methods are more frequently used. These latter methods are generally more computationally time consuming than the former, and it is usually held that this is the price paid to represent adequately severely anisotropic photon scattering. In other words, most neutron solution codes are capable of representing isotropic and linearly anisotropic scattering; these approximations, supplemented by the transport approximation, seem to be adequate for many neutron computations. However, in neutron-shielding and photon-distribution calculations, more precise representation of anisotropic scattering is essential.

Suppose that one wishes to use the same method to compute neutron and photon distributions (in particular, the method of discrete ordinates); the above considerations raise several questions. First, is it even possible, in a multigroup, discrete-ordinates representation of the transport equation, to represent severe anisotropic scattering accurately? Even supposing the existence of perfectly prepared multigroup cross sections, might there be some numerical bound on accuracies obtainable? After all, in seeking the photon distribution emerging from a reactor-shield complex, one is trying to calculate a distribution that is attenuated by many orders of magnitude; and this distribution must surely be very sensitive to how adequately anisotropic scattering is represented. Secondly, if a discrete-ordinates solution is possible, is it economical? That is, must the same computational effort be expended in a discrete-ordinates code as in a Monte Carlo code? Thirdly, what sort of scattering approximation should be used? And fourthly, how should multigroup cross sections be prepared?

This report describes the results of an investigation undertaken to attempt to answer the above questions. The investigation was restricted to

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photon transport, primarily because preparation of gamma-scattering cross sections is more amenable to automation. The investigation consisted of four major phases: 1) selection of an anisotropic scattering approximation, 2) modification of a discrete-ordinates transport code to apply the scattering approximation, 3) development of a code to produce multigroup photon cross sections for use in the scattering approximation, and 4) testing of the complex constructed in 1), 2), and 3).

The Anisotropic Scattering Approximation

Based on a thorough examination of anisotropic scattering recipes in the monoenergetic Boltzmann equation⁽¹⁾ and the failure of certain extended transport approximations, an $N + 1$ term Legendre polynomial expansion was adopted for scattering approximation. Let the collision source term of the Boltzmann equation be written*

$$\iiint \phi(\vec{r}, \vec{\Omega}', E') \sigma_s(E' \rightarrow E, \vec{\Omega}' \cdot \vec{\Omega}) dE' d\Omega', \quad (1)$$

where ϕ is the particle flux as a function of position, direction, and energy, and σ_s is the macroscopic transfer probability for scatter from initial energy E' to energy E through an angle (between initial direction $\vec{\Omega}'$ and final direction $\vec{\Omega}$) with cosine $\mu_0 = \vec{\Omega}' \cdot \vec{\Omega}$. The scattering transfer probability can be expanded in terms of Legendre polynomials of this cosine, giving

$$\sigma_s(E' \rightarrow E, \mu_0) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} \sigma_{sn}(E' \rightarrow E) P_n(\mu_0), \quad (2)$$

where, by orthogonality, the expansion coefficients σ_{sn} are defined by

$$\sigma_{sn}(E' \rightarrow E) = \int_0^{2\pi} \int_{-1}^1 P_n(\mu_0) \sigma_s(E' \rightarrow E, \mu_0) d\mu_0 d\omega. \quad (3)$$

In terms of the unit vectors of a spherical coordinate system (for example), $\vec{e}_r$, $\vec{e}_\theta$, and $\vec{e}_\phi$, and the angles and cosines

$$\begin{aligned} \mu &= \vec{\Omega} \cdot \vec{e}_r; \\ \eta &= \vec{\Omega} \cdot \vec{e}_\theta \equiv \sqrt{1 - \mu^2} \cos \omega; \\ \xi &= \vec{\Omega} \cdot \vec{e}_\phi \equiv \sqrt{1 - \mu^2} \sin \omega, \end{aligned} \quad (4)$$

* σ_s may also be a function of $\vec{r}$. Here, spatial dependence of cross sections is treated by considering a series of homogeneous zones.

the polynomial $P_n(\mu_0)$ can be expanded to give

$$P_n(\mu_0) = P_n(\mu) P_n(\mu') + 2 \sum_{r=1}^n \frac{(n-r)!}{(n+r)!} P_n^r(\mu) P_n^r(\mu') \cos r(\omega - \omega'). \quad (5)$$

Here, the P_n^r are associated Legendre polynomials. Similar expansions can be made with other coordinate systems.

The Legendre scattering approximation truncates the expansion of Eq. (2) after the term $n = N$. The scattering source term of Eq. (1) is then

$$\sum_{n=0}^N \int \sigma_{sn}(E' \rightarrow E) \phi_n(\vec{r}, \vec{\Omega}, E') dE', \quad (6)$$

where

$$\phi_n(\vec{r}, \vec{\Omega}, E') = \frac{2n+1}{4\pi} \iint \phi(\vec{r}, \vec{\Omega}', E') P_n(\mu_0) d\Omega'. \quad (7)$$

The Legendre polynomial expansion requires the evaluation of the coefficients σ_{sn} of Eq. (3) and of the flux moments ϕ_n of Eq. (7). The approximation seems to be accurate with relatively few terms, even for exceptionally anisotropic scattering.⁽¹⁾ Qualitatively, both σ_{sn} and ϕ_n should decrease with increasing n . The σ_{sn} are zero for $n > 0$, in the case of isotropic scattering, and fail to decrease with increasing n only in the case of purely forward scattering for which all σ_{sn} are equal. The ϕ_n should decrease because the P_n are (more and more rapidly) oscillating functions while ϕ is positive. Thus, as n increases, the product $\sigma_{sn} \phi_n$ should decrease, and hence become unimportant, rapidly.

In what follows, the truncation of Eq. (6) is referred to as the P_N scattering approximation; N is the number of terms, in addition to the isotropic term, that are retained. In a discrete-ordinates solution of the transport equation the order of angular quadrature, M , is unrelated to N except that, for consistency, M should be greater than N .

Preparation of a Discrete-ordinates Transport Code to Treat Anisotropic Scattering

The DTF code,⁽²⁾ a one-dimensional, multigroup, discrete-ordinates code, was modified* to accept multigroup transfer cross sections for an

*In addition to the conceptual modification, the code was also rewritten in variable-dimension Fortran IV to permit more flexible use of storage.

arbitrary order, N , of the Legendre scattering approximation and to compute the angular moments ϕ_n . The modified code uses a multigroup analog of Eq. (6) for the source of the g^{th} group, $g = 1, 2, \dots, G$:

$$\sum_{n=0}^N \sum_{h=1}^G \sigma_{sn}^{g \leftarrow h} \phi_{nm}^h. \quad (8)$$

In the above, ϕ_{nm}^h is the h^{th} group, n^{th} Legendre moment of the angular flux in the discrete $\vec{\Omega}_m$:

$$\begin{aligned} \phi_{nm}^h = (2n+1) \sum_{m'=1}^M \omega_{m'} \phi_{m'}^h & \left[P_n(\mu_m) P_n(\mu_{m'}) \right. \\ & \left. + 2 \sum_{r=1}^n \frac{(n-r)!}{(n+r)!} P_n^r(\mu_m) P_n^r(\mu_{m'}) \cos(\omega_m - \omega_{m'}) \right]. \end{aligned} \quad (9)$$

Thus, ϕ_{nm}^h is a discrete-ordinates angular quadrature of the angular flux ϕ_m^h , in group h , analogous to the integration of Eq. (7). The factor 4π is included in the quadrature weight, $\omega_{m'}$. Also, $\sigma_{sn}^{g \leftarrow h}$ is the transfer cross section from group h to group g , the analog of $\sigma_{sn}(E' \rightarrow E)$.

The above modification increases code-execution time mainly in the time required to prepare and store the moments of Eq. (9). Since the group angular flux was already available, this increase is surprisingly modest. Execution time is also increased indirectly because an increased order of angular quadrature is needed to integrate accurately the moments of Eq. (9).

Multigroup Cross Sections

Write the general Boltzmann transport equation, with an N -term scattering approximation, as

$$\nabla \cdot (\vec{\Omega} \phi) + \sigma_t(E) \phi(\vec{r}, \vec{\Omega}, E) = \sum_{n=0}^N \int \sigma_{sn}(E' \rightarrow E) \phi_n(\vec{r}, \vec{\Omega}, E') dE' + S(\vec{r}, \vec{\Omega}, E), \quad (10)$$

where σ_t is the macroscopic total cross section and S represents external sources. Let the average flux and external sources in the energy range $E_{g+1} \leq E \leq E_g$ be defined by

$$\phi^g(\vec{r}, \vec{\Omega}) = \int_{E_{g+1}}^{E_g} \phi(\vec{r}, \vec{\Omega}, E) dE; \quad S^g(\vec{r}, \vec{\Omega}) = \int_{E_{g+1}}^{E_g} S(\vec{r}, \vec{\Omega}, E) dE. \quad (11)$$

Then, in terms of the averages

$$\sigma_t^g(\vec{r}, \vec{\Omega}) = \int_{E_{g+1}}^{E_g} \sigma_t(E) \phi(\vec{r}, \vec{\Omega}, E) dE / \phi^g(\vec{r}, \vec{\Omega}) \quad (12)$$

and

$$\sigma_{sn}^{g \leftarrow h}(\vec{r}, \vec{\Omega}) = \frac{\int_{E_{h+1}}^{E_h} \phi_n(\vec{r}, \vec{\Omega}, E') dE' \int_{E_{g+1}}^{E_g} \sigma_{sn}(E' \rightarrow E) dE}{\int_{E_{h+1}}^{E_h} \phi_n(\vec{r}, \vec{\Omega}, E') dE'}, \quad (13)$$

the group average of Eq. (10) is

$$\nabla \cdot (\vec{\Omega} \phi^g) + \sigma_t^g(\vec{r}, \vec{\Omega}) \phi^g = \sum_{n=0}^N \sum_{h=1}^G \sigma_{sn}^{g \leftarrow h}(\vec{r}, \vec{\Omega}) \phi_n^h(\vec{r}, \vec{\Omega}) + S^g(\vec{r}, \vec{\Omega}), \quad (14)$$

where ϕ_n^h is the denominator of Eq. (13). Equation (14) is a very general multigroup formulation, but the angular flux and its moments are seldom known, even qualitatively.* For the work described here, it is assumed that, at best, only an energy-dependent function is available for the averages of Eqs. (12) and (13). Based on this assumption (as a consequence of which σ_t^g and $\sigma_{sn}^{g \leftarrow h}$ are independent of $\vec{r}$ and $\vec{\Omega}$) a code, GAMLEG,⁽³⁾ was written to prepare multigroup photon cross sections. For photon scattering, the Klein-Nishina⁽⁴⁾ differential scattering cross section is given analytically, and the coefficients $\sigma_{sn}(E' \rightarrow E)$ and their E integrals can be obtained explicitly.⁽³⁾ The GAMLEG code is also designed to prepare the group-averaged total cross section as the sum of the scattering cross-section average

$$\sigma_s^g = \int_{E_{g+1}}^{E_g} f(E) dE \int_{E/(1+zE)}^E \sigma_{s0}(E \rightarrow E') dE' / \int_{E_{g+1}}^{E_g} f(E) dE \quad (15)$$

*Such information can be obtained in an iterative manner. For this purpose the DTF code prints the angular flux moments and their zone averages.

and the absorption cross-section average

$$\sigma_a^g = \frac{\int_{E_{g+1}}^{E_g} f(E) \sigma_a(E) dE}{\int_{E_{g+1}}^{E_g} f(E) dE}. \quad (16)$$

Here, $f(E)$ is the energy-dependent weighting distribution. The code is designed to accept this weighting function, absorption data, coherent-scattering data, and source-energy data as input from which the respective group averages are prepared. The energies at which each of these types of data are specified must also be supplied. The energy-group structure is chosen by the user. Output is in a form suitable for input to the DTF code.

Test Problems

The test problems here considered are designed as consistency checks, in which the results of one numerical scheme are compared to the results of another, and no effort is made to compare with experiment. In this connection the same raw data (absorption and coherent scattering) were used in each computation. The use made of the data, of course, differed. For example, in the second test problem, the same 81 energy-absorption data were used in both solutions. But in the Monte Carlo solution, fluxes were calculated at 81 energies and then condensed for comparison with fluxes, obtained by first-group averaging of the absorption data, of the discrete-ordinates solution. Similarly, treatment of the collision source differed greatly in the two solutions, but both treatments were based on the Klein-Nishina scattering law.

For lack of better information, the cross sections used in all the discrete-ordinates solutions below were prepared with a constant weighting function. An attempt, with unsatisfactory results, to use the source energy distribution as a weighting function is described in Ref. 5.

In a first test problem, the percentage of photons penetrating a 10-cm iron slab was computed. A 6-MeV isotropic source was assumed to impinge upon the left side of the slab. The DTF calculation was made by use of a double P_7 (equivalent to S_{16}) angular quadrature, fifty spatial intervals, and an elementary nine-group representation. Unweighted cross-section sets were prepared for $N = 0, 1, \dots, 5$. Absorption data were taken from the 81-energy United Nuclear Corporation data file used in conjunction with the Monte Carlo codes, SANE-SAGE⁽⁶⁾ and ADONIS.⁽⁷⁾ With unweighted cross sections the only difference between a P_{N-1} and P_N scattering approximation is the addition of the $\sigma_{SN}^{g \leftarrow h}$ scattering transfer matrix. Table I shows the variation of the percentage of the transmitted photons as a function of scattering approximation and group.

Table I
TRANSMISSION PERCENTAGE FOR A 10-cm IRON SLAB^a

Group	Group Energy Bounds (MeV)	P ₀	P ₁	P ₂	P ₃	P ₄	P ₅
1	7 0795-3 5481	2 4574	3 0245	3 10804	3 0553	3 0633	3 0616
2	3 5481-1 7783	0 4979	1 3465	1 4809	1 4285	1 4380	1 4377
3	1 7783-0 89125	0 3703	1 1214	1 2120	1 2032	1 2074	1 2075
4	0 89125-0 44668	0 3424	0 9933	0 9825	0 9953	0 9977	0 9992
5	0 44668-0 22387	0 3854	0 7326	0 6970	0 7064	0 70806	0 7090
6	0 22387-0 11220	0 1671	0 2693	0 2677	0 2699	0 2707	0 2710
7	0 11220-0 05623	0 7127-2	0 9922-2	0 9728-2	0 9810-2	0 9837-2	0 9849-2
8	0 05623-0 02818	0 1916-4	0 2195-4	0 2147-4	0 2163-4	0 2169-4	0 2172-6
9	0 02818-0 01540	0 6433-8	0 6966-8	0 6691-8	0 6715-8	0 6738-8	0 6743-8
Total		4 2277	7 4975	7 7579	7 6685	7 6951	7 6959

^aIn the table, 0 7127-2 $\equiv$ 0 007127

The above results show a relatively swift pattern of convergence, that is, despite the severely anisotropic scattering of 6-MeV photons, the biggest difference between P₃ and P₅ results is 0.64% in the second group. The total P₅ transmission percentage is 2% higher than an ADONIS result. Part of the difference is due to the elementary group structure, which does not do justice to the absorption cross section in the lower energy range (cf. the next test problem), and part due to the fact that the ADONIS code does not admit infinite-slab geometry.

In a second and more ambitious test, the flux was calculated in a spherical reactor mockup. The Monte Carlo code SAGE was used to provide comparison results. Since SAGE does not allow a source distributed in energy (except as a superposition of independent monoenergetic problems), a source energy of 2 MeV was arbitrarily chosen. The material composition, group structure, and source spatial distribution for this problem are given in Table II. Initially, a double P₇ angular quadrature, P₅ scattering and 99 spatial intervals were used in the discrete-ordinates solution.

SAGE and DTF fluxes are compared for group 1 in Fig. 1 and for group 7 in Fig. 2. The fluxes are normalized for plotting, but a single normalization factor is used for both sets of data. The agreement of the two solutions in groups 2 through 6 is as good as that of group 7. In group 9, however, the agreement is not good (see Fig. 3). The discrepancy here is due to the poor resolution of rapidly varying absorption cross sections in this energy range. To check this statement, a revised group structure was used. The first eight groups were retained intact, but

group 9 was replaced with groups 9 (0.25-0.20 MeV), 10 (0.20-0.15 MeV), 11 (0.15-0.10 MeV), 12 (0.10-0.05 MeV), and 13 (0.05-0.02 MeV). Both methods were used to recompute fluxes, with the comparison given in Fig. 4 for new group 9, in Fig. 5 for group 11, and in Fig. 6 for group 13. As shown in the figures, the revised group structure is much more effective than the original.

Table II
REACTOR MOCKUP SPECIFICATIONS

Relative Source Strength	Outer Radius (cm)	Zone	Outer Radius (cm)	Material	Atomic Density ($\times 10^{22}$)	Group Energies (MeV)
1.0	0.97	1	7.74	U ²³⁸	1.96	2.00-1.99
0.98	1.94			Fe	1.18	1.99-1.75
0.96	2.91			Na	0.704	1.75-1.50
0.92	3.87	2	9.37	Fe	6.83	1.50-1.25
0.87	4.84			Na	0.395	1.25-1.00
0.81	5.82	3	11.83	Fe	8.3	1.00-0.75
0.74	6.77	4	12.76	Void	-	0.75-0.50
0.65	7.74	5	25.47	Fe	7.5	0.50-0.25
		6	29.52	Fe	4.0	0.25-0.02
		7	80.08	C	6.77	
				B	0.0302

Fig. 1. Group-1 Fluxes as a Function of Radius.
 $1.99 \leq E_{\gamma} \leq 2.0$ MeV.

Fig. 2. Group-7 Fluxes as a Function of Radius. $0.5 \leq E_\gamma \leq 0.75$ MeV.

Fig. 3. Group-9 Fluxes as a Function of Radius. $0.02 \leq E_\gamma \leq 0.25$ MeV.

Fig. 4. Revised Group-9 Fluxes as a Function of Radius. $0.20 \leq E_\gamma \leq 0.25$ MeV.

Fig. 5. Group-11 Fluxes as a Function of Radius. $0.10 \leq E_\gamma \leq 0.10$ MeV.

Figure 6

Group-13 Fluxes as a Function of Radius. $0.02 \leq E\gamma \leq 0.05$ MeV.

Since in this problem all the fluxes above 0.05 MeV are attenuated by at least six orders of magnitude in traversing the reactor, the right leakage is sensitive to how accurately the transport equation is solved. Table III shows the effect, on the right leakage, of changing the angular quadrature and refining the spatial mesh. The Legendre polynomial P_{15} quadrature is more accurate than the DP_7 quadrature, because the former has a direction cosine closer to 1.0. The differences in the right leakages in the problems above are less than that made in more adequately representing the group structure. In the 13-group, 148-interval calculation, the total system leakage was 0.0685%, compared to the leakage from SAGE of $\sim 0.06\%$ and that of $\sim 0.08\%$ from a run with the Monte Carlo code MCG.⁽⁸⁾

Table III

RIGHT LEAKAGE BY GROUP (PERCENT)

Group	99 Intervals DP_7 Quadrature	99 Intervals P_{15} Quadrature	148 Intervals P_{15} Quadrature
1	0.001809	0.001909	0.001972
2	0.002153	0.002306	0.002363
3	0.002568	0.002723	0.002787
4	0.002946	0.003107	0.003179
5	0.003572	0.003752	0.003838
6	0.004484	0.004682	0.004786
7	0.005936	0.006144	0.006279
8	0.008919	0.009143	0.009339
9	0.042579	0.043474	0.044249
Total	0.074966	0.077240	0.078791

For this problem, the discrete-ordinate solution required 7.5 min (148 intervals, 13 groups, P_{15} angular quadrature, P_5 scattering) whereas the Monte Carlo computations each required at least 2 hr.

A third test calculation was made to examine the effectiveness of the method in problems with energy-distributed sources. A uniform source, in radius, was distributed between 0 and 25 cm in a 70-cm iron sphere. The source was distributed in energy as $\exp[-1.1E]$, with E in MeV. A detailed definition of the problem and a description of the comparison calculations is given in Ref. 5. Figure 7 shows a comparison of group fluxes calculated with the DTF code in two-group representations, one chosen to span all energies and the other chosen to refine the high-energy behavior. Figure 8 shows the results of an energy-deposition calculation made from DTF fluxes, from methods of moments fluxes, and from Monte Carlo fluxes. A much more detailed comparison of the results is made in Ref. 5. The discrete-ordinates solution (DP_7 , 24 groups, 99 intervals, and P_3 scattering) required about 10 min, whereas the Monte Carlo calculation required over 2 hr of comparable time. The moments solution required a great deal of "this problem only" computation, and no fair time comparison can be made.

Fig. 7. Energy Dependence of the Group Fluxes from an $\text{Exp}[-1.1E]$ Source Distributed Uniformly in the Central 25 cm of a 70-cm Iron Sphere.

Fig. 8. Energy Deposition as a Function of Radius; Problem as in Fig. 7.

Conclusions

As Figs. 1, 2, 4, 5, and 8 show, the discrete-ordinates method is able to calculate gamma fluxes in excellent agreement with Monte Carlo and moments solutions. Further, the discrete-ordinates method is computationally much faster, at least in one-dimensional problems. A portion of this edge might be lost in deep-penetration problems; the results of Table III indicate that more care must be taken to calculate emergent fluxes. However, this type of problem is also difficult for Monte Carlo methods since, typically, only a few particles in ten thousand escape.

The results of the test problems also indicate that the Legendre scattering approximations are accurate. Except for deep-penetration problems, for which the P_5 or higher approximation is needed, the P_3 approximation seems to be adequate.

The fact that unweighted cross sections give such accurate results seems surprising. However, the results of Fig. 7 show that refining the energy integration mesh in the high-energy range did not appreciably alter the energy dependence of the flux. In the low-energy range the distribution altered significantly, but the altered distribution gave the accurate results of Fig. 8. Again, in the second test problem, accuracy in flux computations was achieved when the low-energy mesh was refined. From these observations it is concluded that if a fine-enough energy mesh is used, unweighted cross sections can give good accuracy. "Fine enough" is, of course, problem dependent, meaning a relatively coarse group structure in the problems considered.

The investigation described above is by no means exhaustive. The test problems form only a small sample, and even in these problems no attempt was made to examine all combinations of quadratures (space, angle, and energy) and scattering approximations (to determine, say, minimum adequate combinations). However, the success in these test problems of the combination of multigroup cross sections for a Legendre scattering approximation, discrete-ordinates solution of the Boltzmann equation should encourage the use of these methods in other photon transport problems.

Acknowledgments

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Discussion of Paper
Presented by Mr. Lathrop

MR. deBARYSHE(Westinghouse Astronuclear Laboratory): We have tried the same sorts of techniques with a modified 2-D transport code, originating in Los Alamos, DDK, I guess. We find another improvement in running times by an order of magnitude compared to Monte Carlo. We don't, of course, go anywhere near P_5 ; we are using a P_1 approximation, but the matching, even to fairly thick shields, is quite good. I believe a report will be made on this at the Gatlinburg meeting by Mr. R. K. Disney.

The question I have concerns the integration scheme. From what you write, I gather the angular fluxes are expanded only in Legendre polynomials, so there is no need to worry about a consistency or inconsistencies possibly in expanding the angular fluxes with a S_N approximation and the scattering matrix in a P_N approximation.

MR. LATHROP: One has to make sure of one thing. Whatever discrete ordinate quadrature is used will integrate a Legendre polynomial correctly. We have moment-matching S_N sets. I have used the Legendre

set, because, generally speaking, it has directions close to the straight-out directions where it is important to resolve the angular flux.

MR. JORDAN (Douglas Missile and Space Systems Division): Through some techniques I have developed at Douglas, I have run this last problem by Monte Carlo techniques, and I will not say that my points are right on top of the line, because you usually don't get that with Monte Carlo. I ran this problem for 8 min and results were obtained every 2 min. Even after the first 2 min they were within a factor of two, I would say, and after 8 min probably within 25%.

MR. LATHROP: I didn't mean to imply that one should neglect Monte Carlo calculations. Certainly, where geometric versatility is necessary, one has to use Monte Carlo calculations, at least at present. There are a great many calculations, especially of gamma heating, that might well be done with a discrete-ordinate code in a fraction of the time; because, if you are interested only in the absorption in the system, it is not necessary to use nearly as high a scattering approximation. I have been trying to test the method to see what ultimately may be necessary. I think one could get quite reasonable results with the P_1 scattering approximation and not nearly so high an angular quadrature.

MR. UNDERHILL (AERE, Winfrith): I would like to comment on the question of the truncation of the spherical harmonic expansion of the scattering law. I think one must remember that the source term will either truncate because the scattering is properly represented, or because the flux shape is properly represented in the order of approximation used. My impression, based on some work on the Aldermaston S_N code STRAINT, is that in many situations the P_5 approximation is adequate, not because it represents the scattering law, but because it represents the flux shape. This is certainly true for fairly compact geometries, where one is trying to estimate criticality. I am less certain in the case of shielding where, particularly in spherical systems, the unscattered source of the zeroth-collision neutron flux deep in the system is nearly all outward moving. In other words, the flux shape is very strongly peaked forward. I am less certain there that a P_5 approximation is really adequate, since it certainly doesn't represent the scattering law, and under these conditions I am equally sure that it doesn't represent the flux. Whether this is going to be important in any practical situation must depend, I think, on the relative importance of direct neutrons coming out of the system and scattered neutrons. In STRAINT, an attempt is made to get over this situation to some extent by doing a direct calculation of the zero-collision neutrons. This is then used as a distributive source term throughout the whole system on which to do an S_N calculation. Although I cannot recall the precise justifications for this, intuitively it seems to me to be a somewhat sounder and a more generalized approach.

MR. LATHROP: I might remark that for a time, for deep-penetration neutron problems, we had included in this particular code a first-collision source. After some types of calculations similar to those that have been made, we no longer use the first-collision source approximation. We got essentially the same result, and it might be swifter in calculation, but the generality of the Legendre expansion is great. I want to mention that, in the collision source term which is

$$\sum_{n=0}^N \sigma_{sn} P_n(\mu) \frac{2n+1}{2} \int_{-1}^1 \psi(x, \mu') P_n(\mu') d\mu',$$

the order of the angular quadratures performed in the integration is divorced in the discrete ordinate code from the order of the scattering approximation. In P_5 scattering, I kept five of these terms, but did the quadrature with the P_{15} approximation. The justification for the rapid decrease of the terms in the summation is, first, that the flux is positive and the rapidly oscillating Legendre polynomial for large n diminishes the importance of the integral for large n . Secondly, the σ_{sn} presumably should decrease with n ; the only case for which this is not true is when the scattering is purely in the forward direction and the transport approximation is exact. Thus the two effects together eliminate the importance of high- n terms. The only case for which that is not true is when the absorption is high and the flux is collimated in the forward direction, say a delta function. Then the integral becomes unity for each n , but σ_{sn} is quite small compared to the total cross section for a highly absorbing assembly, so that the whole source term isn't very important.

MR. CERTAINE (United Nuclear): Recently I have been using a double P_N in effect. Here, even a lower-order N is sufficient because both the source term and the Legendre polynomial terms of the flux have double P_N expansions. The energy treatment is based on that which was used for the RENUPAK program for treating moments methods. Tremendous accuracy is attained with a rather low approximation for N .

MR. PENNY (Radiation Shielding Information Center, Oak Ridge): I would like to make some comments. First, regarding the moment-method calculation that was done here, the 30-min time should have some explanation. Most of this time is consumed in data preparation which is a once-and-for-all thing. The actual integration over the sphere involves an almost negligible amount of time. However, the use of the moments-method data is really an approximation, because the data were generated for a infinite homogeneous medium. In this particular system, it is a good approximation to use.

The second comment is in regard to the Monte Carlo codes. One can always do better in time by putting enough thought into it; that is, one can

devise importance sampling schemes given a detector located somewhere in the system, either at the outer edge or somewhere in the middle, and tailor the calculations to do very well at that particular space point. This gives a large reduction in computer time. However, the beauty of the S_N method is that you get all the space points at once. In the Monte Carlo system, even if you did elegant importance sampling, you would presumably have to tailor it for each space point, or at least groups of them. The Monte Carlo calculations done at Oak Ridge had no importance sampling schemes incorporated, except that the selection of energies from the source was from a uniform distribution which was then weighted with the actual source distribution to emphasize the high-energy gamma rays which will eventually be the important ones at the edge of the shield. In the SAGE calculations (I presume they were done at Los Alamos), they did incorporate some importance sampling schemes which were splitting in Russian roulette.

MR. LATHROP: That is correct. They were split ten times. That is why the statistics were relatively good at the outside of the system.

MR. CERTAINE: The calculational scheme does not involve the angular dependence, that is, the backward and forward Legendre coefficients are computed directly from differential equations involving the distance variable only, so that the angular integration is done, in a sense, exactly. This is because the Boltzmann equation is reduced into a differential equation involving the coefficients themselves; angular dependence is no longer present.

THE SOLUTION OF THE TRANSPORT EQUATION BY COLLISION PROBABILITY METHODS

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1. Introduction

Methods of calculating the neutron flux within a lattice cell as a function of space and energy have been developed based on a representation of neutron transport in terms of first-collision probabilities. This approach provides a description of neutronics phenomena which is formulated here directly without recourse to the Boltzmann integrodifferential equation.

The method has the considerable advantage that the transport and collision mechanics parts of the problem are completely dissociated; the form of the final equations which are solved numerically is not dependent on the type of geometry.

Thus, the computer code PIP (see Section 5) solves the transport equations as formulated in Section 2 and may be applied to any system whatever its geometry, provided that a method of calculating the appropriate first-collision probabilities is available. One such method, embodied in the code PIJ, is described in Sections 3 and 4. It is based on a purely numerical approach and is such that a change of geometry is accommodated by the provision of a routine to calculate straight-line distances from points to physical boundaries (precisely as is required by Monte Carlo codes; this method does not, however, involve random sampling).

2. Basic Equations

The system under consideration is divided into K regions. Each region is assumed homogeneous with respect to its nuclear properties, but different regions are not necessarily of different materials.

Let $P_{ij}(E)$ be the probability that a neutron of energy E emitted from a collision in region R_j has its next collision in region R_i [by implication, isotropic emission is assumed; further, for the purpose of calculating $P_{ij}(E)$, a flux shape in region R_j must be assumed (see Section 3)]. Let $\phi_\ell(E) dE$ and $\psi_\ell(E) dE$ be the collision and emission rates, respectively, in region R_ℓ for neutrons with energies in the range $(E - \frac{1}{2} dE, E + \frac{1}{2} dE)$.

Let $q_\ell(E', E)$ be such that the average number of neutrons with energies in $(E - \frac{1}{2} dE, E + \frac{1}{2} dE)$ resulting from a collision in region R_ℓ of a

neutron with incident energy E' is $q_{\ell}(E', E) dE$. Further, let $S_{\ell}(E)$ be the source rate in region R_{ℓ} ; the source in each region is assumed uniformly distributed spatially and isotropic.

The equations which determine $\phi_{\ell}(E)$ and $\psi_{\ell}(E)$ are

$$\phi_{\ell}(E) = \sum_{k=1}^K \psi_k(E) P_{\ell k}(E), \quad (2.1)$$

which describes neutron transport and relates the collision rate in region R_{ℓ} to the emission rates in all regions $k(k = 1 \dots K)$, and

$$\psi_{\ell}(E) = \int_{E'=0}^{\infty} dE' \phi_{\ell}(E') q_{\ell}(E', E) + S_{\ell}(E), \quad (2.2)$$

which, following the definition of $q_{\ell}(E', E)$ above, describes the collision processes in region R_{ℓ} .

Formal group averaging is now performed, leading to the following definitions:

$$\int_{E_{g-1}}^{E_g} \phi_{\ell}(E) dE = \phi_{\ell g}; \quad (2.3)$$

$$\int_{E_{g-1}}^{E_g} \psi_{\ell}(E) dE = \psi_{\ell g}; \quad (2.4)$$

$$\int_{E_{g-1}}^{E_g} S_{\ell}(E) dE = S_{\ell g}; \quad (2.5)$$

$$\frac{1}{\psi_{kg}} \int_{E_{g-1}}^{E_g} dE \psi_k(E) P_{\ell k}(E) = P_{\ell kg}; \quad (2.6)$$

$$\frac{1}{\phi_{\ell g'}} \int_{E_{g'-1}}^{E_{g'}} dE' \phi_{\ell}(E') \int_{E_{g-1}}^{E_g} q_{\ell}(E', E) dE = q_{\ell g' g}. \quad (2.7)$$

The group-averaged forms of the basic Eqs. (2.1) and (2.2) are

$$\phi_{lg} = \sum_{k=1}^K \psi_{kg} P_{lkg}; \quad (2.8)$$

$$\psi_{lg} = \sum_{g'=1}^G \phi_{lg'} q_{lg'g} + S_{lg}; \quad (2.9)$$

where G is the total number of energy groups.

Equations (2.8) and (2.9) may be written in matrix notation:

$$\begin{pmatrix} \phi \\ \psi \end{pmatrix} = \begin{pmatrix} O & P \\ Q & O \end{pmatrix} \begin{pmatrix} \phi \\ \psi \end{pmatrix} + \begin{pmatrix} O \\ S \end{pmatrix}, \quad (2.10)$$

where ϕ , ψ , and S are column vectors of KG elements and defined by

$$\phi = \{\phi_{11}, \phi_{21}, \dots, \phi_{K,1}, \phi_{12}, \phi_{22}, \dots, \phi_{KG}\}; \quad (2.11)$$

$$\psi = \{\psi_{11}, \psi_{21}, \dots, \psi_{K,1}, \psi_{12}, \psi_{22}, \dots, \psi_{KG}\}; \quad (2.12)$$

$$S = \{S_{11}, S_{21}, \dots, S_{K,1}, S_{12}, S_{22}, \dots, S_{KG}\}. \quad (2.13)$$

The matrix P is square, consists of K^2G^2 elements, and is defined by

$$P = \text{block diagonal}\{P_1, P_2, \dots, P_G\}, \quad (2.14)$$

where P_g is the collision probability matrix in group g , that is,

$$\{P_g\}_{ij} = P_{ijg}, \quad (2.15)$$

where P_{ijg} is as defined by Eq. (2.6). Since P is a block diagonal matrix, at most K^2G of its elements are nonzero.

The matrix Q is square, consists of G^2 submatrices, and is defined by

$$Q = \text{block}[D_{mn}], \quad (2.16)$$

where the submatrix D_{mn} is $K \times K$ and diagonal; thus,

$$D_{mn} = \text{diagonal}\{q_{1nm}, q_{2nm}, \dots, q_{Knm}\}. \quad (2.17)$$

At most KG^2 elements of Q are nonzero.

The emission vector ψ may be eliminated from the equations

$$\phi = P; \quad \psi = Q\phi + S \quad (2.10)$$

to give

$$\phi = PQ\phi + PS. \quad (2.18)$$

In solving these equations numerically, it is more economical to use Eqs. (2.10) than Eqs. (2.18). This is due to the properties of P and Q which are such that the former procedure requires $KG(K+G)$ words for the storage of matrix elements, whereas the latter procedure requires K^2G^2 . If the solution is effected by means of a first-order iterative process, these are also the approximate numbers of multiplications per iteration.

Moreover, the Eqs. (2.10) may be written as

$$\begin{pmatrix} I & -P \\ -Q & I \end{pmatrix} \begin{pmatrix} \phi \\ \psi \end{pmatrix} = \begin{pmatrix} O \\ S \end{pmatrix}, \quad (2.19)$$

where I is the unit matrix of order KG , in which the matrix

$$\begin{pmatrix} I & -P \\ -Q & I \end{pmatrix} \quad (2.20)$$

possesses "Property A." The equations may therefore be solved numerically by the method of successive over-relaxation (SOR); this is the basis of the PIP code.

3. Formulae for Collision Probabilities

3.1 General

Herein P_{ij} is the probability that a neutron emerging from a collision at a point uniformly distributed in region R_j , and emitted isotropically therefrom, will next undergo a collision in a region R_i . Energy dependence of P_{ij} is implied but not written explicitly. If $\Sigma(\underline{r})$ is the total macroscopic cross section at the point $\underline{r}$ and if, when $\underline{r} \in R_k$, $\Sigma(\underline{r}) = \Sigma_k$, then

$$P_{ij} = \iiint_{R_j} \frac{d\underline{r}_1}{V_j} \iiint_{R_i} \frac{d\underline{r}_2 \Sigma_i}{4\pi |\underline{r}_1 - \underline{r}_2|^2} \exp\{-T(\underline{r}_1, \underline{r}_2)\}, \quad (3.1)$$

where

$$V_k = \iiint_{R_k} d\underline{r}$$

and

$$T(\underline{T}_1, \underline{T}_2) = \int_0^1 \Sigma(\underline{T}_1 + [\underline{T}_2 - \underline{T}_1] t) dt$$

is the "optical distance" between $\underline{T}_1$ and $\underline{T}_2$.

The standard reciprocity theorem

$$V_i \Sigma_i P_{ji} = V_j \Sigma_j P_{ij}$$

follows immediately from Eq. (3.1).

The extension to include surfaces follows. If S is any surface (not necessarily closed) such that no line drawn outwards from a surface point of R_i crosses S more than once,

$$P_{Si} = \iiint_{R_i} \frac{d\underline{T}_1}{V_i} \iint \frac{d\underline{S} \cdot (\underline{T}_1 - \underline{S})}{4\pi|\underline{T}_1 - \underline{S}|^3} \exp\{-T(\underline{T}_1, \underline{S})\} \quad (3.2)$$

is the probability that a neutron emitted from R_i crosses S , and

$$P_{iS} = \iint_S \iiint_{R_i} \frac{d\underline{S} \cdot (\underline{T}_1 - \underline{S})}{\pi S} \frac{d\underline{T}_1 \Sigma_i}{|\underline{T}_1 - \underline{S}|^3} \exp\{-T(\underline{S}, \underline{T}_1)\} \quad (3.3)$$

is the probability that neutrons crossing S isotropically (and therefore with a cosine distribution to the normal) and uniformly will have a first collision in R_i . In this case the reciprocal relationship

$$\frac{1}{4} S P_{jS} = V_j \Sigma_j P_{Sj}$$

holds.

Similarly, if S and U are two surfaces such that no outward line from one intersects the other more than once,

$$P_{US} = \iint_S \iint_U \frac{d\underline{S} \cdot d\underline{U}}{\pi S |\underline{S} - \underline{U}|^2} \exp\{-T(\underline{S}, \underline{U})\} \quad (3.4)$$

and

$$S P_{US} = U P_{SU}.$$

Coordinate System

$$\exp\left\{-\frac{\Sigma_j(AC-y)}{\sin\theta}\right\}\exp\left\{-\frac{T(CD)}{\sin\theta}\right\}\left[1-\exp\left\{-\frac{\Sigma_i t_i}{\sin\theta}\right\}\right],$$
$$P_{ij} = \frac{1}{2\pi V_j \Sigma_j} \int_0^\pi d\phi \int_{-\infty}^\infty dx \int_0^{\pi/2} \sin^2 \theta d\theta F(\phi, x, \theta), \quad (3.5)$$
$$\left[1 - \exp\left\{-\frac{t_j \Sigma_j}{\sin \theta}\right\}\right] \exp\left\{-\frac{T(\text{CD})}{\sin \theta}\right\} \left[1 - \exp\left\{-\frac{t_i \Sigma_i}{\sin \theta}\right\}\right].$$
$$\text{Ki}_n(\mathbf{x}) = \int_0^{\pi/2} \sin^{n-1} \theta \exp\left\{-\frac{\mathbf{x}}{\sin \theta}\right\} d\theta,$$

then

$$P_{ij} = \frac{1}{2\pi V_j \Sigma_j} \int_0^\pi d\phi \int_{-\infty}^\infty dx \sum_{\substack{\text{all pairs} \\ \text{of} \\ \text{entries}}} \left\{ \begin{aligned} &Ki_3(t_j \Sigma_j + t_i \Sigma_i + T) \\ &+ Ki_3(t_j \Sigma_j + t_i \Sigma_i) - Ki_3(t_j \Sigma_j + T) - Ki_3(t_i \Sigma_i + T) \end{aligned} \right\}. \quad (3.6)$$

The self-collision probability of a convex body is given by

$$P_{ii} = 1 - \frac{1}{\pi V_i \Sigma_i} \int_0^\pi d\phi \int_{-\infty}^\infty dx [Ki_3(0) - Ki_3(t_i \Sigma_i)], \quad (3.7)$$

which is identical with

$$P_{ii} = 1 - \chi - \frac{1}{\pi V_i \Sigma_i} \int_0^\pi d\phi \int_{-\infty}^\infty dx [Ki_3(0) - Ki_3(t_i \Sigma_i) - \chi t_i \Sigma_i], \quad (3.8)$$

where χ is a free parameter. The latter form is required for a numerical technique described in Section 4.

If the body is not convex, further terms similar to those of (3.6) are required in (3.7) to account for neutrons which leave and re-enter the body.

4. Computation of Collision Probabilities

4.1 Method

Equations (3.6) and (3.7) suggest a systematic and very general scheme for calculating collision probabilities in a given cylindrical system. The integrations over ϕ and x have inevitably to be performed numerically; accurate polynomial fits exist for the Ki_3 function.⁽¹⁾ The geometrical information required is a map of the appropriate path across the region of interest for every chosen pair of values (ϕ, x) . Thus it is possible to write a digital computer programme which can be adapted to new or unusual geometries by changing only the routine which supplies this map. Moreover, for a given system this routine need be entered only once, however many sets of cross section (i.e., energy groups) are to be processed, as the sets of vectors $t_1, t_2, \dots; m_1, m_2, \dots$, which record the length and region identification of each segment of a line can be stored and used for each case.

The Fortran computer programme PIJ⁽²⁾ uses this method. The standard version deals with systems of concentric annuli within which arbitrarily placed rods are subdivided radially and into annuli, but the programme has been used to analyse experiments in which plutonium "spikes," with rectangular shapes, were placed in various configurations around a fuel rod.

4.2 Accuracy of Calculation

(i) In PIJ the ϕ and x integrations are performed in the simplest possible way, by means of the trapezoidal rule. This is very inefficient when, for example, a simple annular system is considered. The Swedish programme FLURIG,⁽³⁾ which uses effectively the same method and was written exclusively for a single nest of concentric annuli, uses carefully considered Gaussian weights which reduce by a large factor the number of lines required for a given accuracy.

No such improved numerical technique, applicable to all cases which can be accommodated by PIJ, has yet been found.

(ii) A region, the area of which is only a small fraction of that of the whole system, will inevitably be crossed by relatively few of the (x, ϕ) planes. This will seldom affect the flux solution in larger regions, since the density of neutrons arriving from small regions will, in general, be small. It does mean, however, that care must be taken if reaction rates in small regions are required.

An examination of the form of the self-collision probabilities of these small regions reveals the difficulty. The integral is effectively $Ki_3[t(x, \phi)]$

and

$$\frac{\partial}{\partial x} Ki_3[t(x, \phi)] = \left[- \frac{\partial}{\partial x} t(x, \phi) \right] Ki_2[t(x, \phi)].$$

Now $Ki_2(t)$ is bounded for all t , but in most practical cases $\partial t / \partial x$ will have singularities at the edges of the region, and the few sampled values of t will not follow this behavior with sufficient accuracy. If, however, (3.8) is used instead of (3.7), an argument, t , of similar behavior is integrated simultaneously and a multiple, χ (reference Eq. 3.8), of the calculated error in this second integral is subtracted from the first integral. In the Appendix the advantage of this technique is shown. It should be noted that, in the calculations quoted in the Appendix table, the only other collision probability to be changed was that of escape from the system. It would seem, in fact,

that once the new value of P_{11} has been obtained, the best estimate of the other collision probabilities is obtained by scaling them all with that factor which preserves the sum as unity.

4.3 Calculation of Diffusion Coefficients

Benoist⁽⁴⁾ has defined generalised diffusion coefficients in terms of the quantities $P_{ij,x}/\Sigma_i$, where

$$P_{ij,x} = \iiint_{R_j} \frac{d\tau_1}{V_j} \iiint_{R_i} \frac{d\tau_2}{4\pi|\tau_1 - \tau_2|^2} \cdot 3 \left[\frac{(\tau_1 - \tau_2) \cdot \hat{x}}{\tau_1 - \tau_2} \right]^2 \exp\{-T(\tau_1, \tau_2)\} \quad (4.1)$$

and $\hat{x}$ is a unit fixed vector. Then

$$P_{ij} = \frac{1}{3} \sum_k (P_{ij,k}), \quad (4.2)$$

where the summation is over components in three mutually perpendicular directions. In the cylindrical case,

$$P_{ij,z}/\Sigma_i = \frac{3}{2\pi V_j \Sigma_j \Sigma_i} \int_0^\pi d\phi \int_{-\infty}^\infty dx \sum_{\substack{\text{all pairs} \\ \text{of} \\ \text{entries}}} \left\{ \begin{aligned} &Ki_3(T_1) - Ki_5(T_1) + Ki_3(T_2) \\ &- Ki_5(T_2) - Ki_3(T_3) + Ki_5(T_3) - Ki_3(T_4) + Ki_5(T_4) \end{aligned} \right\}, \quad (4.3)$$

where

$$T_1 = t_j \Sigma_j + t_i \Sigma_i + T;$$

$$T_2 = t_j \Sigma_j + t_i \Sigma_i;$$

$$T_3 = t_j \Sigma_j + T;$$

$$T_4 = t_i \Sigma_i + T;$$

$$T = T(CD) \text{ (see Fig. 1).}$$

For a system in which $P_{ij,x}$ and $P_{ij,y}$ are different and required separately, the Ki_3 functions must, following (4.1), be weighted with $\cos^2 \phi$ and $\sin^2 \phi$, respectively; otherwise, (4.2) may be used to deduce the radial diffusion coefficient.

The calculation of these generalised diffusion coefficients between empty regions presents little difficulty since the integral of (4.3) becomes a sum of Ki_4 and Ki_2 function as Σ_1 tends to zero.

5. Solution of the Transport Equation

5.1 General

The neutron transport equations have been expressed (see Section 2) in terms of collision probabilities:

$$\phi = P\psi; \quad \psi = Q\phi + S, \quad (5.1)$$

and it has been observed that these equations are amenable to solution by the method of (point) successive overrelaxation (SOR) for which the iterative scheme is, in this case,

$$\left. \begin{aligned} \phi^{(n+1)} &= (1 - \omega) \phi^{(n)} + \omega P \psi^{(n)}; \\ \psi^{(n+1)} &= (1 - \omega) \psi^{(n)} + \omega S + \omega Q \phi^{(n+1)} \end{aligned} \right\}, \quad (5.2)$$

where ω is a convergence parameter, and $\phi^{(n)}$ and $\psi^{(n)}$ are the n^{th} iterates of ϕ and ψ , respectively. This method of solution has been embodied in the code PIP.⁽⁵⁾

Descriptions of the SOR method are to be found, for instance, in references (6) and (7). The conventional theory is based on the assumption that the eigenvalues λ_i of the matrix

$$\begin{pmatrix} 0 & P \\ Q & 0 \end{pmatrix} \quad (5.3)$$

are real, in which case the following results hold:

- (a) the eigenvalues μ_i of the iteration matrix L described by Eqs. (5.2) are given by

$$(\mu_i + \omega - 1)^2 = \mu_i \omega^2 \lambda_i^2, \quad (5.4)$$

- (b) the value ω_b of ω which minimises η , where

$$\eta = \max\{\mu_i\}, \text{ all } i, \quad (5.5)$$

is given by

$$\omega_b = \frac{2}{1 + \sqrt{1 - \lambda_{\max}^2}}, \quad (5.6)$$

where $\lambda_{\max}$ is the eigenvalue of largest modulus of the matrix (5.3). In this case η takes the value

$$\eta_b = \frac{1 - \sqrt{1 - \lambda_{\max}^2}}{1 + \sqrt{1 - \lambda_{\max}^2}}. \quad (5.7)$$

As is well known, the practical estimation of ω_b may be difficult owing to the proximity to $\lambda_{\max}$ of other eigenvalues or the dominance of other eigenvectors in the error at any stage.

5.2 Complex Eigenvalues

Initial experience with PIP showed that satisfactory convergence could normally be obtained as a result of conventional application of the SOR method. As stated in the previous section, this assumes that the eigenvalues λ_i of the matrix (5.3) are real, that is, the eigenvalues

$$x_i = \lambda_i^2 \quad (5.8)$$

of the matrix PQ are real and positive.

It was found, however, that the method was liable to fail following the application of the diagonal transport correction to the scattering cross sections of light elements, particularly hydrogen. An investigation has been made into the effect of some x_i being negative (λ_i pure imaginary).

In terms of x , Eq. (5.4) for the eigenvalues μ of L is

$$(\mu + \omega - 1)^2 = x\omega^2\mu. \quad (5.9)$$

Thus, the value of $\mu = \mu(\omega, x)$ with the maximum modulus determines the rate of convergence of the method. More particularly, let

$$T_1(\omega) = \max_{x \geq 0} |\mu(\omega, x)| \quad (5.10)$$

and

$$T_2(\omega) = \max_{x < 0} |\mu(\omega, x)|. \quad (5.11)$$

Then if the error $E^{(n)}$ in the solution after the n th iteration is written as

$$E^{(n)} = E^{(n)+} + E^{(n)-}, \quad (5.12)$$

where $E^{(n)+}$ is a sum of the eigenvectors of L associated with positive eigenvalues and $E^{(n)-}$ is a sum of the eigenvectors of L corresponding to negative eigenvalues, it is evident that the asymptotic convergence rate of $E^{(n)+}$ is $T_1(\omega)$ and of $E^{(n)-}$ is $T_2(\omega)$. Now let

$$-a = \min(x) \leq x \leq \max(x) = b < 1 \quad (5.13)$$

and

$$T = \max_{\omega}(T_1, T_2). \quad (5.14)$$

Examination of (5.9) shows that

(i) $T > 1$ unless $0 \leq \omega \leq 2$.

$$(ii) \quad T_1(\omega) = \begin{cases} \omega - 1 & \text{for } \omega \geq w_b = 2/(1 + \sqrt{1-b}), \\ \frac{1}{2} \{2(1-\omega) + b\omega^2 + \sqrt{b\omega^2 \{4(1-\omega) + b\omega^2\}}\} & > |\omega - 1| \\ & \text{for } \omega < w_b. \end{cases}$$

$$(iii) \quad T_2(\omega) = \begin{cases} 1 - \omega & \text{for } \omega \leq w_a = 2/(1 + \sqrt{1+a}) \\ \frac{1}{2} \{a\omega^2 - 2(1-\omega) + \sqrt{a^2\omega^4 - 4a\omega^2(1-\omega)}\} & > |\omega - 1| \\ & \text{for } \omega > w_a. \end{cases}$$

(iv) In the range $w_a < \omega < w_b$, $T_2(\omega)$ increases and $T_1(\omega)$ decreases with ω .

(v) $T_2(\omega) > 1$ for $\omega > w_1 = 2/(1 + \sqrt{a})$.

(vi) The minimum value of T , i.e., the optimum asymptotic convergence rate, occurs when

$$\omega = w_{a,b} = 2/(1 + \sqrt{1+a-b}),$$

in which case

$$T = T_1 = T_2 = H(a/b)(w_{a,b} - 1) = R, \quad (5.15)$$

say, where

$$H(x) = (1 + x^{1/2})^2 / (1 - x). \quad (5.16)$$

Figure 2 shows the principal features in the behaviour of $T_1(\omega)$ and $T_2(\omega)$ in the range $0 \leq \omega \leq 2$.

It will be observed that the introduction of negative eigenvalues of PQ introduces the possibility of divergence even though ω lies in the range $(0, 2)$. Also, and as important in practice, the optimum convergence rate rapidly becomes worse as a increases from zero (see Fig. 3). To illustrate the latter point, consider the case $b = 0.99$. If $a = 0$, then $R = 0.82$, whereas if $a = 0.25$, R has increased to 0.98. The danger of actual divergence is shown when, for example, $b = 0.95$. If $a = 0$ the optimum value of ω is 1.635, but if $a = 0.25$, then $w_1 = 1.333$, and convergence with the previous optimum parameter is now impossible.

Fig. 2. Behaviour of $T_1(\omega)$ and $T_2(\omega)$ in the Range $0 \leq \omega \leq 2$.

Fig. 3. For Various Values of a the One-parameter-method Optimum Convergence Error Reduction is Plotted against b . (Eigenvalues of PQ satisfy $a \leq \lambda \leq b$).

The problem may be ameliorated by making the transformations

$$q'_{g'g} = q_{ig'g} - \delta'_{g'g} \tilde{q}_{ig}, \quad (5.17)$$

where

$$\tilde{q}_{ig} = \begin{cases} 0 & \text{if } q_{igg} \geq 0; \\ q_{igg} & \text{if } q_{igg} < 0, \end{cases}$$

and

$$\psi' = Q'\phi + S. \quad (5.18)$$

Then

$$\phi = P'\psi', \quad (5.19)$$

where

$$P' = (I - P\tilde{Q})^{-1} P. \quad (5.20)$$

Equations (5.18) and (5.19) are of the same form as the original equations. Experiment has shown that the new equations have a slightly larger value of b while the value of a is considerably reduced, although it is still nonzero. For example, a simple water cell gave $b = 0.955$ and $a = 0.26$ in place of $b = 0.95$ and $a = 1.00$.

A special matrix routine has been written to take advantage of the zero columns that appear in $P\tilde{Q}$ in the expression (5.20). Such columns appear when some of the regions do not have negative self-scatters, for then $\tilde{q}_{ig} = 0$. This routine effectively reduces the size of the matrix to be inverted to the number of regions with negative self-scatters. It is evident from (5.20) that the components of P' may be formed group by group and that no modification is necessary if the self-scatters in a group are all positive.

Now the minimum value of $T_2(\omega)$ is

$$1 - w_a = \frac{\sqrt{1+a} - 1}{\sqrt{1+a} + 1}, \quad (5.21)$$

which is small for $1 \geq a > 0$. For example, $1 - w_a$ is 0.172 when $a = 1.0$, and is 0.056 when $a = 0.25$. This means that using a value of $\omega = w_a$ will result in the very rapid reduction of $E^{(n)-}$. Further, because $T_1(\omega) < 1$ always, the contribution $E^{(n)+}$ to the error will never diverge and $E^{(n)+}$ will

in fact decrease, although rather slowly since, $T_1(\omega) > b$ when $\omega < 1$. In practice the value of a is not known and it is necessary to use a conservative guess. By this is meant a value less than w_a , for then $T_2(\omega) = 1 - \omega$ and for many purposes the resulting increase in $T_2(\omega)$ is of no importance. A value of $\omega = 0.9$, for example, will give $T_2(\omega) = 0.1$, representing a very rapid reduction rate, whenever $w_a > 0.9$, i.e., $a < 0.495$ (which has always been a generous overestimate in the many calculations examined). The procedure adopted in PIP is to use under-relaxation for several iterations whenever undesirable effects begin to dominate the calculation. The technique used involves two parameters: $\omega^- < 1$ (preferably ω^- equal to, but certainly not larger than, w_a), and ω^+ (preferably ω^+ equal to, but certainly not less than, w_b). At each iteration either ω^- or ω^+ is used according to a complicated prescription involving a measure of the difference between previous successive iterates.

5.3 Eigenvalue Problems

In previous sections source problems described by Eqs. (5.1) have been considered. The PIP code can, however, solve the eigenvalue problem described by the equations

$$\phi = P\psi; \quad \psi = Q\phi + \nu F\phi, \quad (5.22)$$

where ν is the eigenvalue and $F\phi$ the fission source. The iterative scheme is

$$\begin{cases} \psi^{(n+1)} = (1 - \omega) \psi^{(n)} + \omega \{Q\phi^{(n)} + \nu^{(n)} F\phi^{(n)}\}; \\ \phi^{(n+1)} = (1 - \omega) \phi^{(n)} + \omega P\psi^{(n+1)}, \end{cases} \quad (5.23)$$

and ν is recalculated at each iteration by means of

$$\nu^{(n)} = \frac{\| (I - PQ) \phi^{(n)} \|}{\| PF \phi^{(n)} \|}, \quad (5.24)$$

where $\| x \|$ denotes the sum of the elements of the vector x .

In addition, an experimental technique for the solution of source problems by means of homogeneous equations has been evolved. The conventional method of solving source problems involves inhomogeneous equations, and an iterate to the solution of such equations can be grossly in error simply because it differs from the true solution by a scale factor. The straightforward iterative process does not detect this form of error, and the usual remedy is to apply a scale factor to the iterate so that it will satisfy some single overall equation obtained from the equations to be solved (by addition of such equations, for example).

An attempt to analyse such scaling leads to the method to be described in which homogeneous equations are solved. For such equations the solution is not defined to within a constant factor, and scaling errors can have no influence on convergence rates. If given a solution to the homogeneous equations, the solution of the inhomogeneous equations is obtained by a single scaling of the type just described.

The Eqs. (5.1) are replaced by

$$\phi = P\psi; \quad \psi = Q\phi + S/B(\phi), \quad (5.25)$$

where the "neutron balance factor" is

$$B(\phi) = \frac{\|PS\|}{\|(I - PQ)\phi\|}. \quad (5.26)$$

Since $\|x\|$ gives a linear term, (5.25) may be replaced by the homogeneous equations

$$\phi = P\psi; \quad \psi = Q'\phi. \quad (5.27)$$

The Eqs. (5.27) have $\lambda = +1$ and $\lambda = -1$ amongst their eigenvalues, and it may be shown that

$$\|\phi^{(n+1)} - \phi^{(n)}\| = 0. \quad (5.28)$$

For this reason the code uses $B(\phi) - 1$ as a measure of convergence.

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APPENDIX

The Effect of Varying the Mesh Size and
the Value of the Parameter χ in PIJ

The current version of PIJ requires as data the number of lines to be set across the system, the number of angles at which these lines are to be drawn, and the value of χ . Table 1 shows the effect of varying these quantities in the case of a 22-rod air-filled, unclad cluster. Region 1 is a small central rod, region 2 an inner ring of seven equally spaced larger rods, and region 3 an outer ring of 14 of the larger rods. The (arbitrary) total cross sections used were 1, 2, and 3. For the one-group flux solution (which is available within PIJ), scattering cross sections of 0.5, 1, and 1.5 were taken with source densities within each region of 3, 4, and 5. An isotropic incoming unit current was imposed at the boundary.

Table 1
EFFECT OF VARIATION OF PARAMETERS

Mesh		200 lines, 5 angles		400 lines, 10 angles		1000 lines, 15 angles	
Quantity		Value	% Diff from Best Estimate	Value	% Diff from Best Estimate	Value	% Diff from Best Estimate
P_{11}	$\chi = 0$	0 24608	-2 66	0 25399	0 47	0 25198	-0 37
	$\chi = 1$	0 25200	-0 32	0 25295	0 06	0 25286	0 02
	$\chi = \pi/2$	0 25538	1 02	0 25236	-0 18	0 25336	0 22
	$\chi = 2$	0 25793	2 03	0 25191	-0 36	0 25374	0 37
P_{22}	$\chi = 0$	0 71950		0 71976		0 71974	
	$\chi = 1$	0 71965		0 71977		0 71970	
	$\chi = \pi/2$	0 71973		0 71978		0 71969	
	$\chi = 2$	0 71979		0 71979		0 71968	
P_{33}	$\chi = 0$	0 78993		0 79000		0 78999	
	$\chi = 1$	0 78978		0 78984		0 78989	
	$\chi = \pi/2$	0 78970		0 78976		0 78985	
	$\chi = 2$	0 78964		0 78970		0 78982	
Fluxes	ϕ_1	$\chi = 0$	3 2300	3 2337		3 2320	
		$\chi = 1$	3 2442	3 2293		3 2356	
		$\chi = \pi/2$	3 2583	3 2268		3 2376	
		$\chi = 2$	3 2689	3 2250		3 2392	
	ϕ_2	$\chi = 0$	3 2070	3 2066		3 2067	
		$\chi = 1$	3 2059	3 2066		3 2066	
		$\chi = \pi/2$	3 2063	3 2066		3 2065	
		$\chi = 2$	3 2065	3 2066		3 2065	
	ϕ_3	$\chi = 0$	2 7470	2 7473		2 7474	
		$\chi = 1$	2 7464	2 7468		2 7471	
		$\chi = \pi/2$	2 7462	2 7465		2 7469	
		$\chi = 2$	2 7460	2 7463		2 7468	
	ϕ_2/ϕ_3	$\chi = 0$	1 1675	1 1672	-0 01	1 1672	
		$\chi = 1$	1 1673	1 1674	0 01	1 1673	
		$\chi = \pi/2$	1 1675	1 1675	0 02	1 1673	
		$\chi = 2$	1 1677	1 1676	0 03	1 1673	

The true value of P_{11} , the self-collision probability of a circular cylinder, is known and so, therefore, is the error in the PIJ calculation. The value $\chi = 1$ is apparently the most suitable. The quantities P_{22} and P_{33} are less sensitive to the value of χ .

Discussion of Paper
Presented by Mr. Pull

MR. SUICH (Savannah River Laboratory): The 2-D geometrical collision probability arrangement that you consider is very similar to the experimental 2-D geometry package that Honeck developed and dropped as unworkable. I would like to discover just how it is that this is going to work. The problem that Honeck ran into was that within 32K storage using 30 energy groups you are pretty well restricted to 20 mesh points. If you are going to assign mesh points to a realistic cell, you get 2-D areas which are a mean free path or so in characteristic dimension, and this is too large to represent by a single point. For any practical cell, you get very poor results from assuming the flux flat over this very large material region, and I don't see any way out of the box with your present technique either.

MR. PULL: Can I just make an aside for a moment? This PIJ code contains a routine which is in a plug-in form. It merely calculates distances from points to physical boundaries in the same way as a Monte Carlo code. By changing that routine, one can change one's geometry in the same way one does with a Monte Carlo code. Now to answer your specific question. I am not precisely sure how the code works, but I am perfectly sure that it does. I think that at any one time one needs only K^2 words of storage or less to accumulate collision probabilities. One really processes this information through from tape, building up something less than G^2 words, and puts it out on tape again, and it gets passed to the PIP code. There is no problem of strategy here.

MR. SUICH: That solution is fine. What you have done is to substitute computer time for space points. If you had read-backwards tape, or some other device such as that, along with buffered I/O, so that you could pull these matrices in and manipulate them, you might not pay too big a penalty in machine time. But if that is the only way out (that is, further subdivision of the space points), then you are going to face a fairly large penalty in machine time.

MR. PULL: I did indicate that this set of these PIJ codes appears to take about one minute per group, for realistic systems, and I kept all accuracy.

MR. SUICH: Is that of the order of 20 space points?

MR. PULL: We are talking of regions, not mesh points, and twenty regions will do more for us than 20 mesh points in an S_N .

MR. SUICH: Do I understand that you intend to operate with one point per region, as for instance in a large D_2O or graphite cell with several mean free paths of moderator surrounding the fuel element? One cannot really assign one space point to that entire region.

MR. PULL: There is no question of taking points on lines. If one is considering P_{14} , one considers the two segments involved. One says "What is the probability of going from $1 \rightarrow 4$, in my notation, in one collision step, given neutrons uniformly distributed on the source section, and going in the right direction?"

MR. SUICH: Yes, the whole problem is that if you assume your Q values are constant over several mean free paths, that are spatially uniform, you will not get good results.

MR. PULL: Yes. I still go back to what I said, though. You do better with 20 regions than you do with 20 mesh points in the conventional finite-difference code, and the problem is precisely the same as in a finite-difference code. There you ask how many mesh points you take; here you ask how many regions you take.

MR. SCHAEFER (English Electric Company): I didn't have time in my paper to get around to storage considerations. There are two storage problems: the collision probabilities and the scattering law, and I think Honeck runs out of space mainly because of the scattering-law storage requirements, unless a large number of space points is used, for which the storage is about 50-50. If you don't worship the computer god, you get rid of most of the storage for the energy transfer, but then you still have the collision probabilities left. I didn't explain how you still retain the required amount of accuracy; if you have large moderating regions, combine transport-corrected diffusion theory where it is good enough with collision probabilities where it isn't. In the few zones which are left, even for clusters, the collision probabilities can be calculated in about a hundredth of a second each on the machines we're talking about, by some other cunning devices which don't go through all these calculations but depend upon a few physical parameters.

MR. PULL: I would point out that I have described one method of calculating collision probabilities. With a special kind of geometry for which it is worthwhile to write special routines for calculations, you can calculate them in your better way and feed them directly into the PIP code.

MR. SUICH: That's fine. You can indeed do things like patching together diffusion theory and transport theory, but then you have lost

generality; you are again back to being sure that whoever is using the code knows when and where he can use it. There is a market for a code which an engineer, ignorant of neutron physics, can use.

MR. PULL: There's more to it than that. It's a question of time scale. If someone wants to look at a new system this week, okay, there's the code. Wait for the machine time; so what.

MR. BRISSENDEN (AERE, Winfrith): I think the biggest disadvantage of the collision-probability method is its restriction to isotropic emission. Apart from this, I think that it has certain advantages over the S_N method which will make it win in the end. If we can get away with isotropic calculations, then I feel that the collision-probability method is the one to use for doing multidimensional transport calculations. However, if you have to consider anisotropy of scatter, then it falls down. The reason I say this, is that here with the integral equation, you can write down the equation for the scalar flux and not the angular flux. The scalar flux is a much smoother function than the angular flux, and we don't want the angular flux anyway. If you consider the problem posed by Meneghetti, in which the cell has a very fine structure, perhaps a fifth of a mean free path across, the S_N method falls down very badly, as Meneghetti has shown. This is due to the neutrons which are at high altitude to the azimuthal of the slab. The collision-probability technique solves this problem admirably.

MR. PULL: I think the method can be extended to anisotropic scatter, and the extra complication is certainly no greater than extending the S_N method. It may be, as Mr. Brissenden says, that when one starts looking at anisotropic fluxes one needs to take many more regions to get good accuracy. If that's so, then perhaps our present computers aren't up to it.

A NUMERICAL SOLUTION OF THE GAMMA TRANSPORT EQUATION APPLIED TO CONCRETE SLABS

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ABSTRACT

The gamma transport equation is solved numerically in plane multislabs geometry. A monoenergetic source is assumed on one surface, with isotropic or collimated angular distribution. After computing the unscattered flux, the fluxes at lower energies are calculated from those at higher energies without iteration. Integration of the differential fluxes gives the energy spectra and buildup factors. Source energies ≤ 10 MeV and thicknesses of some dozen mfp can be handled with the present program BIGGI 3.

As an application, buildup factors for normal and heavy concretes are calculated and compared with those of Al, A, and Fe. The so-called Z_{eff} values for heavy concretes are found to be a function of the source energy.

The Integral Form of Boltzmann's Equation.

Most authors start from the integrodifferential transport equation which is, in plane geometry,

$$\omega \frac{\partial}{\partial x} f(\omega, x, \lambda) + \mu(\lambda) f(\omega, x, \lambda) = \int_{\sigma}^{\lambda} \iint_{4\pi} K(\lambda', \vec{\Omega}', \lambda, \vec{\Omega}) f(\omega', x, \lambda') d\Omega' d\lambda' + S(\omega, x, \lambda). \quad (1)$$

Here,

$\vec{\Omega}, \vec{\Omega}'$ = directions of the gammas; Ω' = solid angle;

ω = cosine of the angle between $\vec{\Omega}$ and the normal of the slab;

x = distance from the source plane;

λ, λ' = gamma wavelengths in Compton units $h/m_e c = 0.02426 \text{ \AA}$;

μ = macroscopic total interaction cross section;

$K(\lambda', \vec{\Omega}', \lambda, \vec{\Omega})$ = transference function of the gammas;

$f(\omega, \mathbf{x}, \lambda)$ and $S(\omega, \mathbf{x}, \lambda)$ = space- and energy-dependent angular number flux and source density of the gammas; f in quanta/(cm²-sec-unit λ -sterad), S in quanta/(cm³-sec-unit λ -sterad).

In order to solve this equation directly, we must replace $\partial f / \partial \mathbf{x}$ by a suitable quotient of differences. But in a shield f varies roughly exponentially in $\mathbf{x}$, and this results in increasing errors after some mfp (mean free paths) because of the differences between $\partial f / \partial \mathbf{x}$ and $\Delta f / \Delta \mathbf{x}$ and even rounding errors, or a very fine mesh in $\mathbf{x}$ must be used. But this problem can be avoided by transforming Eq. (1) into a pair of coupled integral equations ([3], pp. 228f, "third form of the Boltzmann Equation"):

$$q(\omega, \mathbf{x}, \lambda) = \int_{\sigma}^{\lambda} \iint_{4\pi} n_{e1} \frac{d\sigma_{KN}}{d\Omega} \delta(1 - \cos \psi + \lambda' - \lambda) f(\omega', \mathbf{x}, \lambda') d\Omega' d\lambda' + S(\omega, \mathbf{x}, \lambda); \quad (2a)$$

$$f(\omega, \mathbf{x}, \lambda) = \int_{\sigma}^{\infty} \exp[-\mu(\lambda)s] q(\omega, \mathbf{x} - \omega \mathbf{s}, \lambda) ds, \quad (2b)$$

where

$q(\omega, \mathbf{x}, \lambda)$ = generalised source density, adding to the real source S the "scattering sources;"

ψ = scattering angle in the Compton process;

s = spatial coordinate opposite to the gamma flight direction.

In Eq. (2a) the transference function has been split into a product of the electron density n_{e1} , the Klein-Nishina cross section for free electrons:

$$\frac{d\sigma_{KN}}{d\Omega} = \frac{1}{2} \left(\frac{e^2}{m_{e1}c^2} \right)^2 \left(\frac{\lambda'}{\lambda} \right)^2 \left[\frac{\lambda'}{\lambda} + \frac{\lambda}{\lambda'} - 1 + (1 + \lambda' - \lambda)^2 \right], \quad (3)$$

and a Dirac δ -function taking account of the Compton relation $\lambda - \lambda' = 1 - \cos \psi$. Further, e and m_{e1} are the electronic charge and mass, respectively, and c the velocity of light. The law of cosines in spherical trigonometry gives (see Fig. 1)

$$\cos \psi = \cos \vartheta \cos \vartheta' + \sin \vartheta \sin \vartheta' \cos \gamma' =$$

$$\omega \omega' + \sqrt{1 - \omega^2} \sqrt{1 - \omega'^2} \cos \gamma'. \quad (4)$$

Figure 1
Geometry of the Scattering
Process ($\vec{\Omega}'$ = Old, $\vec{\Omega}$ = New
Gamma Direction)

We insert Eq. (4) in Eq. (2a) and perform the integration over γ' :

$$q(\omega, \mathbf{x}, \lambda) = n_{e1} \int_{\sigma}^{\lambda} \frac{d\sigma_{KN}}{d\Omega} \int \frac{2f(\omega', \mathbf{x}, \lambda') d\omega' d\lambda'}{[(1 - \omega^2)(1 - \omega'^2) - (1 + \lambda' - \lambda - \omega\omega')^2]^{1/2}} + S(\omega, \mathbf{x}, \lambda). \quad (5)$$

(We use the following property of the δ -function:

$$\int_a^b \delta[f(z)] \, dz = \sum_{i=1}^n \frac{1}{|f'(z_i)|},$$

where $z_1, z_2, \dots, z_n$ are the zeros of $f(z)$ between a and b .)

The integration limits for ω' in Eq. (5) are those values between which the integrand is real. Equation (5) can be integrated numerically, taking account of Eq. (3); but near the ω' -limits the integrand diverges, and it is convenient to integrate the diverging factor $[\dots]^{-1/2}$ analytically. In Eq. (2b) we write

$$f(\omega, \mathbf{x}, \lambda) = \int_{\delta}^{\Delta \mathbf{x}/|\omega|} \dots ds + \int_{\Delta \mathbf{x}/|\omega|}^{\infty} \dots ds,$$

(Δx = spatial integration step), and the second term can be transformed into:

$$\exp[-\mu(\lambda) \frac{\Delta x}{|\omega|}] f(\omega, \mathbf{x} - \Delta \mathbf{x} \text{ sign } \omega, \lambda).$$

We evaluate the first part by a linear interpolation between $\mathbf{x}$ and $\hat{\mathbf{x}} = \mathbf{x} - \Delta \mathbf{x} \text{ sign } \omega$

$$\begin{aligned} f(\omega, \mathbf{x}, \lambda) = & \frac{1}{\mu(\lambda)} \left\{ q(\omega, \mathbf{x}, \lambda) \left(1 - e^{-\frac{\mu(\lambda) \Delta x}{|\omega|}} \right) + \right. \\ & + \frac{q(\omega, \hat{\mathbf{x}}, \lambda) - q(\omega, \mathbf{x}, \lambda)}{\mu(\lambda) \Delta x / |\omega|} \left[1 - \left(1 + \frac{\mu(\lambda) \Delta x}{|\omega|} \right) e^{-\frac{\mu(\lambda) \Delta x}{|\omega|}} \right] + \\ & \left. + e^{-\frac{\mu(\lambda) \Delta x}{|\omega|}} f(\omega, \hat{\mathbf{x}}, \lambda) \right\} \end{aligned} \quad (6)$$

The Numerical Integration

Equations (5) and (3) can be integrated directly. In BIGGI 3 (Boltzmanns Integralgleichung für Gamma-Intensitäten) we use a 3-dimensional mesh: 71 points in λ with up to 5 spacings, 26 points in $\mathbf{x}$ with equal spacing in mfps, and the ω -mesh with up to (usually) 8 points can be chosen arbitrarily. The source is assumed monoenergetic, and λ_1 the lowest λ corresponding to the highest (source-) energy. Let the other wavelengths be $\lambda_2, \lambda_3, \dots, \lambda_{n-1}, \lambda_n$, with $\lambda_1 < \lambda_2 < \lambda_3 < \lambda_4 < \dots < \lambda_{n-1} < \lambda_n$.

The program proceeds like this (we omit the variables $\mathbf{x}$ and ω because of simplicity):

Stage 1 $f(\lambda_1)$

Stage 2 $f(\lambda_1) \rightarrow q(\lambda_2) \rightarrow f(\lambda_2)$

Stage 3 $f(\lambda_1), f(\lambda_2) \rightarrow q(\lambda_3) \rightarrow f(\lambda_3)$

Stage 4 $f(\lambda_1), f(\lambda_2), f(\lambda_3) \rightarrow q(\lambda_4) \rightarrow f(\lambda_4)$

Stage n $f(\lambda_1), f(\lambda_2), \dots, f(\lambda_{n-1}) \rightarrow q(\lambda_n) \rightarrow f(\lambda_n)$

We get the q -values by inserting the f -values into Eq. (5) and the f -values by inserting the q -values in Eq. (6). The boundary condition for f is that the incoming scattered fluxes vanish. This recursion is possible because the gamma energy can only decrease in each scattering process, and therefore the flux at a given energy is not influenced by those at lower energies. In mathematical terms: we have a Volterra integral equation. But in a reproducing medium this simplification is not possible.

Finally, the spectra

$$n(x, \lambda) = 2\pi \int_{-1}^1 f(w, x, \omega) d\omega$$

and the buildup factors are evaluated by simple integrations. The influence of the not-calculated part of the low-energetic spectrum is estimated by an extrapolation.

The Exponential Transformation

In order to save machine time, we make the substitution

$$f(\omega, x, \lambda) = e^{-\alpha\mu_1 x} \tilde{f}(\omega, x, \lambda);$$

$$q(\omega, x, \lambda) = e^{-\alpha\mu_1 x} \tilde{q}(\omega, x, \lambda),$$

where α is a dimensionless quantity in the range from 0.7 to 1. Since $\tilde{f}$ and $\tilde{q}$ do not change as rapidly with x as f and q , we can choose much greater spatial integration steps, such as $\mu_1 \Delta x$ equal to 2.5 instead of $1/3$. Even a trial with $\mu_1 \Delta x = 6$ gave only a 20% error in the buildup factor. Only for boundary effects (e.g., the albedo) are smaller $\mu_1 \Delta x$ needed.

Which are the equations for $\tilde{f}$ and $\tilde{q}$? Equation (5) or (2a) does not change; in (6) or (2b), $\mu(\lambda)$ must be replaced by $\tilde{\mu}(\lambda) = \mu(\lambda) - \alpha\mu(\lambda_1)\omega$ (an anisotropic attenuation of the "transformed rays," roughly comparable with certain crystals). This result is well-known in the Monte Carlo technique.⁽⁴⁾

Results : Spectra

As an example we show in Fig. 2 the energy spectra $n_E(x, \lambda) = n(x, \lambda)/\lambda$ in Al. (The unscattered flux should be a δ -function at $\lambda = \lambda_1 = 0.511$.) The parameters near the curves are the distances from the source plane (with a plane monodirectional source). The discontinuities at $\lambda = \lambda_1 + 2$ and in the derivative at $\lambda = \lambda_1 + 4$ are real; they correspond to the jumps of the Placzek function in neutron physics (even in a head-on collision a gamma cannot lose its whole energy, and therefore in the case of a mono-energetic source at λ_1 the once-scattered flux breaks off at $\lambda_1 + 2$, the twice-scattered at $\lambda_1 + 4$, etc., in accordance with the Compton relation).

The reflected spectrum at $\mu_1 x = 0$ shows two additional jumps at $\lambda_1 + 0.8$ and $\lambda_1 + 0.5$. A detailed analysis shows that for a monodirectional beam the once-scattered reflected spectrum breaks off at $\lambda_1 + 1$ and the twice-scattered at $\lambda_1 + 2 - \sqrt{2} \approx \lambda_1 + 0.586$.

Fig. 2. Spectra in Al, $E_1 = 1.0$ MeV. 4-mfp Thickness;
Source Plane Monodirectional.

In Fig. 2 the cutoffs are shifted because of our nonideal collimation (the machine cannot calculate with a δ -source in ω !). In thin slabs, we see in the transmitted flux, too, a jump at $\lambda_1 + 1$. (But for isotropic and similar sources, we have only the Placzek discontinuities at $\lambda_1 + 2$, $\lambda_1 + 4$, etc.!).

Buildup Factors

From the shielding point of view, the buildup factors are of more interest than spectra. In order to see the limitations of our method, we made an internal check and a comparison with the results of the moments method. Briefly summarized, our method is sensitive neither to changes in the spatial parameters α and $\mu_1 \Delta x$ nor to a change in the λ -mesh. The dependence on the ω -mesh is greater; for most cases, we get good agreement, about 10% or better, with Refs. 1 and 5 by using the values $\omega = \pm 1, \pm 0.925, \pm 0.84, \pm 0.28$. But for low energies (~ 0.5 MeV) in low-Z materials and high energies (~ 10 MeV) in high-Z materials we have differences, internal and compared with the moments method, of up to 30% for deep penetrations. For the moments method, just such error limits were estimated (Ref. 7, p. 115) for deep penetrations in water; and our internal check gave up to 26% in the worst case. So we can say that our results and those of Ref. 5 are compatible within the error limits of both methods.

Application: Buildup Factors in Some Concretes

Instead of calculating the buildup in concrete directly, a reduction of work was tried by substituting for the concrete a material having a suitable effective atomic number Z_{eff} for which the buildup factors can be taken from the moments method (Ref. 5, Chapter 6.2; Ref. 1, p. 221; and Ref. 6, p. 17). With our program we can check this method directly: we evaluate the buildup for three different concretes and the corresponding Z_{eff} materials. We choose, using the nomenclature of (6):

ordinary concrete ($\rho = 2.35 \text{ g-cm}^{-3}$): 04, $Z_{\text{eff}} = 11$ (Na)

ilmenite concrete ($\rho = 3.44 \text{ g-cm}^{-3}$): I-NRUe, $Z_{\text{eff}} = 18$ (A)

barytes concrete ($\rho = 3.50 \text{ g-cm}^{-3}$): Ba-a, $Z_{\text{eff}} = 27$ (Co)

In order to have better known reference materials, we take $Z_{\text{eff}} = 13$ instead of 11, and 26 instead of 27 (Al and Fe, not Na and Co; these variations should have little real effect).⁽⁶⁾ The comparison Al-concrete 04 gives excellent agreement. For the source energies of 0.5, 2, and 8 MeV, and for penetrations up to 20 mfp, B_E , B_D , and B_A show only differences $\leq 3\%$; only the unimportant particle buildup, B_P , yielded $\leq 6\%$.

The comparison ilmenite concrete-argon gives higher divergences. Only for source energies $E_1 \geq 2 \text{ MeV}$, the agreement is good, $\leq 4\%$ in B_E , B_A and B_D . For 1 MeV, $B_E^{(A)}$ can be greater than $B_E^{(I-C)}$ by up to 7% at $\mu_1 x = 20$, and for 0.5 and 0.255 MeV the B_E -ratios are plotted in Fig. 3 as

Fig. 3: Ratio of "Effective-Z-" to Real Energy-buildup Factor

function of penetration; their highest values: 1.2 for 0.5 MeV, and 1.6 for 0.255 MeV. In shielding calculations, factors like these are in most cases unimportant, and the choice $Z_{\text{eff}} = 18$ is still reasonable, even at low source energies. Nevertheless, we should notice that for $E_1 \leq 0.5$ MeV a Z_{eff} of 21 or 22 (Ti or Va) should give better agreement with reality. Besides we can decide with our results for A, Al, and 04 the question whether for the concrete 04 Z_{eff} is 11 or 18, a value found by another author (Ref. 6, p. 20). For $E_1 \geq 2$ MeV, equally good choices are 18, 13, or 11; there is no significant difference among A, Al, Na, and the concrete 04. But for 0.5 MeV, $B_E^{(04)}$ is higher than $B_E^{(A)}$ by up to nearly 40% at deep penetrations. For 0.255 MeV, we have at $\mu_1 x = 20$ B_E , B_A , and B_D ratios of ~ 2 . Because of this, $Z_{\text{eff}}(04) = 11$ or 13 is surely a better choice than 18.

But the comparison barytes concrete-iron gives still worse results. Only for $E_1 = 8$ MeV do we have good agreement: $\lesssim 4\%$ in B_E , B_A , and B_D . For the other source energies, Fig. 3 shows the ratios $B_E^{(\text{Fe})}/B_E^{(\text{Ba-a})}$. Below 1 MeV at deep penetrations this ratio is far from unity, becoming 7 at $\mu_1 x = 20$ for the isotropic source at $E_1 = 0.255$ MeV. This means we cannot replace barytes concrete by iron for all source energies. For low energies, a considerably higher Z_{eff} should be chosen; a rough interpolation of our 0.5-MeV results between those of Ref. 5 at $Z = 26$ and $Z = 50$ gives approximately $Z_{\text{eff}}(\text{Ba-a}) \approx 42$ (Mo).

Discussion of the Results

What is the physical reason for the fact that the results of the effective-Z concept are excellent in one case and bad in another? The reason is to be found in the different chemical compositions (see Table 1).

Table 1
ELEMENTAL COMPOSITIONS OF THE CONCRETES, g/cm³*

Element	Z	04	I-NRue	Ba-a
H	1	0.013	0.009	0.024
C	6	-	0.015	-
O	8	1.165	1.182	1.185
Na	11	0.040	-	-
Mg	12	0.006	0.057	0.004
Al	13	0.107	0.042	0.014
Si	14	0.737	0.066	0.035
S	16	0.003	-	0.364
K	19	0.045	-	-
Ca	20	0.194	0.102	0.167
Ti	22	-	0.649	-
Fe	26	0.029	1.309	0.160
Ba	56	-	-	1.551
ρ_{total}		2.339	3.431	3.504

*Different authors give in some cases different compositions for the same concrete, but the differences are $\lesssim 1\%$ in ρ_{total} , and were neglected in this context.

For 04 the most important constituents lie in the range of Z from 8 to 14 (88% in weight); medium- Z elements like Ca and Fe ($Z=20$ or 26) only give rise to small corrections. Here it is not difficult to find a suitable average, and it is no wonder that $Z_{\text{eff}} = 11$ coincides with the arithmetic mean of 8 and 14.

For I-NRUe the distribution in weight has another form: 60% have medium- Z values from 20 (Ca) to 26 (Fe), and 35% lie in the low- Z range ≤ 8 . As long as the photoeffect ($\sim Z^4 E^{-3.5}$) is only a small correction, a reasonable averaging is possible. But for $E_1 \leq 1/2$ MeV, we must carry down the calculation of the scattered spectra below the single-scattering cutoff (Compton relation) at $\lesssim 1/6$ MeV; here we approach the energy range where in iron the photoeffect predominates [$\sigma_{\text{photo}} > \sigma_{\text{scatt}}$ below 0.11 MeV, (Ref. 1, p. 144)]. In this range the σ values of the heavy elements behave more like Z^4 than like Z in the Compton range. Clearly it is impossible to find one Z_{eff} valid for both ranges; for E_1 well below 0.11 MeV, Z_{eff} will tend more to be 26 instead of 18, where the photoelectric range begins at 0.07 MeV! (For the ordinary concrete 04 this effect is negligible, because the Fe and Ca content is small, only some few %.)

Still more than for I-NRUe these reasons apply for Ba-a: 35% lie in the Z range ≤ 8 , but 44% are Ba with $Z = 56$, and for Ba the photoelectric range begins at 0.31 MeV, as compared with the substitute iron ($Z=26$) at 0.11 MeV. As the single-scattering cutoff lies in any case < 0.255 MeV, we do not only approach the critical range where $\sigma(\text{Ba}) \gg \sigma(\text{Fe})$ (σ per electron), we enter it directly! Only for high source energies will this range give a negligible contribution to the buildup factors; for 2 MeV we already have a visible effect, and for $E_1 \leq 1/2$ MeV the buildup can change even by one order of magnitude.

As a final result we can say that Z_{eff} should be considered as a function of the source energy E_1 ; only for ordinary concretes (more generally, for materials where the main constituents have neighboring atomic numbers) does this function become constant in the interesting source-energy range.

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Discussion of Paper
Presented by Mr. Penkuhn

MR. MacAIRE (Electricite de France): You were speaking of integrodifferential equations, but equations (1) and (2) of the summary are integral equations, not integrodifferential.

MR. PENKUHN: Equations (1) and (2) form a set of two coupled integral equations. These are already the transformed equations. The transformation is made for neutron transport theory in the book by Weinberg and Wigner, and is equally possible for gamma theory.

SESSION II

NUMERICAL ANALYSIS AND REACTOR MATHEMATICS

Monday, May 17, 1965

CHAIRMAN: Richard Ehrlich
Knolls Atomic Power Laboratory

CO-CHAIRMAN: J. Merkwitz
Kernforschungszentrum--Germany

SCIENTIFIC SECRETARIES: Gary Leaf
David Meneghetti
Argonne National Laboratory

ACTIVITIES OF THE ANL-ENEA COMPUTER PROGRAM LIBRARIES AND THE ORNL RADIATION SHIELDING INFORMATION CENTER*

Margaret Butler
Applied Mathematics Division
Argonne National Laboratory
Argonne, Illinois

Betty Maskewitz
Radiation Shielding Information Center
Oak Ridge National Laboratory
Oak Ridge, Tennessee

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ORIGIN AND OPERATION OF THE ARGONNE CODE CENTER

About nine years ago, in 1956, at the Second Annual Meeting of the American Nuclear Society held here in Chicago, the initial meeting of an informal group known as the Nuclear Codes Group was held. A notice posted on the bulletin board prompted the meeting of "all persons interested in the development and use of computer codes for reactor design." This group continued to hold regular though informal meetings in conjunction with the semi-annual ANS meetings, discussing current programming efforts, and exchanging ideas and codes.

A Newsletter was published and distributed containing code abstracts submitted by Group members. These abstracts for the most part followed the format of the now historical Atomic Energy Commission document AECU-3078, A Bibliography of Available Digital Computer Codes for Nuclear Reactor Problems.⁽¹⁾ This format was as shown in Fig. 1.

Approximately 100 codes were included, covering the seven categories as shown in Fig. 2.

During the period from September 1956 to December 1959, the Nuclear Codes Group published and distributed ten Newsletters through the auspices of the AEC Computing Facility at New York University.⁽¹¹⁾

*Work performed in part under the auspices of the U. S. Atomic Energy Commission.

TITLE	Cog. Eng.	Laboratory
Computer	Problem Status	Category
Geometry & dimensions	Typical computing time	Parameters solved
Problem Description		
Limitations of the code		
References		

Fig. 1. Code Abstract Format (AECU-3078)

1. Reactor and Nuclear Physics (P)
2. Reactor Survey (RS)
 - One Dimension
 - One Group
 - Two Group
 - Three Group
 - Multigroup
 - Two Dimension
 - Few Group
 - Multigroup
 - Three Dimension
 - Two Group
3. Shielding (S)
4. Reactor Kinetics (K)
5. Reactor Burnout (RB)
6. Reactor Engineering (E)
7. Miscellaneous (M)

Fig. 2
Category Definitions
(AECU-3078)

In 1959 Ward Sangren and General Atomics personnel collected from Group members approximately 300 abstracts, which they edited and published in the Communications of the Association for Computing Machinery.⁽²⁾ A supplementary list of another 100 abstracts was collected and published in the same journal the following year.⁽³⁾ Additional reactor code collections and references are indicated in the bibliography.⁽⁴⁻¹⁰⁾

It was in 1959 also, after much discussion and heated argument, that the Nuclear Codes Group decided to petition the American Nuclear Society to become the Reactor Mathematics and Computation Division. The official membership list grew from approximately 40 members to over 1000 with this official step.

With stature and membership came a desire for a more formal and routine means for handling the distribution of computer codes and the dissemination of information concerning them.

A format for an official code abstract was agreed upon, and plans were made to publish these abstracts in the Society's journal, Nuclear Science and Engineering. Short notes on applications and problems in the use of codes were to be submitted for publication in the ANS monthly publication, Nuclear News.

During 1960 the plans for a centralized agency to maintain the code-abstract files and to serve as a source of information as to the accessibility of reactor codes and references were discussed. A proposal was made whereby with the cooperation of Division members and computer manufacturers, the Argonne National Laboratory would undertake this effort.

Procedures were drafted defining the material to be collected, reproduced, and disseminated, and the responsibilities of the ANS membership, Code Center installation representatives, computer manufacturers' representatives, and the ANL Code Center.

Two categories of material were defined:

A. The code abstract, which in its present form includes:

1. name or designation of program;
2. computer for which program is designed and others upon which it is operable;
3. nature of physical problem solved;
4. method of solution;
5. restrictions on the complexity of the problem;
6. typical running time;
7. unusual features of the program;
8. related and auxiliary programs;
9. status;
10. references;

11. machine requirements;
12. programming language(s) used;
13. operating system or monitor under which program is executed;
14. any other programming, operating information, or restrictions;
15. name and establishment of author;
16. material available.

B. The "code package," including (as shown in Fig. 3) - for FORTRAN, ALGOL, or other compiler language codes:

Fig. 3. ANS-ANL Code Center Code Package

1. source or statement deck, and object or binary deck, together with any special subroutines required, in the form in which the code is most easily transmitted, i.e., cards or tape;
2. operating instructions, a description of the input data required, and the output information printed, including a sample problem, or test case;
3. reference material, such as reports and memoranda describing the problem for which the code was written, and the code itself, in detail; flow charts, definitions of nomenclature, and code symbols should be included whenever possible;
4. library material required for use of the code, such as cross-section specifications;

- for assembly language or machine-operation-only codes:

1. code deck or tape, including any special subroutines required, in the form in which the code is most easily transmitted, i.e., cards or tape. Items 2, 3, and 4 as above - operating instructions, sample problem, reference material, and library data;
5. symbolic or assembly decks or listing of the code.

The submission of this material to the Code Center is the responsibility of the individual members of the Division, either directly or through

their installation representatives. The Code Center edits and publishes the code abstracts, transmitting them to ANS for distribution to the Division membership. In addition, the Argonne Center collects, reviews, and transmits the "code package" material to the appropriate computer manufacturer's representative for retention and distribution upon request from the Center.

Difficulties have been encountered in relying upon computer manufacturers for the distribution of "code package" material. In addition to the expected communication and associated delay problems, the Center has been forced in many instances to take over complete reproduction and distribution services for many of our library codes which the manufacturer arbitrarily deleted from his library. Reliance upon these manufacturers for performing distribution of "code package" material has proved not only unrealistic, but impractical. The Code Center would like to continue to transmit library programs to the computer manufacturers to make them as generally available as possible, but if financial means could be found would like in the future to answer requests for "code package" material directly.

A list of all material distributed by or through the Center together with the recipient's name and address is maintained for each code contained in the Code Center library, and available to the code author at any time.

The various installation representatives at AEC installations serve as a source of information to the Code Center concerning codes or requests emanating from their installation and it is they, in collaboration with the Code Center personnel, who supply the answers often to the nonroutine inquiries received.

The operation looks something like that in Fig. 4. The Code Center, as you see, is the bottleneck. Currently, that bottleneck represents a portion of my time and the full-time efforts of my assistant, the Code Center secretary, within the Applied Mathematics Division of the Argonne Laboratory.

Fig. 4

Schematic Diagram of
ANS-ANL Code Center
Operation

Since 1961 the Argonne Code Center has published nine distributions containing abstracts of approximately 168 codes.⁽¹²⁾ Something like 1500 "code package" requests have been filled, and we haven't kept track of all those code queries received either unrelated to library material or which required no transmittal of material.

An IBM-1401 KeyWord-In-Context (KWIC) program is used to provide an updated index to available codes with each distribution of abstracts. This index (see Fig. 5) has replaced the categories as defined originally (see Fig. 2). In addition, a CDC 160A program has been developed for library maintenance and retrieval purposes. This program will provide source listings, and source, object, sample problem, and/or library decks upon demand, when the requested material is available in the library.

= S4 CYLINDRICAL CELL CODE, 1-D SOLUTION FOR 1	53
WITHIN A CYL, 2-C FOR 7090 BY CRNL F	67
OR SLAB, CYL, SPH ON 7090 BY HAPD FLOCCO RSB T= G	75
RCH 7090 DAC F RS = PDS, 1-D MULTI-GP	81
SECTION DATA REDUCTION, MARTIN F+FAP	16
RSBP T= DDB, 2-C R-Z DIFFUSION DEPLETION CODE 709	99
2-D 2-GP DEPLETION SLAB CYL 7090 ORNL F	88
JRN, 1-D DEPLETION ON P1 OR SN FOR 7090, MARTIN F+	96
DIFFUSION DEPLETION CODE 7090 GA F+FAP R	99
3 FEW-GP DEPLETION CODE SLAB CYL SPH, 7090, GA F	117
MIT CELL DESIGN CALC. FOR LATTICES FOR 704 BY WAPD	101
OR PLANT DESIGN OPTIMIZATION 7090 AI F RS	112
OR PLANT DESIGN OPTIMIZATION 7090 AI F RS	114
NEAR A DETECTOR, 704, UF F = DETECTO	61
= DETECTOR, DISTURBED FLUX IN OR NEAR A DET	61
IN CYL DETECTOR 704 F = TRG-RS(GAMMA)	68

Fig. 5
KWIC Index

The most recent revision of the abstract format was completed in collaboration with our European counterpart, the ENEA Computer Programme Library, to facilitate the interchange of European and American Library material.

ENEA COMPUTER PROGRAMME LIBRARY

Just one year ago this month, the ENEA Computer Programme Library was installed at the host centre, the Joint Research Center of Euratom at Ispra, Italy. Apart from the head, the staff of the library consists of two programmer-mathematicians, an accountant, a secretary, and a machine operator.

Twelve countries support the Library: Austria, Belgium, Denmark, France, F. R. of Germany, Italy, Netherlands, Norway, Spain, Sweden, Switzerland, and the United Kingdom.

For the first three years of operation, a budget of \$520,000 has been allocated.

Seventy-five establishments from the Member countries form a "users' society." The nomination of establishments to participate in the Library is a national affair and, once nominated, these establishments are represented by a liaison officer, normally one per establishment. The

Library itself has liberal access to the IBM-7090 computer installation at Ispra and, within the users' society, 26 establishments either own or have easy access to a large installation of the computing power of the IBM-7090 series. Included amongst these machines are other makes such as: English Electric KDF-9, ICT ATLAS, CDC 1604 and 3600, GE 625, and UNIVAC 1107. There is also a large variety of other small installations used by the establishments, for example, Olivetti, GIER, IBM-1620, Siemens 2002, and ZUSE. Programmes written for the former type of installation tend to be more easily distributable and easier to implement because they are written mainly in FORTRAN or one of its dialects.

To date, 787 programmes have been offered to the Library of which some 400 are for the larger type of computer. Of a total of 219 programmes available at the Library, 146 have been obtained from the Programmotheque of the Centre de Traitement de l'Information Scientifique (CETIS) of Euratom which the Library was fortunate to be able to take over. It is interesting to note that of the total number of programmes offered to the Library, about 200 are of American origin. During its first year of operation, 22 programmes were received directly from the Argonne Code Center - one result of the co-operation for the interchange of information which exists between the two libraries.

The preparation of a programme package by the author is often a tedious and unattractive task. The Library has found that it appears more worthwhile and is also more efficient if a member of the Library staff visits the contributing centre and assists in this work.

It is part of our policy that the programmes in the Library are routine tested before being distributed, that is, the symbolic programme is compiled and one or more sample problems are executed satisfactorily. In rare cases a more complete testing is carried out in order, for example, to trace more complicated errors or to translate the programme for use on another computer. The Library would like to acknowledge the continuous support of the CETIS personnel in this work.

In one year of operation the Library has dispatched 180 programmes resulting from 47 requests, including 17 European programmes which have been sent to the Argonne Code Center. In fulfilling requests, we attempt to take into account the equipment available at the requester's establishment so that, for instance, programmes are not transmitted on magnetic tape to an installation without tape facilities, or lacking compatibility with our type of tape.

Normally, the distribution of a program package involves the preparation of a tape containing the symbolic version of the programme, together with input data for a sample problem and any library data which might be required. The programme report, any other associated documentation, and the output resulting from the successful execution of the program usually complete the package.

Experience has shown that a fully automatic distribution system is needed to reduce the human repetitive action in this preparation and, to this end, a programme is presently being developed and written.

The Library holds a stock of 500 magnetic tapes. Member establishments are therefore not obliged to return immediately a tape sent to them, but it may be held until the Library requests a programme from the establishment concerned.

To ensure a feedback of information which the Library judges essential for its work in distributing programmes, all programme packages sent out include a questionnaire (to be returned to the Library) requesting details concerning problems encountered during the implementation of the programme, experience gained during its production execution, and the state of the package on its receipt.

Programmes written for computers other than the larger type of installation have proved a problem which we are solving by studying documentation concerning the software used for these machines and by acquiring practical experience on computers owned by participating establishments.

The contents of the Library and the work which is done there are described and circulated to the participating establishments in the following ways:

1. A Newsletter⁽¹³⁾ is distributed three or four times a year; it contains details of the programmes offered to the Library, articles describing the work currently being carried out in participating establishments, announcements of forthcoming conferences, and other matters of general interest.

2. A book of Programme Abstracts,⁽¹⁴⁾ which gives details of the programmes available in the Library, has been published and is updated at frequent intervals. The abstract format used has been developed jointly and adopted by the Argonne Code Center and the Library. This greatly facilitates the interchange of information.

3. A looseleaf folder containing descriptions of the computer installations which are available to the member establishments is currently being prepared.

4. It is intended to hold seminars on relatively confined topics, where programmes will be presented and experience in their use obtained. The object of these meetings will be to examine groups of programmes which have been written to solve a common problem or, alternatively, to examine the programmes originating from a single establishment and little known to the other establishments.

The scope of the Library during its initial period has been purposely confined to its purely functional side. However, after a period of consolidation there are many foreseeable "natural" extensions to its activities. One of these activities in which the Library has already taken some action and which will certainly be expanded in the future is to advise member establishments on the use of different programmes for a given problem. This evaluational aspect will play an increasingly important role. To this end, contact has been made with the European American Committee on Reactor Physics, and a study is being made to enable this Committee to aid the Library in evaluating the relative merits of different programmes. This investigation is concerned with fuel-burnup programmes presently in use at participating establishments. It is intended that the EACRP will also advise us on other types of programmes.

Of course, we also maintain close links with our twin, the ENEA Neutron Data Compilation Centre. In particular, the evolution of an evaluated data file is of great interest to us.

In the field of large shielding programmes, the Library is cooperating closely with the Radiation Shielding Information Center (RSIC) at Oak Ridge. As a result of the direct links which we have established with the RSIC, users of the Library will be able to benefit from the accumulated experience on shielding problems which is available at that Center.

RADIATION SHIELDING INFORMATION CENTER

Mrs. Butler and Mr. Rosen have outlined the history, development, and current activities of the Argonne Code Center and the ENEA Computer Programme Library - two large and wide-scale efforts to collect and distribute reactor codes. May I invite you now to turn your attention to a technical tool which is rapidly gaining attention, the specialized information center.

Many attempts have been made by the technical community to cope with the ever-increasing volume of information which threatens to saturate the individual researcher. The concept of the specialized center received authoritative support from the Panel on Science Information of the President's Science Advisory Committee.⁽¹⁵⁾ It is stated in the report: "The Panel sees the specialized information center as a major key to the information system, as a scientific institute rather than a scientific library. The specialized center will become the accepted retailer of information, switching, interpreting, and otherwise processing information from the large wholesale depositories and archival journals to the individual user." The Panel envisioned the ideal information center as "a technical institute manned by working scientists who make it their business to know as much as possible about a certain specialized area of science, and who critically compact, review, and synthesize information for the technical community."

The RSIC is such a scientific information center.⁽¹⁶⁾ It is manned by working scientists whose major goal is to aid in advancing the art of shielding.

The Radiation Shielding Information Center was established at ORNL by the U. S. Atomic Energy Commission in November 1962. Sponsored by the Neutron Physics Division, E. P. Blizard, Director, the Center was organized by S. K. Penny and D. K. Trubey. An advisory board of Coordinators, comprised of members selected from organizations having significant radiation shielding problems, was named to aid the overall program of the Center.

The purpose of RSIC was to assist the scientist in solving radiation shielding problems. Information, including that related to digital computer codes, was to be collected, evaluated, and disseminated by the Center. The primary function of the Center was to be that of technical operations. The functions associated with the necessary special library operations were to be well formulated but secondary in importance. The initial effort was directed toward accumulating a "store" of information on shielding against radiation from reactors and toward the development of an information-retrieval system.⁽¹⁷⁾

In March 1963 a Computer Code Section was established to collect, evaluate, and disseminate computer codes useful for shielding calculations. By June 1963, RSIC completed its first shielding bibliography,⁽¹⁸⁾ published a newsletter,⁽¹⁹⁾ and had underway several activities in connection with computer codes.

The announced purpose and the working philosophy initially proposed are current RSIC operating policy. The scope has since been enlarged to include accelerator shielding, shielding from nuclear weapons radiation (supported by the Defense Atomic Support Agency), and shielding from radiation encountered in space (supported by the National Aeronautics and Space Administration). The staff consists of S. K. Penny (Director), D. K. Trubey, a secretary, and myself, assisted by several ORNL physicists and nuclear engineers, and by the advisory board of 77 coordinators. Programming and computer services are supplied by a staff of five full-time employees experienced in nuclear codes and additional part-time assistance as needed.

The RSIC now has a total distribution of over 400 individuals, serving 160 installations in the USA, Australia, Belgium, Brazil, Canada, Czechoslovakia, England, France, Germany, Holland, Hungary, Israel, Italy, Japan, Norway, South Africa, Sweden, and West Germany.

How does the RSIC function? What do we do? What services do we give?

The Center's activities may be divided into three areas: library functions, technical functions, and publishing functions. This is the natural order in which these functions were formulated, and each will be described in turn in more detail.

The Center has identified the shielding literature, and this literature is constantly being scanned for the relevant articles. This scan includes articles which must be translated into English. The literature is reviewed, and the bibliographic and indexing information is entered into a computer-oriented information-retrieval system. The selected literature is also placed in an archival microfiche file.

The collection of digital-computer codes written to perform shielding calculations is of great interest and presently consists of 57 code packages. The requirements for codes to be placed in the collection are complete documentation, availability of source decks, and sample input and output. The Center has defined the code package to include the subject program, any auxiliary routines that have been written to assist in data preparation for input to it, and any analysis routines written to deal with output. We never "freeze" a code package, but continue to add to or modify it as long as the programme is of interest. Additions or modifications are announced in the monthly RSIC Newsletter for the benefit of current users.

After a trial period of 18 months of distributing codes through computer manufacturers, and another trial of about 6 months of distributing directly from RSIC, we have chosen the latter as our future course. We have found that direct contact with the individual shielding scientist in both giving and receiving is essential toward achieving our goal of making the Center a technical institute. Very few of our requests are as simple as "send me code package so-and-so."

The RSIC staff has decided that it cannot ignore the existence of computer shielding codes which, for various reasons, have restricted distribution. Having complete control of distribution, we can consider the efforts of a larger group of shielders. We have found that we can easily handle the distribution, since only about 75 code packages were shipped in the six-month period.

You are perhaps thinking: "What about your cooperative agreements with the other code libraries?" We propose to be even more useful to them than originally planned. We propose to give them abstracts of our reactor shielding code packages; to give them any documentation they want; and to distribute shielding code packages for them upon request. An exception would be made in the event the library wanted a code package for its own use. We feel that direct distribution keeps open the lines of communication with the individual scientist, and we deem this communication very necessary to our overall program.

The technical functions of the RSIC are oriented toward the determination of the state-of-the-art of shielding calculations and design. Consequently, an important goal is to make use of the literature and code collections to publish state-of-the-art reports on various topics of interest in shielding. Other functions include: checkout of codes; preparation of code packages; adding to the documentation of codes; comparison of the results of various calculation methods with each other and with experimental information; technical advice and answers to inquiries; review and selection of shielding literature and the subsequent analysis and indexing in depth; special or restrictive literature searches with the aid of the computer information-retrieval system; production of data⁽²⁰⁾ whenever the need is apparent and a large amount of research is not necessary.

The Center is often asked for advice concerning the selection of a code to do a specific problem. Other special services include effecting the transition from one computer monitor system to another very different monitor system, aiding in an economic feasibility study to determine whether a code should be changed so that it could be operated on a computer which was different from the computer for which it was originally written, and "trouble shooting" input data for codes which require very complicated and exact input.

Since the overall subject of this meeting deals in computation methods, you may be interested in more detail concerning RSIC's program for evaluation and comparison in connection with computer codes. We had to make a choice between two different philosophies: code comparison, in which one would undertake to compare all codes representing a given method; or method comparison, where one would select one or two codes representing each calculation method and compare results. We believed the latter philosophy to be more useful to the RSIC program. In evaluating methods, the RSIC finds it desirable to make use of aid from other installations. This is especially necessary when codes not operable at Oak Ridge and codes under development are to be utilized.

Comparisons have been made of fission-neutron transport in water⁽²¹⁾ and concrete,⁽²²⁾ and fission-gamma-ray transport in iron.⁽²³⁾ Results so far show very good agreement when the individual peculiarities of each code have been understood. It has been our experience that perseverance is required with almost all codes before success is achieved. It is anticipated that an increased amount of continuing effort will go into the comparison work.

The publications of the RSIC include the following: formal reports such as state-of-the-art reports,⁽²⁴⁾ results of evaluation and comparison programs,⁽²¹⁻²³⁾ bibliographies of the shielding literature⁽²⁵⁾ and the shielding codes literature; literature abstracts,⁽²⁶⁾ informal printed matter

such as newsletters,⁽²⁷⁾ brochures, computer code abstracts, and a selective dissemination of information aimed at informing the individual researcher of current literature more rapidly than the issuance of bibliographies affords.

In addition to the three main activities, RSIC attempts to keep abreast of current developments by attending symposia where shielding work is presented, visiting installations where some shielding activity is evident, and making inquiries to individuals who are developing calculation methods or producing experimental data.

I have attempted to define for you the specialized information center and the need it fills in our modern technology. I have outlined the purpose and program of RSIC, its functions, and RSIC's relationship with the great code libraries described here today. I would like to close with a tribute and a request for your cooperation.

For every frontier there must be a pathfinder. In the area of the collection and dissemination of nuclear codes, in the area of promoting the idea of sharing our efforts and so avoid much duplication of effort, no one has done more than Margaret Butler. To have built the Argonne Code Center on the proverbial shoestring, and with no outside financial support, is a real achievement. I earnestly hope that you now have understanding and a new appreciation of the efforts of such people as Margaret and Johnny Rosen.

Where do you come in?

Much credit for the rapid development of nuclear reactors is due to the free exchange of data and codes which has characterized the industry. We believe that the limitations on code exchange which arise from their treatment as proprietary property is to be regretted and to be avoided whenever possible. We deplore the tendency on the part of some programmers to take a code which is generally distributed, make minor changes, change the name and then distribute the results without giving credit to the original author. We feel that each scientist should receive his due credit. We make a plea for more and better documentation of your computer codes. Along with the utilization - instructions on data preparation and on operating the code - the physics, the mathematics, and the numerical methods should be described. We urge the continuing march in the direction of universal coding languages.

In these and all our efforts - we solicit your continued cooperation.

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SOME NEW NONLINEAR ITERATION TECHNIQUES FOR SOLVING NEUTRON-DIFFUSION PROBLEMS

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1. THEORY

Variational principles provide a basis for nonlinear acceleration of linear iterative methods for solving homogeneous (eigenvector) and inhomogeneous (fixed-source) linear-equation systems, both of which occur in neutron-diffusion computations: The outer iteration on the fission-neutron source is used to solve the homogeneous coupled-group-diffusion equations, and an inner iteration procedure is applied to solve successively the inhomogeneous diffusion equation for each group of every outer iteration.

Let $\{y_i\}$ be a sequence of successive approximations (obtained by a linear iterative procedure) to the vector $\underline{y}$ which is the fundamental neutron-flux mode of the discrete coupled-group-diffusion equations

$$A\underline{y} = \lambda B\underline{y}.$$

Let $\{y_i^+\}$ be a sequence of approximations for the adjoint equations

$$A^*\underline{y}^+ = \lambda B^*\underline{y}^+.$$

If we were to choose $\underline{z} = \sum_1^I a_i \underline{y}_i$ and $\underline{z}^+ = \sum_1^I a_i^+ \underline{y}_i^+$ as trial functions for the functional

$$F[\underline{z}^+, \underline{z}] = (\underline{z}^+, [A - \lambda B]\underline{z})$$

and determine $\{a_i\}$ and $\{a_i^+\}$ by applying the stationarity conditions

$$\frac{\partial F}{\partial a_i} = \frac{\partial F}{\partial a_i^+} = 0,$$

we would obtain a vector after I iterations identical with that computed by Lanczos' method (or the method of "conjugate gradients") after I iterations.

In the absence of adjoint approximations, we may choose $\underline{y}_i^+ = \underline{y}_i$ and obtain in many cases reasonably good values for $\{a_i\}$. This is known as Galerkin's method.

*Operated by The General Electric Company for the U. S. Atomic Energy Commission.

Chebyshev extrapolation gives results of comparable accuracy for most neutron-diffusion problems and has the advantage of not requiring the auxiliary computations (based on inner products of successive approximations) needed for Lanczos' method. Both Chebyshev and Lanczos extrapolations are linear acceleration techniques despite the nonlinear computation of the Lanczos coefficients of combination.

Another degree of freedom may be introduced by partitioning the n -space of $\underline{y}$ into M orthogonal subspaces so that $\underline{y}_i$ can be expressed as a direct sum of its projections on these subspaces:

$$\underline{y}_i = {}_1\underline{y}_i \oplus {}_2\underline{y}_i \oplus \dots \oplus {}_M\underline{y}_i.$$

For a particular partitioning, we may choose subsets $\{\underline{y}_j\}$ and $\{\underline{y}_j^+\}$ of the direct and adjoint approximations to $\underline{y}$ and $\underline{y}^+$, for the following trial functions:

$$\underline{Z} = \sum_j [a_{1j}({}_1\underline{y}_j) \oplus a_{2j}({}_2\underline{y}_j) \oplus \dots \oplus a_{Mj}({}_M\underline{y}_j)];$$

$$\underline{Z}^+ = \sum_j [a_{1j}^+({}_1\underline{y}_j^+) \oplus a_{2j}^+({}_2\underline{y}_j^+) \oplus \dots \oplus a_{Mj}^+({}_M\underline{y}_j^+)].$$

The stationarity conditions yield the matrix equations

$$[A' - \lambda B']\underline{a} = 0$$

for the $\{a_{mj}\}$.

Astute partitioning leads to block tri-diagonal matrices A' and B' , and when the number of vectors in $\{\underline{y}_j\}$ is small, $\underline{a}$ can be found readily by Wielandt's method. The linear iterative method can then be continued with $\underline{Z}$ and $\underline{Z}^+$ as trial vectors.

Suppose consistently ordered successive overrelaxation (SOR) is used to obtain successive approximations $\{\underline{x}_i\}$ to the vector $\underline{x}$ which satisfies the discrete group equation: $A\underline{x} = \underline{k}$, where $\underline{k}$ is a known n -vector and A is a real, positive-definite matrix of order n . The functional

$$F[\underline{z}] = (\underline{z}, A\underline{z}) - 2(\underline{z}, \underline{k})$$

is stationary about $\underline{x}$. We may use the trial vector

$$\underline{Z} = \sum_j [a_{1j}({}_1\underline{x}_j) \oplus a_{2j}({}_2\underline{x}_j) \oplus \dots \oplus a_{Mj}({}_M\underline{x}_j)],$$

and apply the stationarity conditions $\partial F / \partial a_{mj} = 0$ to obtain the equation

$$A' \underline{a} = \underline{k}'.$$

Consistent ordering implies the existence of a convenient partitioning which results in a tri-diagonal A' matrix. A more refined partitioning can be chosen to yield a block tri-diagonal A' matrix. In either case, the vector $\underline{a}$ is readily computed.

2. APPLICATION TO NOVA

a. Inner Iteration

In the NOVA Program,⁽²⁾ successive overrelaxation (with all points on each horizontal line of a rectangular grid improved simultaneously) is used as a base linear iteration. For every t iterations (t is input), block renormalization factors (M factors for each horizontal line where $M \leq 10$ is input) are computed by solving a coarse-mesh problem with equations derived from the last SOR iterate.

The fine grid consists of points (ij) , where $i = 1, 2, \dots, I$ and $j = 1, 2, \dots, J$, and the five-point difference equation at point ij is

$$b_{ij}x_{ij} - c_{ij}x_{i+1j} - e_{ij}x_{ij+1} - c_{i-1j}x_{i-1j} - e_{ij-1}x_{ij-1} = s_{ij}.$$

Several columns are coalesced into a single column for the coarse-mesh computation. The coarse mesh has points (mj) , where $m = 1, 2, \dots, M$. Suppose the K fine-mesh columns from $i = a$ to $i = a + K - 1$ are coalesced to form column m and that x_{ij} is the latest SOR iterate. Then the coarse-mesh coefficients for point mj are

$$s_{mj} = \sum_{i=a}^{a+K-1} x_{ij}s_{ij}; \quad e_{mj} = \sum_{i=a}^{a+K-1} e_{ij}x_{ij}x_{ij+1};$$

$$c_{mj} = c_{a+K-1,j}x_{a+K-1,j}x_{a+K,j};$$

$$b_{mj} = \sum_{i=a}^{a+K-1} b_{ij}x_{ij}^2 - 2 \sum_{i=a}^{a+K-2} c_{ij}x_{ij}x_{i+1j},$$

Computation of these coefficients requires about eight multiplications and five additions per point in NOVA. The arithmetic for generating coarse-mesh equations is comparable with that of one SOR iteration. These equations are solved by a block LDU scheme⁽¹⁾ similar to that used for two-line SOR. An approximate relationship between the arithmetic for the entire acceleration computation and arithmetic of a single SOR iteration is the following:

$$\left(\begin{array}{c} \text{Variational} \\ \text{Acceleration} \\ \text{Arithmetic} \end{array} \right) \div \left(1 + \frac{M^3 + 3M^2 + 2M}{5.5I} \right) \left(\begin{array}{c} \text{Arithmetic} \\ \text{for a Single} \\ \text{SOR Iteration} \end{array} \right)$$

A variety of problems has been investigated with the NOVA Program, and a considerable gain in efficiency over SOR has been observed in most cases. The acceleration often decreases computation time by a factor of two or three for a prescribed accuracy, depending upon problem size and other properties of the configuration (see Fig. 1).

Fig. 1

Characteristic Convergence with Variational Acceleration

Several parameters must be chosen in advance for the iteration. Convergence is not as sensitive to the SOR extrapolation parameter as when SOR is applied without variational acceleration so that a cruder estimate of this parameter, ω_b , is adequate. Convergence does not depend strongly on the number of SOR iterations in a cycle, and $t = 10$ was found to be effective for problems studied. The upper bound of ten on the number of columns in the coarse grid was chosen on the basis of memory requirements, and even though fewer columns may increase efficiency for some problems, it has been found that use of the maximum allowable coarse grid is an effective strategy. The number of cycles is determined by other considerations, such as the convergence rate of the outer iteration on the fission-neutron source.

b. Outer Iteration

We note that the coarse-mesh coefficients from the last acceleration computation in each group may be used for the diffusion component of a coarse-mesh outer-iteration matrix. The only other matrix elements required for the outer iteration are the coarse-mesh terms coupling the groups:

$$(A_{gg'})_{mj} = \sum_{(i \text{ in } m)} (A_{gg'})_{ij} X_{ijg} X_{ijg'};$$

$$(F_{gg'})_{mj} = \sum_{(i \text{ in } m)} (F_{gg'})_{ij} X_{ijg} X_{ijg'}.$$

In the above equations, the slowing-down cross section from group g to $g + 1$ is denoted by $A_{g+1,g}$. If χ_g is the fraction of the fission-neutron source introduced in group g and $F_{g'}$ is the fission cross section for group g' , then $F_{gg'} = \chi_g F_{g'}$.

The eigenvalue λ_p for outer iteration p is determined by solving the coarse-mesh problem by Wielandt's method of fractional iteration.

The flux vector obtained from the coarse-mesh solution consists of a set of renormalization factors $\{\beta_{mjg,p}\}$ which are applied to the fine-mesh fluxes to generate the "upper" source (that is, from group $g' \geq g$ to group g) and the flux guess for the next outer iteration. The computation strategy is indicated by the following equations:

$$X_{ijg,p+1}^{(0)} = \beta_{m(i)jg,p} \cdot X_{ijg,p}^{(\text{iterated})};$$

Flux guess for inner iterations which precede outer iteration $p+1$	Result of coarse- mesh outer iteration p	Fine-mesh result of inner iterations just prior to outer iteration p
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$$S_{ijg,p+1}^{(0)} \text{ (upper source)} = \left[\sum_{g' > g} A_{gg'} X_{g,p+1}^{(0)} + \lambda_p \sum_{g' \geq g} F_{gg'} X_{g,p+1}^{(0)} \right]_{ij};$$

$$S_{ijg,p+1}^{(g')} \text{ (accumulated group source)} = S_{ijg,p+1}^{(g'-1)} + \left[(A_{gg'} + \lambda_p F_{gg'}) X_{g',p+1}^{(\text{iterated})} \right]_{ij};$$

($g' = 1, 2, \dots, g-1$ for each g).

In this notation, the group source used for group g during outer iteration $(p+1)$ is

$$S_{ijg,p+1}^{(g-1)}.$$

A NOVA two-space-dimension neutron-diffusion computation proceeds as outlined in Fig. 2.

Fig. 2. Strategy for NOVA Neutron-diffusion Computation

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RITZ DIFFERENCE EQUATIONS ON A TRIANGULATION

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1. Introduction

In obtaining approximate solutions to the two-dimensional multi-group diffusion equations, it is sometimes desirable to use a set of mesh points which does not form a rectangular pattern. For a general distribution of mesh points, Ritz variational methods are a convenient means of deriving difference equations. It is important to be able to judge the accuracy of the difference equations, and it seems that the truncation error is not a useful concept in this regard. As a contribution to this problem we consider the one-group neutron-diffusion equation

$$-(pu_x)_x - (pu_y)_y + qu = f \quad (1)$$

in a region R with boundary condition

$$u(x,y) = 0, \quad (x,y) \in \Gamma, \quad (2)$$

on the boundary Γ of R , and we prove two theorems (Theorem 3 and Theorem 4) giving estimates for the error in the approximate solution of (1) and (2) obtained by a variational method.

It will be assumed that the mesh points come from a triangulation of the region R . (The notion of a triangulation is defined in Section 4). If the interfaces between regions of different material composition lie on the sides of mesh triangles, Theorem 4, which says that a certain norm of the error is bounded by ch , where h is the maximum mesh spacing, applies. If the material interfaces do not lie on the sides of mesh triangles, Theorem 3, which says that the norm of the error tends to 0 as the mesh spacing tends to 0, applies. Theorem 4 involves a certain hypothesis concerning the second derivatives of the solution $u(x,y)$ of (1) and (2). It is conjectured that u always satisfies this hypothesis when $f(x,y)$ is square integrable on R , and when Γ and the material interfaces are polygons. The same hypothesis for u is required in Ref. 7, in which a similar analysis is made of the error coming from the MacNeal difference equations on a triangulation.

These results are obtained by first considering variational approximations from the point of view of functional analysis, and proving a convergence theorem (Theorem 2) in this case. This abstract theorem is then specialized to the boundary value problem (1) and (2).

The use of these variational difference equations in the computer program PDQ-6 is described in Ref. 1 and 2. A similar application of mesh triangulations is described in Ref. 3.

2. The Abstract Formulation

The mathematical analysis of the boundary value problem described by (1) and (2) and of the variational approximations to this problem is greatly simplified if a few elementary properties of Hilbert spaces are used. We follow the notation of Ref. 4 in writing down the facts necessary for our analysis.

Consider the bilinear expression

$$a(u,v) = \iint_R (p \nabla u \cdot \nabla v + quv) dx dy. \quad (3)$$

If both sides of (1) are multiplied by a continuously differentiable function $v(x,y)$ which vanishes on Γ , and if the left side is integrated over R , using Green's theorem and the continuity of u and $p \nabla u \cdot \underline{n}$ across curves of discontinuity of $p(x,y)$, one obtains

$$a(u,v) = \iint_R f v dx dy. \quad (4)$$

The collection of Eq. (4) for all continuously differentiable v which vanish on Γ may be regarded as an equivalent statement of the boundary value problem given by (1) and (2). This statement is simpler in that (4) involves only first derivatives of u and in that (4) contains implicitly the requirements of continuous flux and current.

Let H be the real Hilbert space of real functions $f(x)$ such that $\iint_R f(x)^2 dx dy < \infty$. The inner product and norm of functions in H are written as

$$(f,g) = \iint_R f(x)g(x) dx dy$$

and

$$|f| = (f,f)^{1/2},$$

respectively. Included in the space H is the set $D(R)$ of functions which are infinitely differentiable on R and each of which vanishes in a neighborhood of Γ . The set $D(R)$ is a dense subset of H . On $D(R)$ we may define an inner product and norm by

$$((v, w)) = \iint_R (vw + v_x w_x + v_y w_y) dx dy$$

and

$$||v|| = ((v, v))^{1/2},$$

respectively.

Now $D(R)$ is not a Hilbert space because it is not complete with this norm. It may be completed to a Hilbert space V by adjoining Cauchy sequences to $D(R)$. Since $|v| \leq ||v||$, one has $V \subset H$, and V is a dense subset of H in the norm of H .

It will be assumed that $p(x, y)$ and $q(x, y)$ are bounded and strictly positive. Then one may deduce the inequalities

$$\left. \begin{aligned} |a(v, w)| &\leq c_1 ||v|| \cdot ||w||, \quad v \in V; \\ a(v, v) &\leq c_2 ||v||^2, \quad v \in V. \end{aligned} \right\} \quad (5)$$

These inequalities may be proved for $v \in D(R)$, and then for any $v \in V$ by a passage to the limit.

The following theorem is proved in Ref. 4

Theorem 1. Let H and V be Hilbert spaces satisfying the conditions

- (i) $V \subset H$, V is dense in H in the topology of H ;
- (ii) there is a $c > 0$ such that $||v|| \leq c|v|$, $v \in V$.

Let a be a bilinear functional on V satisfying (4). Then for each $f \in H$, there is one and only one $u \in V$ such that

$$a(u, v) = (f, v), \quad v \in V. \quad (6)$$

Moreover, there is a $c^1 > 0$ such that $||u|| \leq c^1 |f|$.

In terms of the original boundary value problem, Theorem 1 asserts the existence of a unique solution of (4), even if $p(x, y)$ and $q(x, y)$ are discontinuous.

3. The Method of Weighted Residuals

To describe the method of weighted residuals (Bubnov-Galerkin method) for finding approximate solutions to the abstract problem (6), we

suppose there is given a sequence of finite-dimensional subspaces V_n of the Hilbert space V satisfying the following conditions:

$$\left. \begin{array}{l} V_1 \subset V_2 \subset \dots; \\ \bigcup_{n=1}^{\infty} V_n \text{ is dense in } V. \end{array} \right\} \quad (7)$$

The second condition of (7) means that for any $v \in V$, and for any $\epsilon > 0$, there is an index n and a $w \in V_n$ such that $\|v - w\| < \epsilon$.

Given $f \in H$, the n -th approximate solution of the problem (6) is defined to be the solution $u_n \in V_n$, if any exists, of the equations

$$a(u_n, v) = (f, v), \quad v \in V_n. \quad (8)$$

Note that (8) is a system of N linear equations in N unknowns, where N is the dimension of V_n . To see this one may pick a basis of N linearly independent elements of V_n , say $v_1, \dots, v_N$. If u_n is represented as $u_n = \sum a_i v_i$, and if in (7) $v = v_j$, $1 \leq j \leq N$, then one obtains N equations in the N unknown coefficients $a_1, \dots, a_N$.

The variational method (8) is known as Galerkin's method for finding an approximate solution of (6). If $a(u, v)$ is given by (3), then (8) is the Ritz method for finding an approximate solution of the boundary value problem (1) and (2).

Lemma 1. If the hypotheses of Theorem 1 are satisfied, and if V_n is a finite dimensional subspace of V , then the system of Eqs. (8) has a unique solution $u_n \in V_n$.

Proof. For $v, w \in V_n$, the bilinear form $a(v, w)$ may be written $a(v, w) = (Av, w)$, where A is an N by N matrix. Since $(Av, v) = a(v, v) > 0$ when $v \neq 0$, A is a nonsingular matrix. Since (7) implies $Au_n = f$, the system (8) has a unique solution.

Theorem 2. With the hypotheses of Theorem 1, let $\{V_n\}$ be a sequence of finite-dimensional subspaces of V which satisfies (7), let u be the solution of (6), and let $u_n \in V_n$ be the n -th approximate solution of (6). For any $\epsilon > 0$, there is an n_0 such that if $n \geq n_0$, then $\|u_n - u\| \leq \epsilon$.

Proof. From (7) there is an n_0 and a $\tilde{u} \in V_{n_0}$ such that

$$\|\tilde{u} - u\| \leq \frac{\epsilon}{2} \min(1, c_2/c_1). \quad (9)$$

Then $\tilde{u} \in V_n$ for $n \geq n_0$. If $v \in V_n$, then $a(u_n, v) = a(u, v) = (f, v)$. Hence

$$a(\tilde{u} - u_n, v) = a(\tilde{u} - u, v) \leq \frac{1}{2} c_2 \epsilon \|v\|, \quad v \in V_n.$$

Setting $v = \tilde{u} - u_n$ and using (5), we obtain $\|\tilde{u} - u_n\| \leq \epsilon/2$. Using (9) and the triangle inequality, we have

$$\|u_n - u\| \leq \|u_n - \tilde{u}\| + \|\tilde{u} - u\| \leq \epsilon,$$

and the theorem is proved.

In Ref. 5 it is proved under additional assumptions that $\|u - u_n\| \leq \epsilon|f|$ for $n \geq n_0$, where n_0 does not depend upon f . The additional assumptions are that $a(u, v) = a(v, u)$ is a symmetric bilinear form, and that the mapping $f \rightarrow u$ defined by Theorem 1 is completely continuous when considered as a mapping from H into H . These conditions are satisfied when $a(u, v)$ is given by (3).

When the bilinear form $a(u, v)$ is symmetric and comes from a positive definite quadratic form as in (3), the method of weighted residuals reduces to the Ritz variational method. Therefore, the difference approximation to (1) and (2) which is derived in the next section will be called the Ritz difference approximation to (1) and (2). (See also Ref. 8.)

4. The Triangulation

To apply the general Theorem 2 to the boundary value problem (1) and (2), we must define the subspaces V_n of V . This will be done in terms of triangulations of the region R .

Assume that the boundary Γ of R is a polygon. By a triangulation $\underline{T}$ of R is meant a finite collection of triangles contained in $\bar{R}$, the closure of R , such that $\bar{R}$ is the union of all the triangles in $\underline{T}$, and such that any two triangles of $\underline{T}$ have either no points in common, a vertex in common, or a side in common. We use $\underline{S}$ to denote the set of vertices of triangles of $\underline{T}$, and $\underline{S}_0$ to denote the set of vertices not lying on Γ . Two points P and Q in $\underline{S}$ will be called neighbors of one another if there is a triangle $T \in \underline{T}$ such that both P and Q are vertices of T . The points of $\underline{S}$ will be the mesh points of our difference approximation. The maximum mesh spacing, $h(\underline{T})$, is defined to be the maximum distance between neighboring mesh points.

For $P \in \underline{S}_0$, let $\alpha_P(x, y)$ be the unique function defined by the conditions

$$\alpha_P(x, y) = 1, \quad (x, y) = P;$$

$$\alpha_P(x, y) = 0, \quad (x, y) = Q \neq P, \quad Q \in \underline{S};$$

$$\alpha_P(x, y) \text{ is linear in each triangle } T \in \underline{T}.$$

Let $V(\underline{T})$ be the collection of all finite linear combinations of the functions $\alpha_P(x,y)$, $P \in \underline{S}_0$. $V(\underline{T})$ is a finite-dimensional subspace of the Hilbert space V ; the dimension of $V(\underline{T})$ is the number of points in $\underline{S}_0$.

A triangulation $\underline{T}_1$ is called a refinement of $\underline{T}$ if the vertices of triangles of $\underline{T}$ are also vertices of triangles of $\underline{T}_1$. In this case, $V(\underline{T}_1) \supset V(\underline{T})$. By taking a sequence of triangulations $\underline{T}_n$, each of which is a refinement of the preceding, we obtain an increasing sequence of finite-dimensional subspaces $V_n = V(\underline{T}_n)$ of V . To use these subspaces in Theorem 2 we must show that their union is dense in V ; that is, given $v \in V$ and given $\epsilon > 0$, we must show that there is an $n(\epsilon, v)$ and a $v_n \in V_n$ such that $\|v - v_n\| < \epsilon$. At the same time, a more precise idea of the function $n(\epsilon, v)$ will be given, for use in a more refined version of Theorem 2.

Let $\underline{T}$ be a triangulation of R and let $v \in D(R)$ be an infinitely differentiable function on R which vanishes on Γ . Let $\tilde{v}$ be the unique function in $V(\underline{T})$ which agrees with v on the set $\underline{S}$ of mesh points, that is,

$$\tilde{v}(x,y) = \sum v(P) \alpha_P(x,y), \quad P \in \underline{S}_0.$$

Let $a(\underline{T})$ be the minimum value of $|\sin \phi|$, where ϕ is any one of the angles of any of the triangles in $\underline{T}$.

Lemma 2. There is a constant $c_3 > 0$ depending only on $a(\underline{T})$ such that, if $T \in \underline{T}$,

$$\iint_T [(v - \tilde{v})^2 + (v_x - \tilde{v}_x)^2 + (v_y - \tilde{v}_y)^2] dx dy \leq c_3 h(\underline{T})^2 \iint_T (v_{xx}^2 + v_{xy}^2 + v_{yy}^2) dx dy. \quad (10)$$

Proof. Let the vertices of the triangle T be P_1 , P_2 , and P_3 , and let a system of coordinates be given so that $P_1 = (0,0)$, $P_2 = (e,0)$, $P_3 = (f,g)$, with $e > 0$ and $g > 0$. In T , we have

$$\tilde{v}(x,y) = v(P_1) + \frac{v(P_2) - v(P_1)}{e} x + \frac{e[v(P_3) - v(P_1)] - f[v(P_2) - v(P_1)]}{eg} y.$$

From a Taylor's series expansion,

$$v(P_1) = v(x,y) - xv_x(x,y) - yv_y(x,y) + F(x,y);$$

$$v(P_2) = v(x,y) + (e-x)v_x(x,y) - yv_y(x,y) + G(x,y);$$

$$v(P_3) = v(x,y) + (f-x)v_x(x,y) + (g-y)v_y(x,y) + H(x,y);$$

where

$$F(x,y) = \int_0^1 t [x^2 v_{xx}(xt,yt) + 2xy v_{xy}(xt,yt) + y^2 v_{yy}(xt,yt)] dt,$$

and $G(x,y)$ and $H(x,y)$ are given by similar expressions. Thus, we find that

$$\begin{aligned}\tilde{v}_x - v_x &= \frac{1}{e} (G - F); \\ \tilde{v}_y - v_y &= \frac{1}{g} H - \frac{e-f}{eg} F - \frac{f}{eg} G; \\ \tilde{v} - v &= \frac{eg - gx + (f-e)y}{eg} F + \frac{gx - fy}{eg} G + \frac{y}{g} H.\end{aligned}$$

It will be shown that

$$\left. \begin{aligned}\iint_T F^2 dx dy &\leq 6 h(\underline{T})^4 \iint_T (v_{xx}^2 + v_{xy}^2 + v_{yy}^2) dx dy; \\ \iint_T G^2 dx dy &\leq 6 h(\underline{T})^4 \iint_T (v_{xx}^2 + v_{xy}^2 + v_{yy}^2) dx dy; \\ \iint_T H^2 dx dy &\leq 6 h(\underline{T})^4 \iint_T (v_{xx}^2 + v_{xy}^2 + v_{yy}^2) dx dy.\end{aligned}\right\} \quad (11)$$

From this (10) follows easily.

To prove the first inequality of (11), note that several applications of Schwarz's inequality gives

$$\begin{aligned}|F(x,y)| &\leq (x^4 + 4x^2y^2 + y^4)^{1/2} \int_0^1 t(v_{xx}^2 + v_{xy}^2 + v_{yy}^2)^{1/2} dt \\ &\leq 6^{1/2} h(\underline{T})^2 \left\{ \int_0^1 t^2 [v_{xx}(tx,ty)^2 + v_{xy}(tx,ty)^2 + v_{yy}(tx,ty)^2] dt \right\}^{1/2}.\end{aligned}$$

The inequality will follow if we show that, for any non-negative integrable function $w(x,y)$ defined on T ,

$$\iint_T \left\{ \int_0^1 t^2 w(tx,ty) dt \right\} dx dy \leq \iint_T w(x,y) dx dy. \quad (12)$$

To prove (12), if one defines w to be 0 outside T , and if the integral over T is extended to an integral over the entire (x,y) plane, the left side of (12) is increased. Changing to polar coordinates (r,θ) , one finds that the left side of (12) is bounded by

$$I = \int_{\theta=0}^{2\pi} \int_{r=0}^{\infty} \int_{t=0}^1 r t^2 w(rt, \theta) dt dr d\theta.$$

If we introduce the variable $p = rt$, we have

$$\begin{aligned}
 I &= \int_{\theta=0}^{2\pi} \int_{r=0}^{\infty} \int_{p=0}^r \frac{p^2}{r^2} w(p, \theta) \, dp \, dr \, d\theta \\
 &= \int_{\theta=0}^{2\pi} \int_{p=0}^{\infty} \int_{r=p}^{\infty} \frac{p^2}{r^2} w(p, \theta) \, dr \, dp \, d\theta \\
 &= \int_{\theta=0}^{2\pi} \int_{p=0}^{\infty} p w(p, \theta) \, dp \, d\theta \\
 &= \iint_T w \, dx \, dy.
 \end{aligned}$$

This proves (12) and, hence, the first inequality of (11). The other two inequalities of (11) are proved in the same way, and the proof of Lemma 2 is finished.

Let $\{\underline{T}_n\}$ be a sequence of triangulations satisfying the conditions

$\underline{T}_{n+1}$ is a refinement of $\underline{T}_n$;

$h(\underline{T}_n) \rightarrow 0$; (13)

$a(\underline{T}_n)$ is bounded away from 0.

Let $V_n = V(\underline{T}_n)$ and $h_n = h(\underline{T}_n)$.

Lemma 3. $\bigcup_1^{\infty} V_n$ is dense in V .

Proof. Let $v \in D(R)$, and let $\tilde{v}_n \in V_n$ be the function in V_n agreeing with v on the mesh points of $\underline{T}_n$. If (1) is summed over all mesh triangle $T \in \underline{T}_n$ and the square root of the result taken, we find that

$$||v - \tilde{v}_n|| \leq h_n \left\{ c_3 \iint_R (v_{xx}^2 + v_{xy}^2 + v_{yy}^2) \, dx \, dy \right\}^{1/2}. \quad (14)$$

Now let $w \in V$ and let $\epsilon > 0$. Since $D(R)$ is dense in V , let $v \in D(R)$ be such that $||v - w|| \leq \epsilon/2$. Using (14), let n be so large that $||\tilde{v}_n - v|| \leq \epsilon/2$. Then $||v_n - w|| \leq \epsilon$, so the lemma is proved.

5. The Discretization Error

We are now ready to estimate the discretization error for the Ritz approximate solution of (1) and (2). The first theorem says that, under general conditions, the norm of the discretization error tends to zero.

Theorem 3: Let $p(x,y)$ and $q(x,y)$ be bounded and bounded away from zero, let $f \in H$, and let $u \in V$ be the solution of (3) and (4). Let $\{\underline{T}_n\}$ be a sequence of triangulations satisfying (13), and let $u_n \in V_n$ be the corresponding sequence of approximate solutions. Then

$$\lim_{n \rightarrow \infty} \|u - u_n\| = 0.$$

Proof. This follows from Theorem 2 and Lemma 3.

The next theorem requires the existence, in some sense, of second derivatives of the solution $u(x,y)$ of (3) and (4). If $p(x,y)$ is sufficiently differentiable and if the boundary Γ is sufficiently smooth, it is known (see Ref. 6) that this is the case. Since it is important to allow $p(x,y)$ to be discontinuous, we make a hypothesis concerning the solution in this case. We further conjecture that this hypothesis is satisfied for all solutions of (3) and (4), but we do not know how to prove this.

Let the region R be decomposed into a number of subregions $R_1, \dots, R_J$, and let the boundary of $\bar{R}_j$ be Γ_j . Suppose that Γ_j is a polygon. Suppose that $p(x,y)$ is continuously differentiable in $\bar{R}_j$, $j = 1, \dots, J$, but that p is discontinuous across the boundaries Γ_j . Our hypothesis concerning the solution $u(x,y)$ is that, in each subregion R_j , there is a sequence $v_{j,i} \in D(R)$, $i = 1, 2, \dots$, such that

$$\lim_{i \rightarrow \infty} \iint_{R_j} [(u - v_{j,i})^2 + (u_x - v_{j,i,x})^2 + (u_y - v_{j,i,y})^2] dx dy = 0;$$

$$\lim_{i,k \rightarrow \infty} \iint [(v_{j,i,xx} - v_{j,k,xx})^2 + (v_{j,i,xy} - v_{j,k,xy})^2 + (v_{j,i,yy} - v_{j,k,yy})^2] dx dy = 0.$$

If this is true, then the sequences $v_{j,i,xx}$, $v_{j,i,xy}$, and $v_{j,i,yy}$ converge in the mean to square integrable functions on R_j which may be identified with the corresponding second derivatives u_{xx} , u_{xy} , and u_{yy} of the solution. Furthermore, $u(x,y)$ is uniformly continuous in R_j , and $v_{j,i}(x,y)$ converges uniformly to $u(x,y)$. Using the fact that $u \in V$, it may be shown that if the boundaries of subregions R_j and R_k have a nonempty intersection, the values of u on this intersection agree whether considered as a continuous function on $\bar{R}_j$ or $\bar{R}_k$. Thus, u is a continuous function on all of R . This hypothesis will be described by saying that $u(x,y)$ has generalized second derivatives on each subregion R_j .

A triangulation $\underline{T}$ will be called consistent with the family of subregions R_j if each triangle T in $\underline{T}$ is contained entirely in one of the $\bar{R}_j$. If $\underline{T}$ is consistent with the family of subregions R_j , and if $u(x,y)$ has generalized second derivatives on each R_j , then on each R_j the interpolating

functions $\tilde{v}_{j,i}$ converge to a piecewise linear function $\tilde{u}$ on R_j , which agrees with u on the mesh points in $\bar{R}_j$. Since the values of $\tilde{u}$ agree on common boundaries of different subregions, we obtain in this manner a function $\tilde{u} \in V(\underline{T})$ which agrees with u on the set $\underline{S}$ of mesh points of the triangulation.

Lemma 4. There is a constant $c_3 > 0$ depending only on $a(\underline{T})$ such that

$$\|u - \tilde{u}\|^2 \leq c_3 h(\underline{T})^2 \iint_R (u_{xx}^2 + u_{xy}^2 + u_{yy}^2) dx dy. \quad (15)$$

Proof. If Lemma 2 is applied to each of the functions $v_{j,i}$, the limit is taken as $i \rightarrow \infty$, and the result is summed over j , the inequality (15) is obtained.

Theorem 4. Let $p(x,y)$ and $q(x,y)$ be bounded away from 0, let $f \in H$, and let the solution $u \in V$ of (3) and (4) have generalized second derivatives on each subregion R_j . Let $\{\underline{T}_n\}$ be a sequence of triangulations which satisfies (13), and each of which is consistent with the family of subregions R_j . Let $u_n \in V_n$ be the corresponding sequence of approximate solutions. Then there is a constant $c_4 > 0$ depending only on c_1, c_2 , and c_3 such that

$$\|u - u_n\| \leq c_4 h_n \left\{ \iint_R (u_{xx}^2 + u_{xy}^2 + u_{yy}^2) dx dy \right\}^{1/2}.$$

Proof. Let $\tilde{u}_n \in V_n$ be the function which agrees with u on the mesh points of $\underline{T}_n$. Then one has, following the proof of Theorem 2,

$$c_1 \|\tilde{u} - u_n\|^2 \leq a(\tilde{u} - u, \tilde{u} - u_n) \leq c_2 \|\tilde{u} - u\| \cdot \|\tilde{u} - u_n\|; \quad \|\tilde{u} - u_n\| \leq \frac{c_2}{c_1} \|\tilde{u} - u\|,$$

so from the triangle inequality and (15),

$$\begin{aligned} \|u - u_n\| &\leq \left(1 + \frac{c_2}{c_1}\right) \|\tilde{u}_n - u\| \\ &\leq c_4 \left(1 + \frac{c_2}{c_1}\right) h_n \left\{ \iint_R (u_{xx}^2 + u_{xy}^2 + u_{yy}^2) dx dy \right\}^{1/2}, \end{aligned}$$

and the theorem is proved.

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VARIATIONAL METHODS FOR THE SOLUTION OF PROBLEMS OF REACTOR KINETICS

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1. Introduction

The solution of the time-dependent multigroup, multiregion diffusion equations may be obtained by searching for the functions which render stationary a particular functional.

These functions are determined numerically by Kantorovich's method and by Euler's method.

With the Kantorovich method the flux and the adjoint flux are expanded in a set of space-dependent trial functions with time-dependent coefficients. These coefficients are determined by solving with a "one-step method" a system of ordinary differential equations.

The Euler method consists in searching for the functions which render stationary the above functional in the class of piecewise linear functions. These functions satisfy a large system of ordinary differential equations and are determined numerically by three different methods: the "implicit method," the "implicitly explicit method," and the "alternating method of Saul'yev."

A comparison between the Kantorovich method and the Euler method is made by means of some numerical examples.

2. Statement of the Problem

Let the domain of the nuclear reactor R be a finite connected region with exterior boundary Γ . We suppose that

$$\bar{R} = \bigcup_{k=1}^r \bar{R}_k$$

(the bar denotes the topological closure in the Euclidean metric), where the R_k are regular, open, simply-connected, disjoint regions. With

$$\gamma = \left\{ \bigcup_{k=1}^r (\bar{R}_k - R_k) - \Gamma \right\}$$

we indicate the internal boundaries between the regions R_k .

The time-dependent diffusion equations (or kinetic equations) in the two-group approximation have the form

$$\begin{cases} \frac{1}{V_1} \frac{\partial \phi_1}{\partial t} = \text{div}(D_1 \text{grad } \phi_1) - A_{11}\phi_1 + A_{12}\phi_2 + (s+g); \\ \frac{1}{V_2} \frac{\partial \phi_2}{\partial t} = \text{div}(D_2 \text{grad } \phi_2) + A_{21}\phi_1 - A_{22}\phi_2, \end{cases} \quad (1)$$

with

$$s \equiv s(\underline{x}t) = \mu \exp(-\lambda t) \int_0^t H(\underline{x}\tau) \phi_2(\underline{x}\tau) \exp(\lambda\tau) d\tau. \quad (2)$$

The initial-boundary conditions are ($i = 1, 2$)

$$\begin{cases} \phi_i(\underline{x}0) = f_i(\underline{x}) & \text{for } \underline{x} \in R; \\ \phi_i(\underline{x}t) = 0 & \text{for } \underline{x} \in \Gamma_1 \text{ and } 0 \leq t \leq t^*, \end{cases} \quad (3)$$

and

$$\frac{\partial \phi_i(\underline{x}t)}{\partial n} = 0 \quad \text{for } \underline{x} \in \Gamma_2 (\Gamma_2 = \Gamma - \Gamma_1) \text{ and } 0 \leq t \leq t^* \quad (4)$$

(the normal n refers to the outward pointing normal).

We suppose that the length of Γ_1 is different from zero.

The coefficients $V_i \equiv V_i(\underline{x}t)$, $D_i \equiv D_i(\underline{x}t)$, $A_{ij} \equiv A_{ij}(\underline{x}t)$, with $(i, j = 1, 2)$, $H \equiv H(\underline{x}t)$, and $g \equiv g(\underline{x}t)$ are continuous with their first-order derivatives in each region $\bar{R}_k (1 \leq k \leq r)$.

For $\underline{x} \in R$ and all t , $0 \leq t \leq t^*$, the functions $V_i(\underline{x}t)$ and $D_i(\underline{x}t)$ are positive, and the functions $A_{ij}(\underline{x}t)$, $H(\underline{x}t)$, and $g(\underline{x}t)$ are non-negative ($i, j = 1, 2$).

The functions $\phi_i \equiv \phi_i(\underline{x}t)$ belong to the class C , that is, for $i = 1, 2$:

- a) $\phi_i(\underline{x}t)$ is a function of t continuously differentiable in the interval $0 \leq t \leq t^*$;
- b) $\phi_i(\underline{x}t)$ and $\partial \phi_i(\underline{x}t) / \partial t$ are continuous with their first- and second-order derivatives inside the regions $\bar{R}_k (1 \leq k \leq r)$ for all values of t , $0 \leq t \leq t^*$;

- c) $\phi_i(\underline{x}t)$, $\partial\phi_i(\underline{x}t)/\partial t$, and the normal component of $[D_i(\underline{x}t) \cdot \text{grad } \phi_i(\underline{x}t)]$ are continuous across the interfaces γ between the regions R_k for all values of t , $0 \leq t \leq t^*$.

The constants λ and μ are non-negative. We wish to determine numerically the solution of class C of the system (1) with the initial boundary conditions (3)-(4).

3. A Variational Principle for the Neutron Kinetic Equations

The adjoint problem of the problem (1)-(4) is expressed by the equations

$$\begin{cases} -\frac{\partial}{\partial t}\left(\frac{1}{V_1}\phi_1^*\right) = \text{div}\left(D_1 \text{grad } \phi_1^*\right) - A_{11}\phi_1^* + A_{21}\phi_2^*; \\ -\frac{\partial}{\partial t}\left(\frac{1}{V_2}\phi_2^*\right) = \text{div}\left(D_2 \text{grad } \phi_2^*\right) + A_{12}\phi_1^* - A_{22}\phi_2^* + s^*, \end{cases} \quad (5)$$

with

$$s^* \equiv s^*(\underline{x}t) = \mu H(\underline{x}t) \exp(\lambda t) \int_t^{t^*} \phi_1^*(\underline{x}\tau) \exp(-\lambda\tau) d\tau. \quad (6)$$

The initial-boundary conditions are ($i = 1, 2$):

$$\begin{cases} \phi_i^*(\underline{x}t) = 0 & \text{for } \underline{x} \in R; \\ \phi_i^*(\underline{x}t) = 0 & \text{for } \underline{x} \in \Gamma_1 \text{ and } 0 \leq t \leq t^*, \end{cases} \quad (7)$$

and

$$\frac{\partial\phi_i^*(\underline{x}t)}{\partial n} = 0 \quad \text{for } \underline{x} \in \Gamma_2 \text{ and } 0 \leq t \leq t^*. \quad (8)$$

The functions $\phi_i^*(\underline{x}t)$, ($i = 1, 2$) belong to the class C.

Let the following functional⁽¹⁾ be given:

$$\begin{aligned} \mathcal{J}[\phi_1 \phi_2 \phi_1^* \phi_2^*] = & \int_0^{t^*} dt \left\{ \sum_{k=1}^r \int_{R_k} d\sigma \left(\phi_1^* \left[\frac{1}{V_1} \frac{\partial\phi_1}{\partial t} \right] + \text{grad } \phi_1^* [D_1 \text{grad } \phi_1] \right. \right. \\ & + \phi_1^* [A_{11}\phi_1 - A_{12}\phi_2 - (s+g)] + \phi_2^* \left[\frac{1}{V_2} \frac{\partial\phi_2}{\partial t} \right] \\ & \left. \left. + \text{grad } \phi_2^* [D_2 \text{grad } \phi_2] + \phi_2^* [-A_{21}\phi_1 + A_{22}\phi_2] \right) \right\}, \end{aligned} \quad (9)$$

whose admissible functions ϕ_i and ϕ_i^* ($i = 1, 2$) belong to the class K.

A function $\psi(\underline{x}t)$ belongs to the class K if:

- a) $\psi(\underline{x}t)$ is a function of t continuously differentiable in the interval $0 \leq t \leq t^*$;
- b) $\psi(\underline{x}t)$ and $\partial\psi(\underline{x}t)/\partial t$ are continuous inside the domain $\bar{R}$ and possess first- and second-order derivatives continuous in the regions $\bar{R}_k$ ($1 \leq k \leq r$) for all values of t , $0 \leq t \leq t^*$.

Using the theory of the calculus of variations, we can prove the following theorem 1:

If the admissible functions ϕ_i and ϕ_i^* ($i = 1, 2$) of class K constrained to satisfy, respectively, the conditions (3) and (7) render stationary the functional (9), then the functions ϕ_i ($i = 1, 2$) satisfy the equations (1)-(4), and the functions ϕ_i^* ($i = 1, 2$) satisfy the equations (5)-(8). In addition, ϕ_i and ϕ_i^* ($i = 1, 2$) belong to the class C.

For this theorem, the solution of the system (1)-(4) can be determined by searching for the functions ϕ_i and ϕ_i^* ($i = 1, 2$) of class K which render stationary the functional (9). We will determine these functions by the Kantorovich method and by the Euler method⁽²⁾.

From this time forward we will consider the "source term" (2) in this way.

We subdivide the interval $[0, t^*]$ into ℓ equal parts in steps $\Delta t = t^*/\ell$, and we suppose that in the interval $(t - \Delta t, t)$ the function $H(\underline{x}t) \phi_2(\underline{x}t)$ varies weakly, so that it may be represented by $H(\underline{x}t - \Delta t) \phi_2(\underline{x}t - \Delta t)$. Then we can write

$$\begin{cases} s(\underline{x}t) = \alpha s(\underline{x}t - \Delta t) + \beta H(\underline{x}t - \Delta t) \phi_2(\underline{x}t - \Delta t); \\ s(\underline{x}0) = 0, \end{cases} \quad (10)$$

where

$$\alpha = \exp(-\lambda \Delta t); \quad \beta = \mu(1 - \alpha)/\lambda.$$

4. The Kantorovich Method

In the Kantorovich method the flux $\phi_i(\underline{x}t)$ and the adjoint flux $\phi_i^*(\underline{x}t)$ are expanded in a set of linearly independent trial functions with time-dependent coefficients:

$$\begin{cases} \phi_i(\underline{x}t) = \sum_{n=1}^N c_n^i(t) W_n(\underline{x}); \\ \phi_i^*(\underline{x}t) = \sum_{n=1}^N c_n^{*i}(t) W_n(\underline{x}). \end{cases} \quad (i = 1, 2) \quad (11)$$

The functions $W_n(\underline{x})$ are continuous in $\bar{R}$, possess first- and second-order derivatives continuous in $\bar{R}_k (1 \leq k \leq r)$, and are vanishing on Γ_1 .

We suppose that the functions $g(\underline{x}t)$ and $f_i(\underline{x})$ ($i = 1, 2$) have the form

$$g(\underline{x}t) = \sum_{n=1}^N h_n(t) W_n(\underline{x}); \quad f_i(\underline{x}) = \sum_{n=1}^N \gamma_n^i W_n(\underline{x}).$$

We define the following matrices ($i, j = 1, 2$):

$$Z_i(t) \equiv \left(z_{mn}^i(t) \right)_{m,n=1}^N; \quad R_{ij}(t) \equiv \left(r_{mn}^{ij}(t) \right)_{m,n=1}^N,$$

and the following vectors:

$$\begin{aligned} C_i(t) &\equiv \{c_1^i(t) c_2^i(t) \dots c_N^i(t)\}; \\ C_i^*(t) &\equiv \{c_1^{*i}(t) c_2^{*i}(t) \dots c_N^{*i}(t)\}; \\ Q_1(t) &\equiv \{q_1(t) q_2(t) \dots q_N(t)\}, \end{aligned} \quad (i = 1, 2)$$

where (δ_{ij}) is the symbol of Kronecker;

$$\begin{aligned} z_{mn}^i(t) &= \sum_{k=1}^r \int_{R_k} d\sigma \left[\frac{1}{V_i(\underline{x}t)} W_m(\underline{x}) W_n(\underline{x}) \right]; \\ r_{mn}^{ij}(t) &= \sum_{k=1}^r \int_{R_k} d\sigma \left(\delta_{ij} [D_i(\underline{x}t) \operatorname{grad} W_m(\underline{x}) \operatorname{grad} W_n(\underline{x})] \right. \\ &\quad \left. + A_{ij}(\underline{x}t) W_m(\underline{x}) W_n(\underline{x}) \right); \\ q_m(t) &= \sum_{k=1}^r \int_{R_k} d\sigma W_m(\underline{x}) \left[\sum_{n=1}^N W_n(\underline{x}) (K_n(\underline{x}t) + h_n(t)) \right]; \end{aligned}$$

$$K_n(\underline{x}t) = \alpha K_n(\underline{x}t - \Delta t) + \beta H(\underline{x}t - \Delta t) c_n^2(t - \Delta t);$$

$$K_n(\underline{x}0) = 0.$$

If we substitute the expressions (11) into (9), the functional becomes

$$\begin{aligned} \mathcal{J}[C_1(t) C_2(t) C_1^*(t) C_2^*(t)] = \int_0^{t^*} dt & \left(C_1^*(t) \left[Z_1(t) \frac{dC_1(t)}{dt} + R_{11}(t) C_1(t) \right. \right. \\ & \left. \left. - R_{12}(t) C_2(t) - Q_1(t) \right] + C_2^*(t) \left[Z_2(t) \frac{dC_2(t)}{dt} \right. \right. \\ & \left. \left. - R_{21}(t) C_1(t) + R_{22}(t) C_2(t) \right] \right). \end{aligned} \quad (12)$$

The Euler-Lagrange equations of (12) are

$$\begin{vmatrix} Z_1(t) & 0 \\ 0 & Z_2(t) \end{vmatrix} \begin{vmatrix} \frac{dC_1(t)}{dt} \\ \frac{dC_2(t)}{dt} \end{vmatrix} + \begin{vmatrix} R_{11}(t) & -R_{12}(t) \\ -R_{21}(t) & R_{22}(t) \end{vmatrix} \begin{vmatrix} C_1(t) \\ C_2(t) \end{vmatrix} = \begin{vmatrix} Q_1(t) \\ 0 \end{vmatrix}, \quad (13)$$

with

$$c_n^i(0) = \gamma_n^i \quad (i = 1, 2; 1 \leq n \leq N).$$

Taking into account that $V_i(\underline{x}t)$ and $D_i(\underline{x}t)$ are positive and that $A_{ij}(\underline{x}t)$ are non-negative, it is easy to prove that the matrices $Z_i(t)$ and $R_{ii}(t)$ are positive definite ($i = 1, 2$).

In the numerical examples of Section 7, we will use as trial functions the eigenfunctions (corresponding to the dominant eigenvalues) of the problem

$$\Delta W(\underline{x}) + \mu W(\underline{x}) = 0 \quad \text{for } \underline{x} \in R;$$

$$W(\underline{x}) = 0 \quad \text{for } \underline{x} \in \Gamma_1; \quad \frac{\partial W(\underline{x})}{\partial n} = 0 \quad \text{for } \underline{x} \in \Gamma_2.$$

The numerical solution of (13) is found by solving the following algebraic system:

$$\begin{vmatrix} \left(\frac{1}{\Delta t} Z_1(t) + R_{11}(t) \right) & -R_{12}(t) \\ -R_{21}(t) & \left(\frac{1}{\Delta t} Z_2(t) + R_{22}(t) \right) \end{vmatrix} \begin{vmatrix} C_1(t) \\ C_2(t) \end{vmatrix} = \begin{vmatrix} \frac{1}{\Delta t} Z_1(t) C_1(t - \Delta t) + Q_1(t) \\ \frac{1}{\Delta t} Z_2(t) C_2(t - \Delta t) \end{vmatrix}$$

5. The Euler Method

For clarity of exposition we suppose that R is a rectangular domain in the xy plane. We suppose that:

- 1) a network of horizontal and vertical lines is introduced on the xy plane (we do not assume equal spacing for these lines);
- 2) the domain R and each region $R_k (1 \leq k \leq r)$ of R are the union of rectangular meshes of the net. Thus we shall permit interfaces between regions R_k to occur on link of the net;
- 3) the coefficients of (1)-(2) are constant in each region $R_k (1 \leq k \leq r)$;
- 4) $\phi_i(\underline{x}t) = 0$ for $\underline{x} \in \Gamma$ and all t , $0 \leq t \leq t^*$ ($i = 1, 2$).

Without loss of generality we may take each R_k to be one rectangular mesh of the net.

We will indicate by $\psi_{mn}^i(t)$ the value of the function $\psi_i(xyt)$ at the mesh-point $(x_n y_m)$, and by $V_{mn}^1(t)$, $D_{mn}^i(t)$, $A_{mn}^{ij}(t)$, and $H_{mn}^i(t)$ ($i, j = 1, 2$) the values of the coefficients of (1)-(2) in the middle point $(\bar{x}_n \bar{y}_m)$: $\bar{x}_n = (x_{n+1} + x_n)/2$; $\bar{y}_m = (y_{m+1} + y_m)/2$.

The Euler method (which may be regarded as a particular case of the Kantorovich method) consists in searching for the functions which render stationary the functional (9) in the class of piecewise linear functions. The domain R is decomposed into triangular subregions, as shown in Fig. 1. For any choice of values $\phi_{mn}^i(t)$ and $\phi_{mn}^{*i}(t)$ at mesh-points $(x_n y_m)$ of R [where $\phi_i(xyt)$ and $\phi_i^*(xyt)$ are not specified], we can define the functions $\phi_i(xyt)$ and $\phi_i^*(xyt)$ in R in such a way that $\phi_i(xyt)$ and $\phi_i^*(xyt)$ are continuous in R and linear in each triangular subregion of R .

Fig. 1
Triangular Subregions of R

In the shaded triangular subregion of Fig. 1, we have ($i = 1, 2$) or

$$\begin{aligned}\phi_i(x, y, t) &= \phi_{mn}^i(t) + (x - x_n) \left[\frac{\phi_{m, n+1}^i(t) - \phi_{mn}^i(t)}{x_{n+1} - x_n} \right] + (y - y_m) \left[\frac{\phi_{m+1, n}^i(t) - \phi_{mn}^i(t)}{y_{m+1} - y_m} \right]; \\ \phi_i^*(x, y, t) &= \phi_{mn}^{*i}(t) + (x - x_n) \left[\frac{\phi_{m, n+1}^{*i}(t) - \phi_{mn}^{*i}(t)}{x_{n+1} - x_n} \right] + (y - y_m) \left[\frac{\phi_{m+1, n}^{*i}(t) - \phi_{mn}^{*i}(t)}{y_{m+1} - y_m} \right].\end{aligned}\quad (14)$$

If we substitute these quantities into (9), the functional becomes

$$\mathcal{J}[\phi_{mn}^i(t), \phi_{mn}^{*i}(t)] = \int_0^{t^*} dt F\left(t, \phi_{mn}^{*i}(t), \phi_{mn}^i(t), \frac{d\phi_{mn}^i(t)}{dt}\right). \quad (15)$$

The Euler-Lagrange equations of (15) are

$$\frac{\partial F}{\partial \phi_{mn}^{*i}(t)} = 0 \quad (i = 1, 2; 1 \leq m \leq M, 1 \leq n \leq N), \quad (16)$$

or, in extenso,

$$\begin{aligned}\Lambda_{mn} \left\{ Z^1(t) \frac{d\phi^1(t)}{dt} \right\} + \Lambda_{mn} \left\{ R^{11}(t) \phi^1(t) \right\} - \Lambda_{mn} \left\{ R^{12}(t) \phi^2(t) \right\} \\ = \Lambda_{mn} \left\{ S(t) \theta(t) \right\} + \Lambda_{mn} \left\{ T(t - \Delta t) \phi^2(t - \Delta t) \right\}; \\ \Lambda_{mn} \left\{ Z^2(t) \frac{d\phi^2(t)}{dt} \right\} - \Lambda_{mn} \left\{ R^{21}(t) \phi^1(t) \right\} + \Lambda_{mn} \left\{ R^{22}(t) \phi^2(t) \right\} = 0,\end{aligned}\quad (17)$$

where

$$\begin{aligned}\Lambda_{mn} \left\{ X^i(t) \psi^i(t) \right\} \equiv X_{(1)mn}^i(t) \psi_{m-1, n+1}^i + X_{(2)mn}^i(t) \psi_{m-1, n}^i \\ + X_{(3)mn}^i(t) \psi_{m, n-1}^i + X_{(4)mn}^i(t) \psi_{m+1, n-1}^i \\ + X_{(5)mn}^i(t) \psi_{m+1, n}^i + X_{(6)mn}^i(t) \psi_{m, n+1}^i \\ + X_{(0)mn}^i(t) \psi_{mn}^i(t)\end{aligned}$$

and, for $\ell = 0, 1, \dots, 6$ (δ_{ij} is the symbol of Kronecker),

$$Z_{(\ell)mn}^i(t) \equiv W_{(\ell)mn} \left\{ \frac{1}{V_i} \right\}$$

$$R_{(\ell)mn}^{ij}(t) \equiv W_{(\ell)mn} \{A_{ij}\} - \delta_{ij} \chi_{(\ell)mn} \{D_i\};$$

$$S_{(\ell)mn}(t) \equiv W_{(\ell)mn} \{1\}; \quad T_{(\ell)mn}(t) \equiv W_{(\ell)mn} \{\beta H\}.$$

We have put

$$W_{(1)mn} \{X\} \equiv \frac{K_{m-1}}{12} X_{m-1 \ n}(t) h_n;$$

$$W_{(2)mn} \{X\} \equiv \frac{K_{m-1}}{24} (X_{m-1 \ n}(t) h_n + X_{m-1 \ n-1}(t) h_{n-1});$$

$$W_{(3)mn} \{X\} \equiv \frac{h_{n-1}}{24} (X_{m-1 \ n-1}(t) K_{m-1} + X_{m \ n-1}(t) K_m);$$

$$W_{(4)mn} \{X\} = W_{(1)m+1 \ n-1} \{X\}; \quad W_{(5)mn} \{X\} = W_{(2)m+1 \ n} \{X\};$$

$$W_{(6)mn} \{X\} = W_{(3)m \ n+1} \{X\}; \quad W_{(0)mn} \{X\} = \sum_{\ell=1}^6 W_{(\ell)mn} \{X\};$$

$$\chi_{(2)mn} \{D_i\} \equiv (D_{m-1 \ n}^i(t) h_n + D_{m-1 \ n-1}^i(t) h_{n-1}) / 2K_{m-1};$$

$$\chi_{(3)mn} \{D_i\} \equiv (D_{m-1 \ n-1}^i(t) K_{m-1} + D_{m \ n-1}^i(t) K_m) / 2h_{n-1};$$

$$\chi_{(5)mn} \{D_i\} = \chi_{(2)m+1 \ n} \{D_i\}; \quad \chi_{(6)mn} \{D_i\} = \chi_{(3)m \ n+1} \{D_i\};$$

$$\chi_{(1)mn} \{D_i\} = \chi_{(4)mn} \{D_i\} = 0; \quad \chi_{(0)mn} \{D_i\} = \sum_{\ell=1}^6 \chi_{(\ell)mn} \{D_i\};$$

$$h_n = x_{n+1} - x_n; \quad K_m = y_{m+1} - y_m;$$

$$\theta_{mn}(t) = \alpha s_{mn}(t - \Delta t) + g_{mn}(t).$$

If in the functional (9) we approximate the functions $\phi_i^* \psi$ with the expression [ψ indicates the function ϕ_i or $\partial \phi_i / \partial t$ or $(s+g)$]

$$\begin{aligned} \phi_i^*(x y t) \psi(x y t) = & \phi_{mn}^{*i}(t) \psi_{mn}(t) + (x - x_n) \left[\frac{\phi_{m n+1}^{*i}(t) \psi_{m n+1}(t) - \phi_{mn}^{*i}(t) \psi_{mn}(t)}{x_{n+1} - x_n} \right] \\ & + (y - y_m) \left[\frac{\phi_{m+1 n}^{*i}(t) \psi_{m+1 n}(t) - \phi_{mn}^{*i}(t) \psi_{mn}(t)}{y_{m+1} - y_m} \right], \end{aligned}$$

then the Euler-Lagrange equations (16) become

$$\begin{aligned} Z_{mn}^1(t) \frac{d\phi_{mn}^1(t)}{dt} + \Lambda_{mn} \{R^{11}(t) \phi^1(t)\} - R_{mn}^{12}(t) \phi_{mn}^2(t) \\ = S_{mn}(t) \theta_{mn}(t) + T_{mn}(t - \Delta t) \phi_{mn}^2(t - \Delta t); \end{aligned} \quad (18)$$

$$Z_{mn}^2(t) \frac{d\phi_{mn}^2(t)}{dt} + \Lambda_{mn} \{R^{22}(t) \phi^2(t)\} - R_{mn}^{21}(t) \phi_{mn}^1(t) = 0,$$

where

$$Z_{mn}^i(t) = 2W_{(0)mn}^i \left\{ \frac{1}{V_i} \right\}; \quad R_{mn}^{ij}(t) = 2W_{(0)mn} \{A_{ij}\} \quad (i \neq j);$$

$$S_{mn}(t) = 2W_{(0)mn} \{1\}; \quad T_{mn}(t) = 2W_{(0)mn} \{\beta H\};$$

$$R_{(\ell)mn}^{ii}(t) = -\chi_{(\ell)mn} \{D_i\}; \quad (1 \leq \ell \leq 6);$$

$$R_{(0)mn}^{ii}(t) = \chi_{(0)mn} \{D_i\} + 2W_{(0)mn} \{A_{ii}\}.$$

The system (18) is called the "reduced Euler-Lagrange system."

The following problem is solved by means of the "Euler-Lagrange system" (17) and the "reduced Euler-Lagrange system" (18).

Problem W (see Fig. 2)

$$a = 210 \quad a' = 140$$

$$b = 130.5 \quad b' = 72.5$$

$$\frac{\partial \phi_i(x 0 t)}{\partial y} = \frac{\partial \phi_i(0 y t)}{\partial x} = 0$$

$$\phi_i(x b t) = \phi_i(a y t) = 0$$

$$\phi_i(x, y, 0) = 1 \quad (i = 1, 2)$$

$$g(x, y, t) = e^{-t}; \quad \mu = \lambda = 1.$$

Fig. 2

Problem W

For all t , $0 \leq t \leq 0.3$, the coefficients of (1)-(2) have the values:

Region	V_1	D_1	A_{11}	A_{12}	H
R_1	$1 \cdot 10^7$	1.066	2.132	0.002474	0.00098
$R_2 + R_3$	$1 \cdot 10^7$	1.1	2.2	0	0.00075
Region	V_2	D_2	A_{21}	A_{22}	
R_1	$1 \cdot 10^7$	0.955	2.132	9.002	
$R_2 + R_3$	$1 \cdot 10^7$	0.986	2.2	5.86	

In Table I are given the values of

$$\bar{\phi}_i(t) = \frac{1}{ab} \int_0^a dx \int_0^b dy \phi_i(x, y, t)$$

determined by solving the system (17) and (18).

Table I

SOLUTIONS OF PROBLEM W

Time	Euler-Lagrange System (17)		Reduced Euler-Lagrange System (18)	
	$\bar{\phi}_1(t)$	$\bar{\phi}_2(t)$	$\bar{\phi}_1(t)$	$\bar{\phi}_2(t)$
0.02	0.4118	0.1297	0.4126	0.1306
0.05	0.3997	0.1259	0.4004	0.1268
0.07	0.3917	0.1234	0.3924	0.1243
0.10	0.3802	0.1198	0.3808	0.1206
0.12	0.3726	0.1174	0.3733	0.1182
0.15	0.3616	0.1139	0.3622	0.1147
0.17	0.3544	0.1117	0.3551	0.1124
0.20	0.3440	0.1084	0.3446	0.1091
0.22	0.3372	0.1062	0.3377	0.1070
0.25	0.3272	0.1031	0.3278	0.1038
0.27	0.3207	0.1010	0.3213	0.1017
0.30	0.3112	0.0980	0.3118	0.0987

It has to be noted that there are problems in which the agreement between the solutions of system (17) and (18) is not as good as that shown in this problem.

In the next paragraph we will study only the numerical solution of system (18).

6. Numerical Solution of the "Reduced Euler-Lagrange System"

The "reduced Euler-Lagrange system" (18) can be written in matrix form:

$$\begin{vmatrix} Z_1(t) & 0 \\ 0 & Z_2(t) \end{vmatrix} \begin{vmatrix} \frac{d\Phi_1(t)}{dt} \\ \frac{d\Phi_2(t)}{dt} \end{vmatrix} + \begin{vmatrix} R_{11}(t) & -R_{12}(t) \\ -R_{21}(t) & R_{22}(t) \end{vmatrix} \begin{vmatrix} \Phi_1(t) \\ \Phi_2(t) \end{vmatrix} = \begin{vmatrix} Q_1(t) \\ 0 \end{vmatrix},$$

where

$$\Phi_i(t) \equiv \left\{ \phi_{i1}^i(t) \phi_{i2}^i(t) \dots \phi_{iN}^i(t), \dots, \phi_{iM_1}^i(t) \phi_{iM_2}^i(t) \dots \phi_{iMN}^i(t) \right\}.$$

We can express the matrix $R_{ii}(t)$ as the matrix sum

$$R_{ii}(t) = P_i(t) + E_i(t) + F_i(t),$$

where

$$P_i(t) \equiv \text{diag} \left\{ R_{(0)11}^{ii}(t) \dots R_{(0)1N}^{ii}(t), \dots, R_{(0)M_1}^{ii}(t) \dots R_{(0)MN}^{ii}(t) \right\},$$

and $E_i(t)$ and $F_i(t)$ are, respectively, strictly lower and upper triangular matrices, whose entries are the entries of $R_{ii}(t)$, respectively, below and above the main diagonal of $R_{ii}(t)$. [The matrix $\Omega \equiv (\omega_{ij})$ is a strictly lower triangular matrix if $\omega_{ij} = 0$ for $j \geq i$.] It is convenient to specify that the diagonal $P_i(t)$ be composed by the sum of three diagonal matrices:

$$P_i(t) = P_i^{(1)}(t) + P_i^{(2)}(t) + P_i^{(3)}(t),$$

where

$$P_i^{(1)}(t) \equiv \text{diag} \left\{ a_{11}^i a_{12}^i \dots a_{1N}^i, \dots, a_{M_1}^i a_{M_2}^i \dots a_{MN}^i \right\},$$

$$P_i^{(2)}(t) \equiv \text{diag} \left\{ b_{11}^i b_{12}^i \dots b_{1N}^i, \dots, b_{M_1}^i b_{M_2}^i \dots b_{MN}^i \right\},$$

$$P_i^{(3)}(t) \equiv \text{diag} \left\{ c_{11}^i c_{12}^i \dots c_{1N}^i, \dots, c_{M_1}^i c_{M_2}^i \dots c_{MN}^i \right\}.$$

We have put

$$a_{mn}^i = (\chi_{(2)mn}\{D_i\} + \chi_{(3)mn}\{D_i\}); \quad b_{mn}^i = 2W_{(0)mn}\{A_{ii}\};$$

$$c_{mn}^i = (\chi_{(5)mn}\{D_i\} + \chi_{(6)mn}\{D_i\}).$$

If we write

$$Z(t) = \begin{vmatrix} Z_1(t) & 0 \\ 0 & Z_2(t) \end{vmatrix}; \quad L(t) = \begin{vmatrix} E_1(t) & 0 \\ -R_{21}(t) & E_2(t) \end{vmatrix}; \quad U(t) = \begin{vmatrix} F_1(t) & -R_{12}(t) \\ 0 & F_2(t) \end{vmatrix};$$

$$P(t) = \begin{vmatrix} P_1(t) & 0 \\ 0 & P_2(t) \end{vmatrix}; \quad P^{(\ell)}(t) = \begin{vmatrix} P_1^{(\ell)}(t) & 0 \\ 0 & P_2^{(\ell)}(t) \end{vmatrix} \quad (\ell = 1, 2, 3);$$

$$R(t) = L(t) + P(t) + U(t); \quad P(t) = P^{(1)}(t) + P^{(2)}(t) + P^{(3)}(t),$$

the system (19) may be written

$$Z(t) \frac{d\Phi(t)}{dt} + R(t) \Phi(t) = Q(t), \quad (20)$$

where

$$\Phi(t) \equiv \{\Phi_1(t) \Phi_2(t)\}; \quad Q(t) \equiv \{Q_1(t) 0\}.$$

A method for solving (19) is to approximate

$$\frac{d\Phi_i(t)}{dt} = [\Phi_i(t) - \Phi_i(t - \Delta t)]/\Delta t$$

and to determine the unknown vectors $\Phi_i(t)$ of the resulting algebraic system with a "block Gauss-Sidel" iterative procedure. In each iteration we have to solve two algebraic systems of the form

$$\left[\frac{1}{\Delta t} Z_i(t) + R_{ii}(t) \right] \Phi_i(t) = \sigma_i(t) \quad (i = 1, 2)$$

which are solved by a "successive over-relaxation method." If $A_{ii} \geq A_{ij}$ for all t , $0 \leq t \leq t^*$, the block Gauss-Sidel method is convergent.

This method of solving (19) is called the "implicit method." In order to reduce the computing time for solving (19), we have experimented with the "implicitly explicit method" and the "alternating method of Saul'yev."⁽³⁾

The main feature of the "implicitly explicit method" is to solve (20) with an "explicit method" at time t and to solve (20) with an "implicit method" at time $t + \Delta t$. This method is described by the system

$$\begin{cases} \frac{1}{\Delta t} Z(t) \Phi(t) = \left[\frac{1}{\Delta t} Z(t) - R(t) \right] \Phi(t - \Delta t) + Q(t); \\ \left[\frac{1}{\Delta t} Z(t) + R(t) \right] \Phi(t + \Delta t) = \frac{1}{\Delta t} Z(t) \Phi(t) + Q(t + \Delta t). \end{cases} \quad (21)$$

The "alternating method of Saul'yev" is described by the system

$$\begin{cases} \left\{ \left[\frac{1}{\Delta t} Z(t) + P^{(1)}(t) + P^{(2)}(t) \right] + L(t) \right\} \Phi(t) = \left\{ \left[\frac{1}{\Delta t} Z(t) - P^{(3)}(t) \right] - U(t) \right\} \Phi(t - \Delta t) + Q(t); \\ \left\{ \left[\frac{1}{\Delta t} Z(t) + P^{(2)}(t) + P^{(3)}(t) \right] + U(t) \right\} \Phi(t + \Delta t) = \left\{ \left[\frac{1}{\Delta t} Z(t) - P^{(1)}(t) \right] - L(t) \right\} \Phi(t) + Q(t + \Delta t). \end{cases}$$

This scheme is explicit.

Using the theory of non-negative matrices it is possible⁽⁴⁾ to prove the following theorems:

Theorem 2 If $\mu = 0$ and $A_{ii} \geq A_{ij} > 0$ ($i \neq j$) for all t , $0 \leq t \leq t^*$, the "implicit method" and the "implicitly explicit method" are stable.

Theorem 3 If $\mu = 0$ and $A_{ii} \geq A_{ij} > 0$ ($i \neq j$) for all t , $0 \leq t \leq t^*$, for

$$\Delta t \leq \left[\min_{t,i,m,n} \left\{ Z_{mn}^i(t) \right\} \right] / \max \left\{ \left(\max_{t,i,m,n} a_{mn}^i \right), \left(\max_{t,i,m,n} c_{mn}^i \right) \right\}$$

the "alternating method of Saul'yev" is stable.

7. Numerical examples

We compare the Kantorovich method with the Euler method in the following problems.

We define the "normalized flux" as the quantity

$$\bar{\phi}_i(t) = \left(\int_R d\sigma \phi_i(\underline{x}t) \right) / \int_R d\sigma; \quad (i = 1, 2).$$

Problem A

The domain R is the union of three rectangular regions as shown in Fig. 3. Take

$$a = 130.0 \text{ cm}; \quad b = 261.0 \text{ cm};$$

$$b' = 58.0 \text{ cm}; \quad b'' = 203.0 \text{ cm}.$$

Now

$$\operatorname{div}(D_i \operatorname{grad} \phi_i) \equiv \frac{1}{r} \frac{\partial}{\partial r} \left[r D_i(r, z, t) \cdot \frac{\partial \phi_i(r, z, t)}{\partial r} \right] + \frac{\partial}{\partial z} \left[D_i(r, z, t) \cdot \frac{\partial \phi_i(r, z, t)}{\partial z} \right].$$

The coefficients of system (1)-(2) are as follows:

Region	$V_1(0 \leq t \leq 0.2)$	$D_1(0 \leq t \leq 0.2)$	$A_{11}(0 \leq t \leq 0.2)$	$A_{12}(0 \leq t \leq 0.1)$	$(0.1 < t \leq 0.2)$	$H(0 \leq t \leq 0.2)$
$R_1 + R_3$	$0.3080 \cdot 10^7$	1.1	0.002582	0	0	0
R_2	$0.3080 \cdot 10^7$	1.066	0.002652	0.004506	0.002482	$0.3067 \cdot 10^{-4}$
Region	$V_2(0 \leq t \leq 0.2)$	$D_2(0 \leq t \leq 0.2)$	$A_{21}(0 \leq t \leq 0.2)$	$A_{22}(0 \leq t \leq 0.1)$	$(0.1 < t \leq 0.2)$	
$R_1 + R_3$	$0.2486 \cdot 10^6$	0.986	0.002582	0.0003287	0.002629	
R_2	$0.2486 \cdot 10^6$	0.955	0.002652	0.002542	0.002763	

Also

$$\mu = \lambda = 0.07679.$$

Fig. 3
Problem A

The initial boundary conditions are:

$$\phi_1(r, z, 0) = 0.100678 \cdot 10^{14} \psi(r, z);$$

$$\phi_2(r, z, 0) = 0.733648 \cdot 10^{13} \psi(r, z);$$

$$\frac{\partial \phi_i(0, z, t)}{\partial r} = \phi_i(r, 0, t) = \phi_i(r, b, t) = \phi_i(a, z, t) = 0; \quad (i = 1, 2)$$

$$g(r, z, t) = e^{-t} \psi(r, z) (0.225 \cdot 10^7) \exp(1 - \lambda) t,$$

where

$$\psi(r, z) = \left[J_0\left(\xi_1 \frac{r}{a}\right) \sin\left(\frac{\pi z}{b}\right) \right] / \sqrt{\frac{\pi a^2 b}{4}} J_1(\xi_1)$$

and $\xi_1 = 2.40482$ is the first zero of the Bessel function $J_0(x)$.

In Table II are given the values of $\bar{\phi}_i(t)$ obtained by solving the system (14) with $N = 25$ and $\Delta t = 10^{-3}$, and the system (18) by the "implicit method" and with the "implicitly explicit method."

Table II
SOLUTIONS OF PROBLEM A

Time $t =$	Kantorovich Method ($N = 25, \Delta t = 10^{-3}$)		Euler Method			
			Implicit Method ($\Delta t = 10^{-3}$)		Implicitly Explicit Method ($\Delta t = 10^{-3}$)	
	$\bar{\phi}_1(t)$	$\bar{\phi}_2(t)$	$\bar{\phi}_1(t)$	$\bar{\phi}_2(t)$	$\bar{\phi}_1(t)$	$\bar{\phi}_2(t)$
0.01	0.697 E+10	0.607 E+10	0.696 E+10	0.603 E+10	0.674 E+10	0.584 E+10
0.02	0.286 E+11	0.249 E+11	0.285 E+11	0.247 E+11	0.253 E+11	0.220 E+11
0.03	0.116 E+12	0.102 E+12	0.116 E+12	0.101 E+12	0.947 E+11	0.822 E+11
0.04	0.475 E+12	0.414 E+12	0.472 E+12	0.409 E+12	0.354 E+12	0.307 E+12
0.05	0.193 E+13	0.169 E+13	0.192 E+13	0.166 E+13	0.132 E+13	0.114 E+13
0.06	0.787 E+13	0.687 E+13	0.780 E+13	0.676 E+13	0.493 E+13	0.428 E+13
0.07	0.321 E+14	0.280 E+14	0.317 E+14	0.275 E+14	0.184 E+14	0.160 E+14
0.08	0.130 E+15	0.114 E+15	0.129 E+15	0.112 E+15	0.687 E+14	0.596 E+14
0.09	0.531 E+15	0.164 E+15	0.524 E+15	0.455 E+15	0.257 E+15	0.223 E+15
0.10	0.216 E+16	0.189 E+16	0.213 E+16	0.185 E+16	0.958 E+15	0.831 E+15
0.11	0.127 E+15	0.180 E+15	0.125 E+15	0.177 E+15	0.982 E+14	0.117 E+15
0.12	0.829 E+13	0.117 E+14	0.816 E+13	0.115 E+14	0.362 E+13	0.567 E+13
0.13	0.570 E+12	0.786 E+12	0.563 E+12	0.772 E+12	0.231 E+12	0.267 E+12
0.14	0.699 E+11	0.788 E+11	0.705 E+11	0.786 E+11	0.261 E+11	0.288 E+11
0.15	0.374 E+11	0.330 E+11	0.386 E+11	0.337 E+11	0.215 E+11	0.173 E+11
0.16	0.352 E+11	0.300 E+11	0.365 E+11	0.308 E+11	0.198 E+11	0.170 E+11
0.17	0.352 E+11	0.298 E+11	0.364 E+11	0.306 E+11	0.203 E+11	0.169 E+11
0.18	0.351 E+11	0.298 E+11	0.363 E+11	0.305 E+11	0.201 E+11	0.169 E+11
0.19	0.351 E+11	0.297 E+11	0.363 E+11	0.305 E+11	0.201 E+11	0.169 E+11
0.20	0.351 E+11	0.297 E+11	0.363 E+11	0.305 E+11	0.201 E+11	0.169 E+11

Problem R

The domain R of this problem and the coefficients of system (1)-(2) at time $t = 0$ are the same as for Problem A. For $t > 0$ the coefficients V_i , D_i , A_{ij} , and H are functions of the temperature of the reactor. The initial functions $\phi_i(r, z, 0)$ ($i = 1, 2$) and $g(r, z, t)$ are given in tabular form.

In Figs. 4, 5, and 6 are given the normalized fluxes $\bar{\phi}_i(t)$ and the fluxes $\phi_i(r, z, t)$ at time $t = 0.025$ and $t = 0.055$ obtained by the Kantorovich method and by the Euler method ("implicit method" and "alternating method of Saul'yev"). The functions $\bar{\phi}_i(t)$ obtained by the Kantorovich method and the implicit method have the same shape within a precision of 0.5%.

Fig. 4. Normalized Flux $\bar{\phi}_1(t)$ for Problem R

Fig. 5. Flux ϕ_i as Function of x for Problem R

Fig. 6. Flux ϕ_i as Function of y for Problem R

In Table III we give the computing time required for the various methods considered above.

Table III

ENTIRE TIME OF CALCULATION ON IBM 7090 (in minutes)

Method	Problem A	Problem R
Kantorovich Method ($N = 25$, $\Delta t = 10^{-3}$)	10 (without the pointwise calculation of fluxes at each time step) 50 (with the calculation of fluxes)	52
Implicit Method ($\Delta t = 10^{-3}$)	40	50
Alternating Method of Saul'yev	25	30
Implicitly Explicit Method ($\Delta t = 10^{-3}$)	30	

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THE APPLICATION OF THE EQUIPOISE ITERATIVE METHOD TO DIFFUSION AND TRANSPORT THEORY*

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I. Introduction

The iterative procedure known as Equipoise⁽¹⁾ is probably the simplest technique in current use for the solution of the finite-difference analogs of the neutron-diffusion equations. Less well known is the fact that the original method and variants upon it have shown remarkable success in transport calculations of the discrete-ordinate type.

The Equipoise method is based on the common-sense idea that error modes in an iterative calculation will be significantly reduced if known facts concerning the final solution to the problem are made a part of the problem-solving process. For example, with any method it is generally considered wise to begin with an initial guess for the solution that is as close as possible to the final answer. Also, if the solution possesses a symmetry axis, the equations themselves should embody such a condition. A further condition which can be used as an accelerative device is the requirement that final answers should contain the idea of balance, that is, that all residues should be as close to zero as permitted by round-off error in the machine computation. The central concept of the Equipoise method is that iterative procedures can often be significantly accelerated if blocks of equations are forced to satisfy this overall balance condition.

II. Application to Diffusion-theory Calculations

In group-diffusion-theory calculations the idea of balance occurs in an obvious and natural way. The customary difference equations contain terms easily identifiable for neutrons of a given energy group as the net leakage, absorption, fissions, in-scattering, and out-scattering over a volume element of the system. In two dimensions, the five-point finite-difference analogs of the diffusion equations have the form

$$a_{I,J,K}(\phi_{I-1,J,K} - \phi_{I,J,K}) + b_{I,J,K}(\phi_{I+1,J,K} - \phi_{I,J,K}) + c_{I,J,K}(\phi_{I,J+1,K} - \phi_{I,J,K}) + d_{I,J,K}(\phi_{I,J-1,K} - \phi_{I,J,K}) \\ - e_{I,J,K}\phi_{I,J,K} - f_{I,J,K}\phi_{I,J,K} + \sum_{\substack{k=1 \\ k \neq K}}^{KMAX} p_{I,J,k} e_{I,J,k} \phi_{I,J,k} + \lambda \chi_K \sum_{k=1}^{KMAX} g_{I,J,k} \phi_{I,J,k} = 0. \quad (1)$$

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This equation expresses a neutron balance over a volume element in the finite-difference mesh for neutrons of a particular energy group. Here, I and J are, respectively, the row and column number of a point in the finite-difference mesh, and K is the group number, the total number of groups being $KMAX$. Also, a , b , c , and d are leakage constants determined by the composition of materials around point I, J in group K and by the geometry of the mesh. (The programs we have developed treat x - y , r - z , and r - θ geometries.) The constant $e_{I,J,K}$ represents the cross section volume-weighted around point I, J for removing neutrons from group K to other groups, whereas $f_{I,J,K}$ is the volume-weighted cross section for neutron absorption. The constant $p_{I,J,k}$ is the fraction of neutrons removed from group k which appear in group K ($p_{I,J,K} = 0$ and $\sum_k p_{I,J,k} \equiv 1$); $g_{I,J,k}$ is the volume-weighted fission cross section for group k , while χ_K is the fission spectrum constant. The constant λ is the eigenvalue of the problem and may be regarded as the inverse multiplication constant. As a neutron balance, the equation may be read

$$\begin{aligned} &(\text{in-leakage}) - (\text{out-scattering}) - (\text{absorption}) + (\text{in-scattering}) \\ &+ \lambda(\text{fission source}) = 0. \end{aligned} \quad (2)$$

If, as is easy and natural to do, the leakage constants are constructed such that the leakage out of the faces of volume elements is equal to the leakage into the faces of adjacent volume elements, that is, if

$$\begin{aligned} a_{I,J,K} &= b_{I-1,J,K}; & b_{I,J,K} &= a_{I+1,J,K}; \\ c_{I,J,K} &= d_{I,J+1,K}; & d_{I,J,K} &= c_{I,J-1,K}. \end{aligned}$$

then the sum of the "in-leakage" terms for all the difference equations will cancel to the extent that only the leakage at the outside surface of the reactor will remain. The sum of the in-scattering and out-scattering terms will likewise cancel. The sum of all the difference equations thus represents a neutron balance over the reactor:

$$\lambda(\text{fission source}) = \text{absorptions} + \text{leakages}. \quad (3)$$

The procedure used for solving the above difference equations employing point-wise successive over-relaxation consists of solving Eq. (1) for $\phi_{I,J,K}$ by transposing all the $\phi_{I,J,K}$ terms over to the right-hand side except that in the fission source term. The most recently computed values of fluxes are used wherever possible. It is seen that the newly computed flux will be positive if all the other fluxes are positive. Upon computing such a flux, over-relaxation is applied immediately:

$$\phi_{n+1} = \phi_n + \beta(\phi_{n+1}^* - \phi_n), \quad (4)$$

where the subscript n denotes the number of the mesh sweep, ϕ_{n+1}^* is the value of the flux before over-relaxation, and β is the over-relaxation coefficient. Since it is possible at this point to obtain a negative value for the flux, the over-relaxation process has been modified by a device due to Vondy:⁽²⁾

$$\phi_{n+1} = \phi_n \exp \left[-\beta \left(1 - \frac{\phi_{n+1}^*}{\phi_n} \right) \right] \quad \text{for } \phi_{n+1}^* < \phi_n; \quad (5a)$$

$$\phi_{n+1} = \phi_n \left[2 - \exp \beta \left(1 - \frac{\phi_{n+1}^*}{\phi_n} \right) \right] \quad \text{for } \phi_{n+1}^* > \phi_n. \quad (5b)$$

In this way, ϕ_{n+1} will lie in the range $e^{-\beta} \phi_n$ to $2\phi_n$ and will never be negative if ϕ_n is positive. When the argument of the exponential becomes small, Eqs. (5) revert to Eq. (4).

When a complete set of new fluxes has been obtained, the eigenvalue of the problem is estimated from Eq. (3) on the basis of the new fluxes:

$$\lambda = \frac{\text{Absorptions} + \text{leakages}}{\text{Fission source}}. \quad (3')$$

The iterative process is then continued until the absolute value of the following convergence indicator falls below a prescribed value, usually about 10^{-4} :

$$\epsilon_n = \left(\frac{\phi_n - \phi_{n-1}}{\phi_{n-1}} \right)_{\max}. \quad (6)$$

The right-hand side of Eq. (6) is the largest fractional change which appears among the fluxes. In addition, the behavior of another convergence indicator, which we call the "absolute" flux convergence, is also observed. In this it is assumed that the error decay rate follows the law

$$\phi_n = \phi_\infty + A\mu^n. \quad (7)$$

It is easy to show, under this assumption, that

$$\mu = \frac{\epsilon_n}{\epsilon_{n-1}} (1 + \epsilon_{n-1}), \quad (8)$$

where the so-called "absolute" convergence indicator is defined by

$$e_n = \left| \epsilon_n \left(\frac{1}{1 - \mu} \right) \right| \approx \left| \frac{\phi_\infty - \phi_n}{\phi_n} \right|. \quad (9)$$

(It is our practice to be certain that $|\mu| < 1$.) Should convergence be too slow, the value of μ computed from Eq. (8) is used to extrapolate fluxes

according to the assumption expressed by Eq. (7). The formula for this extrapolation is

$$\phi_{\infty} = \phi_n + \frac{\mu}{1-\mu} (\phi_n - \phi_{n-1}). \quad (10)$$

The procedure outlined above may also be stated in matrix form. The set of equations represented by Eq. (1) may be written as

$$A\phi = \lambda M\phi, \quad (11)$$

where A is a matrix whose diagonal elements are all positive and whose off-diagonal elements are all either negative or zero. The sum of the elements in any column of A is non-negative. M is a non-negative matrix. With these restrictions, it is not difficult to see that $A^{-1}M$ is a non-negative matrix, which we assume to be irreducible. It therefore possesses a real positive eigenvalue equal to its spectral radius and an associated all-positive eigenvector.

The process outlined above amounts to performing the iterative sequence

$$\phi_{t+1} = (D - \beta\lambda_t S - \beta L)^{-1} [\lambda_t \beta T + \beta U + D(1 - \beta)]\phi_t; \quad (12)$$

$$\lambda_t = \frac{e^T A \phi_t}{e^T M \phi_t}, \quad (13)$$

where the matrices D , S , L , T , and U are obtained by partitioning A and M as follows:

$$A = D - L - U; \quad M = S + T. \quad (14)$$

The matrix D is diagonal, and its elements are the diagonal elements of A . The matrices $-L$ and $-U$ are, respectively, lower triangular and upper triangular matrices containing the off-diagonal elements of A . The matrices S and T are likewise lower and upper triangular, and contain, respectively, the elements below the diagonal of M and those above and including the diagonal of M . The coefficient β is the over-relaxation constant of Eq. (4), and e^T is a row vector, $[1 \ 1 \ 1 \ \dots \ 1]$, with as many elements as the vector ϕ .

The use of Eq. (13), which is Eq. (3') in matrix form, represents an attempt to make the source iterates, $\lambda_t M \phi_t$, and the flux iterates conform to one another simultaneously, rather than make the fluxes conform to a source guess by the conventional "inner iteration" procedure. In this way, a known fact about the required answer, the idea of balance, has been introduced into the iterative procedure.

The idea of balance may be further elaborated by dividing the equations represented by Eq. (11) into blocks which may refer to geometric regions and/or neutron groups in the physical problem. In each of these blocks it is often possible to multiply the flux vector by one of a set of easily computed numbers which will force a balance over each such region as well as produce the overall balance represented by Eq. (4). This process, when applied to neutron groups, is particularly helpful in cell calculations if the coupling between groups is relatively weak. When applied to regions, it has been found very useful in transport-theory calculations for deep-penetration problems.

To illustrate this "rebalancing" technique as applied to groups, an example of its use in two groups is given. Instead of using Eq. (13) to estimate λ_t , the balance form of two-group equations could be written:

$$d_1 L_1 + A_1 d_1 + R_1 d_1 - R_2 d_2 = \lambda \chi_1 (S_1 d_1 + S_2 d_2); \quad (15)$$

$$d_2 L_2 + d_2 A_2 + d_2 R_2 - d_1 R_1 = \lambda (1 - \chi_1) (S_1 d_1 + S_2 d_2); \quad (16)$$

$$d_1 L_1 + d_2 L_2 + d_1 A_1 + d_2 A_2 = \lambda (S_1 d_1 + S_2 d_2), \quad (17)$$

where L , A , and R refer to leakage, absorption, and removal out of the indicated group, χ_1 is the fraction of fission source neutrons born in group 1, and S_1 and S_2 are the productions of source neutrons in groups 1 and 2. The factors d_1 and d_2 are to be found by which fluxes are to be multiplied so that all three balance equations are satisfied, i.e., balance is obtained over the groups individually and over both groups together. Since substitution of the overall balance Eq. (17) into Eqs. (15) and (16) produces a pair of homogeneous equations in d_1 and d_2 , one of the multipliers, say d_1 , may be set equal to unity, and d_2 and λ may then be determined. This process can be extended to any number of groups so long as a single fission spectrum is used. It is possible to show that the d_i for group rebalancing will always be positive if the absorption, leakage, and removal terms are positive.

As has already been pointed out, this technique is primarily useful in cell problems. In one such case which would have required thousands of iterations to obtain a reasonable level of convergence, the number of sweeps was reduced to 70. This case was a two-group, rectangular-cell problem containing 225 mesh points. The flux in both groups was approximately flat, a fact soon evident after a relatively small number of iterations. The difficulty, which was remedied by the rebalancing process, lay in the fact that the effect of each group upon the other due to in-scattering was "swamped" by the relatively large leakage terms. In effect, neither group "knew" that the other was there.^(3,4)

III. Application to Transport-theory Calculations

Our experience has shown us that little, if anything, is gained in using regionwise rebalancing in diffusion-theory calculations. Such is not the case in transport-theory calculations. An experimental discrete-ordinates transport-theory code (SWAPS) has been programmed for one-dimensional slab geometry, utilizing the same methods we have outlined for diffusion-theory calculations.⁽⁵⁾ In this treatment the Boltzmann equation has been considered from the standpoint of neutrons traveling along rays, that is,

$$\frac{dN}{ds} + \Sigma_T N = S, \quad (18)$$

where N is the neutron flux per unit solid angle at a given position and traveling in a given direction, Σ_T is the total cross section, and S is the source composed of in-scattering from other directions, fission neutrons, and fixed sources. As the code was set up, Eq. (18) was used in difference form:

$$\frac{N(s + \Delta s) - N(s)}{\Delta s} + \Sigma_T \frac{1}{2} [N(s) + N(s + \Delta s)] = S, \quad (19)$$

where S is now the average source over the interval Δs . By solving the equation for $N(s + \Delta s)$, the following relation is obtained:

$$N(s + \Delta s) = \frac{S\Delta s + N(s) \left[1 - \frac{\Sigma_T \Delta s}{2} \right]}{1 + \frac{\Sigma_T \Delta s}{2}}. \quad (20)$$

It is apparent that $N(s + \Delta s)$ will always be positive if $\Sigma_T \Delta s < 2$, so that it can be ensured that the iterative scheme will always compute positive fluxes from positive flux guesses if the restriction is met. Even this restriction can be removed if Eq. (18) is solved as a differential equation assuming S to be constant over the interval Δs . The following result is obtained:

$$N(s + \Delta s) = N(s) e^{-\Sigma_T \Delta s} + \frac{S}{\Sigma_T} (1 - e^{-\Sigma_T \Delta s}). \quad (21)$$

The use of Eq. (21) permits the use of arbitrarily wide increments without fear of negative fluxes occurring. It is not difficult to see that Eq. (21) reduces to Eq. (20) if e^{-x} is approximated by $[1 - (x/2)]/[1 + (x/2)]$. The same iterative scheme expressed by Eqs. (12) and (13) has been applied to the discrete-ordinates system of equations. As long as deep-penetration problems are not considered, it may be noted that Eqs. (20) or (21) are highly

"forward" in character, that is, $N(s + \Delta s)$ depends mostly on $N(s)$ and convergence is very rapid. Over-relaxation is difficult to apply in such cases and has been found, in fact, to be unnecessary. On the other hand, when the method is applied to deep-penetration problems such as the Milne problem, convergence is quite slow. In one example, a nonabsorbing slab with a thickness of 78 mean free paths was set up with an isotropic plane source at one face and zero incoming current at the other. Although the correct angular distribution was soon obtained at the surface opposite the source, the convergence criteria indicated very sluggish behavior. Examination of the total flux distribution revealed that a very large bulge, resulting from the original flux guess, still existed and was slowly decaying. After 200 sweeps, the point-wise flux-convergence level was about 0.02. By dividing the slab into eight subregions and computing rebalancing factors to force neutron balances over each such region, the bulge was removed and the convergence level was found to be 8×10^{-4} after 90 sweeps.

In this problem four angular increments were used. The emergent angular flux at the face of zero incoming current and the spatial distribution of the total flux are compared in Table 1 with results obtained by the Wiener-Hopf method.^(6,7) The quantities $-\mu$, μ_{avg} , and $(\mu^2)_{\text{avg}}$ are defined as in Sections 16 and 18 of Ref. 6.

Table 1
COMPARISON OF THEORETICAL SOLUTION TO
MILNE'S PROBLEM WITH RESULTS OBTAINED WITH
SWAPS USING FOUR ANGULAR INCREMENTS

	SWAPS Result	Wiener-Hopf	Percent Error
<u>a. Total Flux</u>			
<u>Distance from Boundary, Mean Free Paths</u>			
0	1	1	-
0.2	1.4445	1.4714	-1.83
0.4	1.8491	1.8587	-0.52
0.6	2.2320	2.2271	+0.22
0.8	2.6031	2.5868	+0.63
1.0	2.9680	2.9419	+0.89
2.0	4.7609	4.6902	+1.51
<u>b. Emergent Angular Flux</u>			
<u>$-\mu$</u>			
0.25	0.76422	0.773	-1.1
0.75	1.23578	1.232	+0.3
μ_{avg}	0.55894	0.5774	-3.2
$(\mu^2)_{\text{avg}}$	0.37144	0.4102	-9.4

Table 2 compares results obtained by Carlson⁽⁸⁾ and Dresner⁽⁹⁾ with those obtained using the SWAPS program for calculations on the critical thickness of slabs in which scattering is isotropic or linearly anisotropic.

Table 2

COMPARISON OF ANALYTICAL ESTIMATES OF
CRITICAL NUMBER OF SECONDARIES PER COLLISION
WITH RESULTS OBTAINED USING SWAPS

Total Slab Thickness, Mean Free Paths	Critical Number of Secondaries per Collision	
	Analytical Methods ⁽⁸⁾	SWAPS
<u>a. Isotropic Scattering</u>		
5.665	1.02	1.020
0.7366	1.4	1.400
0.3108	2.0	2.003

b. Anisotropic Scattering

$$\bar{\mu} = 0.3$$

$$\text{where } \bar{\mu} = \frac{\int_{-1}^1 \mu(\nu\sigma_f + \sigma_s) d\mu}{\int_{-1}^1 (\nu\sigma_f + \sigma_s) d\mu}$$

Total Slab Thickness, Mean Free Paths	Critical Number of Secondaries per Collision	
	Variational Estimate ⁽⁹⁾	SWAPS
0.2	3.931	3.99456
0.4	2.601	2.61314
1.0	1.667	1.67240
2.0	1.312	1.31627
4.0	1.127	1.13077
8.0	1.044	1.04641
20.0	1.009	1.00969

An additional problem used to check the performance of the program was the calculation of thermal utilization in a slab lattice. The particular

case chosen was that given on p. 642 of Ref. 7, where an exact result of $f = 0.8560$ is given. Using a special version of the SWAPS code, f was calculated to be 0.8557.

IV. Final Remarks

The methods described here have been used as the basis of a series of codes, the latest of which is a multigroup, two-dimensional diffusion-theory code called EXTERMINATOR,⁽²⁾ which uses successive line over-relaxation and permits scattering from any group to any other group. This program also solves fixed-source and criticality search problems. We are also using these methods in efforts to construct discrete-ordinates transport-theory programs. Although the methods described are simple to state and apply, we have no proofs that the iterative processes they represent will always converge. The most important control over convergence rates is provided by the over-relaxation coefficient β , which is determined empirically in EXTERMINATOR. (The details of the β -estimation method may be found in Ref. 2.) As Kristiansen⁽¹⁰⁾ has shown, it is not difficult to construct examples which diverge with $\beta = 1$. One of the simplest we have been able to construct is given by using the matrices

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \quad M = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

in Eq. (13). (It is to be noted incidentally that the eigenvalues of this problem are 1 and $\frac{1}{2} \pm \frac{1}{2}\sqrt{3} i$. As these are all equal in modulus, any method which relies on the real positive eigenvalue having the largest modulus will fail.) The Equipoise method with $\beta = 1$ gives the desired eigenvalue immediately, but successive flux values oscillate indefinitely. With $\beta = 3/4$, on the other hand, convergence is quite rapid. The question remains, however, whether such a value of β always exists under the restrictions we have placed on the problem. As far as our experience with reactor problems is concerned, we have not yet encountered a case for which a value of β could not be found which would permit convergence. Particularly worthy of mention is the fact that the procedure works well when up-scattering is permitted. We have, in fact, run the same problem both with all down-scattering and with all up-scattering by reversing the order of the groups, and produced exactly the same answers in both cases with the same number of sweeps.

To sum up, we have outlined here a series of techniques which make use of the neutron balance as an accelerative device. These techniques contrast with the conventional "inner-outer" iteration methods in that a continual attempt is made to make sources and fluxes conform to one another. When

used in combination with successive over-relaxation and extrapolation, these methods have enabled us to solve both simple and complex problems in reasonable amounts of time. The techniques appear to be useful in both diffusion and transport theory, and have been applied to eigenvalue, constant source, and criticality search calculations.

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Discussion of Paper
Presented by Mr. Tobias

MR. SEGAL (Atomic Power Development Associates, Inc.): Have you made any progress with the adjoint problem? You wrote recently that you believed the adjoint could, and I believe you actually said should, be solved simultaneously with the real problem and may be done with no increase in computing time.

MR. TOBIAS: I think that there is perhaps a little misunderstanding. We have in some of our codes, e.g., the TWENTY GRAND program, which is a predecessor of the EXTERMINATOR program, solved the adjoint problem after having done the direct problem; that is, we calculated the eigenvalue of the direct problem, then inserted the eigenvalue into the equations, flipped them around the diagonal, and calculated the fluxes for the adjoint problem. We built this into the TWENTY GRAND program, and it works with considerable success. A great degree of improvement was made by C. W. Nestor in a program EQUIPOISE 3-A. Not only could the adjoint flux be calculated by means of EQUIPOISE, but also the change in k with respect to a variation, which is part of the input, of any neutron physics constant. We have not done this for the EXTERMINATOR code because so far there has not been a great demand for that type of calculation, and it would take a great deal of time to do so. It should be done, and it could be done in the same way.

MR. McWHORTER (General Electric APED): You mentioned that the block spatial rebalancing didn't work too well for diffusion problems. What class of diffusion problems have you examined? Have you considered, in particular, large systems with relatively low leakage and relatively weak spatial coupling?

MR. TOBIAS: In such a case, I believe the circumstances in which we applied that method were not those that you describe. When I said it did not work too well I meant that there was no significant acceleration. The problem didn't need this information; there was already a balance over the region. The type of problem that you describe is not very different from the cell calculation where we have had success, and I would recommend a similar approach. It was built into some of our codes so that one can use it as an option. It is not in the EXTERMINATOR code. The group rebalancing, however, is in the EXTERMINATOR code.

VARIATIONAL SYNTHESIS WITH DISCONTINUOUS TRIAL FUNCTIONS

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I. INTRODUCTION

Several methods have been devised for solving higher-dimensional problems approximately with the aid of solutions of related lower-dimensional problems. Two of the more sophisticated methods for neutron-diffusion problems are variational synthesis⁽¹⁾ and multichannel flux synthesis.⁽²⁾ In the former, the solution at an elevation is approximated by a linear combination of trial functions obtained by solving a set of lower-dimensional problems. The coefficients of combination are related by means of a variational principle and are found by solving a system of simultaneous linear equations. In the multichannel synthesis method, regions are represented by nodes and nodal-difference equations are derived with the aid of the lower-dimensional results. For neutron-diffusion computations, a heuristic argument was used initially for obtaining these difference equations in terms of partial currents along region interfaces. The nodal equations are a system of simultaneous linear equations which may be solved by conventional methods.

It should be possible, by a suitable choice of a functional and trial functions, to derive nodal-difference equations from a variational principle. Such a derivation will be made in this paper. The trial functions used, however, are not continuous. The discontinuities lead to infinite contributions to certain integrals in variational principles such as that used in Ref. 1.

Selengut⁽³⁾ has shown how this difficulty may be avoided. Instead of seeking the second-order diffusion equations as Euler equations, he seeks the simultaneous first-order partial differential equations for flux and current. In this formulation, the discontinuities yield finite contributions.

The new variational formulation is more general than the synthesis techniques of Ref. 1 and 2. In the case of continuous trial functions and a single "channel," the procedure is equivalent to the variational synthesis of Kaplan et al.⁽¹⁾ In the case of one trial function per channel, the nodal difference equations are identical in structure to the multichannel synthesis of Wachspress et al.⁽²⁾ The new formulation thus includes the earlier formulations as special cases, and is more general than either.

An important consequence of the admissibility of discontinuous trial functions is that several free parameters can be introduced with each

*Operated by the General Electric Company for the U. S. Atomic Energy Commission.

continuous "base" trial function, whereas only one free parameter can be introduced per base trial function when only continuous trial functions are admissible. In synthesis computations, each base trial function is obtained by solving a detailed two-dimensional problem. Obtaining these base functions is a large contributor to the machine time consumed in the overall computation. The use of several free parameters per base function results in an increase of efficiency in the use of the base function and, therefore, in a reduction in consumption of machine time.

In Section II, we present Selengut's variational principle, with particular attention paid to the contributions of discontinuities. In Section III, we give a simple illustrative problem using discontinuous trial functions. In Section IV, we describe a particular trial function which may be used to derive equations for a generalized model involving multi-channel synthesis, and in Section V we show how this synthesis procedure may be coupled to a variational depletion analysis.

II. THE VARIATIONAL PRINCIPLE

Following Selengut, we rewrite the second-order differential equation:

$$-\nabla \cdot D\nabla\phi + \Lambda\phi = 0 \quad (1)$$

(Λ represents the nondiffusion components of the group diffusion operator) as coupled first-order equations:

$$\Lambda\phi + \nabla \cdot \underline{j} = 0; \quad \underline{j} + D\nabla\phi = 0. \quad (2)$$

The net current $\underline{j}$ is defined by the last equation. We may express the first-order equations in matrix form:

$$H\psi = \begin{bmatrix} \Lambda & \nabla \cdot \\ -\nabla & -D^{-1} \end{bmatrix} \begin{bmatrix} \phi \\ \underline{j} \end{bmatrix} = \underline{0}. \quad (3)$$

We define the inner product

$$(a \ \underline{b}) \begin{pmatrix} c \\ \underline{d} \end{pmatrix} = \int_{\text{all space}} (ac + \underline{b} \cdot \underline{d}) \, dr, \quad (4)$$

and use the functional

$$F[\psi^+, \psi] = (\psi^+, H\psi) = \int_{\text{all space}} [(\phi^+ \Lambda \phi) + \phi^+ \nabla \cdot \underline{j} - \underline{j}^+ \cdot \nabla \phi - \underline{j}^+ \cdot D^{-1} \underline{j}] \, dr. \quad (5)$$

There are contributions to the functional from discontinuities in the trial functions. Consider, for example, the one-dimensional case with discontinuities in both j^+ and ϕ at x_0 . We will evaluate the contribution to the third term on the right-hand side of (5) arising from these discontinuities. Let*

$$\begin{aligned}\phi(x) &= \frac{\phi(x_0 + \epsilon) + \phi(x_0 - \epsilon)}{2} + \frac{(x - x_0)}{2\epsilon} [\phi(x_0 + \epsilon) - \phi(x_0 - \epsilon)]; \\ j^+(x) &= \frac{j^+(x_0 + \epsilon) + j^+(x_0 - \epsilon)}{2} + \frac{(x - x_0)}{2\epsilon} [j^+(x_0 + \epsilon) - j^+(x_0 - \epsilon)]; \quad |x - x_0| \leq \epsilon.\end{aligned}\tag{6}$$

Then

$$\begin{aligned}\int_{x_0 - \epsilon}^{x_0 + \epsilon} j^+(x) \frac{d\phi(x)}{dx} dx &= \int_{-\epsilon}^{+\epsilon} \left[\frac{\phi(x_0 + \epsilon) - \phi(x_0 - \epsilon)}{2\epsilon} \right] \left[\left(\frac{j^+(x_0 + \epsilon) + j^+(x_0 - \epsilon)}{2} \right) \right. \\ &\quad \left. + \frac{(x - x_0)}{2\epsilon} (j^+(x_0 + \epsilon) - j^+(x_0 - \epsilon)) \right] dx \\ &= \frac{j^+(x_0 + \epsilon) + j^+(x_0 - \epsilon)}{2} [\phi(x_0 + \epsilon) - \phi(x_0 - \epsilon)].\end{aligned}\tag{7}$$

As $\epsilon \rightarrow 0$, this remains finite and is given by

$$\bar{j}^+(x_0) [\phi(x_0)],$$

where $\bar{j}^+(x_0)$ is the average of the left and right limits at x_0 and where $[\phi(x_0)]$ denotes the jump in ϕ at x_0 .

[Conventional variational procedures for solving (1) involve integrals of the form

$$\int \phi + \frac{d^2\phi}{dx^2} dx,$$

which can be integrated by parts to yield $\int \frac{d\phi^+}{dx} \frac{d\phi}{dx} dx$ plus boundary terms.

*Contributions from discontinuities can be evaluated by various techniques, and there is some arbitrariness in the final equations.

When ϕ^+ and ϕ are discontinuous at x_0 , we can write ϕ^+ and ϕ as in (6) and obtain

$$\int_{x_0-\epsilon}^{x_0+\epsilon} \frac{d\phi^+}{dx} \frac{d\phi}{dx} dx = \frac{[\phi^+(x_0+\epsilon) - \phi^+(x_0-\epsilon)][\phi(x_0+\epsilon) - \phi(x_0-\epsilon)]}{4\epsilon^2} 2\epsilon.$$

This expression becomes infinite as $\epsilon \rightarrow 0$.

Given two piecewise-continuous functions $u(x)$ and $v(x)$ with a discontinuity at $x = b$, it is easy to show that

$$\begin{aligned} \int_a^c dx u \frac{dv}{dx} &= \int_a^b dx u \frac{dv}{dx} + \int_b^c dx u \frac{dv}{dx} + \bar{u}(b)[v(b)] \\ &= - \int_a^b dx v \frac{du}{dx} - \int_b^c dx v \frac{du}{dx} - \bar{v}(b)[u(b)] = - \int_a^c dx v \frac{du}{dx}. \end{aligned} \quad (8)$$

If we make use of (8), it follows that for (5) to be stationary with respect to arbitrary variations in ϕ^+ , j^+ , ϕ , and j , we should require that (2) and

$$\begin{aligned} \Lambda \phi^+ + \nabla \cdot j^+ &= 0; \\ -\nabla \phi^+ - D^{-1} j^+ &= 0 \end{aligned} \quad (9)$$

be satisfied for $a < x < b$ and $b < x < c$ with appropriate boundary conditions on ϕ and ϕ^+ at the outer boundary, and with the interface condition that ϕ , ϕ^+ , j , and j^+ be continuous at $x = b$.

III. A SIMPLE ILLUSTRATIVE PROBLEM

Consider the boundary-value problem:

$$\begin{aligned} -\frac{d}{dx} \left[D(x) \frac{d\phi}{dx} \right] &= \lambda \phi; \quad \phi(0) = \phi(\pi) = 0; \\ D > 0 \text{ for } x \in [0, \pi]; \quad \phi \text{ and } D \frac{d\phi}{dx} &\in C[0, \pi]. \end{aligned} \quad (10)$$

We seek the minimum λ .

If $D(x)$ is constant for $x \in [0, \pi]$, the solution is $\lambda = D$. The corresponding eigenfunction is $\phi = \sin x$.

Now let

$$D = D_1 \text{ for } 0 \leq x \leq \pi/2$$

and

$$D = D_2 \text{ for } \pi/2 < x \leq \pi.$$

A straightforward variational estimate of λ is found by using $\phi = \sin x$ as a trial function in

$$\frac{\int_0^\pi D(x) \left(\frac{d\phi}{dx} \right)^2 dx}{\int_0^\pi \phi^2 dx} = \lambda_{\text{est}}.$$

Thus

$$\lambda_{\text{est}} = \frac{\int_0^{\pi/2} D_1 \cos^2 x dx + \int_{\pi/2}^\pi D_2 \cos^2 x dx}{\int_0^\pi \sin^2 x dx} = \frac{D_1 + D_2}{2}.$$

This problem can be solved directly to any desired accuracy. The solution, correct through $O(\epsilon^2)$, when $D_2 = D_1(1 + \epsilon)$ is

$$\lambda = D_1 \left(1 + \frac{\epsilon}{2} - \frac{\epsilon^2}{16} \right). \quad (11)$$

Thus,

$$\frac{D_1 + D_2}{2} = D_1 \left(1 + \frac{\epsilon}{2} \right)$$

is correct through $O(\epsilon)$. The problem is self-adjoint so that $\psi^+ = \psi$. We now use (5) with the direct trial function:

$$\phi = a_1 \sin x \quad \text{for } 0 \leq x \leq \frac{\pi}{2};$$

$$\phi = a_2 \sin x \quad \text{for } \frac{\pi}{2} < x \leq \pi;$$

$$j = b_1 + c_1 \cos x \quad \text{for } 0 \leq x \leq \frac{\pi}{2};$$

$$j = b_2 + c_2 \cos x \quad \text{for } \frac{\pi}{2} < x \leq \pi.$$

The adjoint trial function is of the same form with a^+ , b^+ , and c^+ replacing a , b , and c . We have:

$$\begin{aligned} -F[\psi^+, \psi] &= \int_0^{\pi/2} \left[+\lambda a_1^+ a_1 \sin^2 x + a_1^+ c_1 \sin^2 x + (b_1^+ + c_1^+ \cos x) a_1 \cos x \right. \\ &\quad \left. + \frac{(b_1^+ + c_1^+ \cos x)(b_1 + c_1 \cos x)}{D_1} \right] dx + \int_{\pi/2}^{\pi} \left[+\lambda a_2^+ \sin^2 x + a_2^+ c_2 \sin^2 x \right. \\ &\quad \left. + (b_2^+ + c_2^+ \cos x) a_2 \cos x + \frac{(b_2^+ + c_2^+ \cos x)(b_2 + c_2 \cos x)}{D_2} \right] dx \\ &\quad + \frac{a_1^+ + a_2^+}{2} (b_1 - b_2) + \frac{b_1^+ + b_2^+}{2} (a_2 - a_1). \end{aligned}$$

The last two terms arise from the discontinuity at $\pi/2$. Note that these terms vanish when $b_1 = b_2 = 0$. These constants were added to the cosine term to allow for a non-zero j at $\pi/2$.

We evaluate the integrals and get

$$\begin{aligned} -F[\psi^+, \psi] &= +\frac{\lambda a_1^+ a_1 \pi}{4} + \frac{a_1^+ c_1 \pi}{4} + b_1^+ a_1 + c_1^+ a_1 \frac{\pi}{4} + \frac{b_1^+ b_1}{D_1} \frac{\pi}{2} + \frac{b_1^+ c_1}{D_1} + \frac{c_1^+ b_1}{D_1} \\ &\quad + \frac{c_1^+ c_1}{D_1} \frac{\pi}{4} + \frac{\lambda}{4} a_2^+ a_2 \pi + \frac{a_2^+ c_2 \pi}{4} - b_2^+ a_2 + c_2^+ a_2 \frac{\pi}{4} + \frac{b_2^+ b_2 \pi}{2D_2} - \frac{b_2^+ c_2}{D_2} \\ &\quad - \frac{c_2^+ b_2}{D_2} + \frac{c_2^+ c_2}{D_2} \frac{\pi}{4} + \frac{a_1^+ + a_2^+}{2} (b_1 - b_2) + \frac{b_1^+ + b_2^+}{2} (a_2 - a_1). \end{aligned}$$

Setting the partial derivatives with respect to a_1^+ , b_1^+ , and c_1^+ equal to zero, we get

$$\frac{\partial F}{\partial a_1^+} = 0 \rightarrow \frac{\lambda a_1 \pi}{4} + \frac{c_1 \pi}{4} + \frac{1}{2} (b_1 - b_2) = 0;$$

$$\frac{\partial F}{\partial b_1^+} = 0 \rightarrow a_1 + \frac{b_1 \pi}{2D_1} + \frac{c_1}{D_1} + \frac{a_2 - a_1}{2} = 0; \quad (12)$$

or

$$\frac{b_1 \pi}{2D_1} + \frac{c_1}{D_1} + \frac{a_1 + a_2}{2} = 0; \quad (13)$$

$$\frac{\partial F}{\partial c_1^+} = 0 \rightarrow a_1 \frac{\pi}{4} + \frac{b_1}{D_1} + \frac{c_1 \pi}{4D_1} = 0. \quad (14)$$

From (13) and (14) we obtain the relationships

$$\left. \begin{aligned} c_1 &= -D_1 a_1 - \frac{4b_1}{\pi}; \\ b_1 &= \frac{D_1 \pi (a_1 - a_2)}{\pi^2 - 8} \end{aligned} \right\}. \quad (15)$$

We obtain similarly from the partials with respect to b_2^+ and c_2^+ :

$$\left. \begin{aligned} c_2 &= -D_2 a_2 + \frac{4b_2}{\pi}; \\ b_2 &= \frac{D_2 \pi (a_1 - a_2)}{\pi^2 - 8} \end{aligned} \right\}. \quad (16)$$

By substituting (15) into (12), and (16) into the equation resulting from setting $(\partial F / \partial a_2^+) = 0$, we get the simultaneous equations

$$\left. \begin{aligned} \left[D_1 + \frac{2(D_1 + D_2)}{\pi^2 - 8} - \lambda \right] a_1 - \frac{2(D_1 + D_2)}{\pi^2 - 8} a_2 &= 0; \\ -\frac{2(D_1 + D_2)}{\pi^2 - 8} a_1 + \left[D_2 + \frac{2(D_1 + D_2)}{\pi^2 - 8} - \lambda \right] a_2 &= 0 \end{aligned} \right\}. \quad (17)$$

The smaller eigenvalue is

$$\left. \begin{aligned} \lambda &= \frac{D_1 + D_2}{2} + \beta - \sqrt{\left(\frac{D_1 - D_2}{2} \right)^2 + \beta^2}, \\ \text{where} \\ \beta &= \frac{2(D_1 + D_2)}{\pi^2 - 8} \end{aligned} \right\}. \quad (18)$$

When $D_2 = D_1(1 + \epsilon)$, we obtain, through terms of $0(\epsilon^2)$,

$$\lambda = D_1 \left(1 + \frac{\epsilon}{2} - \frac{\epsilon^2}{17.1} \right), \quad (19)$$

which may be compared with the exact expansion through $0(\epsilon^2)$ given in (11).

Considerably more computation was required than for the conventional variational method with $\sin x$ as a trial function. Comparable accuracy can be obtained by choosing $(\sin x + b \sin 2x)$ as a trial function with b as a free parameter in the conventional formulation. In more practical problems, however, the times required to generate second trial functions outweigh the extra computation time.

IV. THREE-DIMENSIONAL MULTICHANNEL SYNTHESIS

Let $\{\phi_m^+\}$ and $\{\phi_m\}$, $m = 1, 2, \dots, M$, be precomputed two-dimensional adjoint and direct flux distributions. Each element of these sets has a component at every (x, y) point of a two-dimensional grid. We partition the (x, y) plane into disjoint channels: $n = 1, \dots, N$. We superimpose a grid on the z axis:

$$z_i = \sum_{j=1}^{i-1} h_j,$$

where h_j are the increments of this grid.

We choose as the three-dimensional trial functions for the variational synthesis computation the following functions:

$$\left. \begin{aligned} \psi^+(x, y, z) &= \left[\begin{aligned} \phi^+(x, y, z) &= \sum_{m(z)} a_m^+(x, y, z) \phi_m^+(x, y) \\ \underline{J}^+(x, y, z) &= \sum_{m(z)} \underline{b}_m^+(x, y, z) \phi_m^+(x, y) - C_m^+(x, y, z) D_m^+(x, y) \nabla \phi_m^+(x, y) \end{aligned} \right] \\ \psi(x, y, z) &= \left[\begin{aligned} \phi(x, y, z) &= \sum_{m(z)} a_m(x, y, z) \phi_m(x, y) \\ \underline{J}(x, y, z) &= \sum_{m(z)} \underline{b}_m(x, y, z) \phi_m(x, y) - C_m(x, y, z) D_m(x, y) \nabla \phi_m(x, y) \end{aligned} \right] \end{aligned} \right\} \cdot (20)$$

These expressions need clarification. The z -axis is partitioned into a set of "trial-function zones," and within each zone a subset $\{m(z)\}$, of the indices $\{m\}$ of the base direct- and adjoint-fluxes, is designated. These zones intersect on planes midway between mesh points.

We define the domains

$$\begin{aligned}
 &G_{ni} \left\{ x, y, z \mid \left(z_i - \frac{h_{i-1}}{2} \right) < z < \left(z_i + \frac{h_i}{2} \right) \text{ and} \right. \\
 &\quad \left. (x, y) \text{ ranging over all points in channel } n \right\}; \\
 &G'_{ni} \left\{ x, y, z \mid z_i < z < (z_i + h_i) \text{ and} \right. \\
 &\quad \left. (x, y) \text{ ranging over all points in channel } n \right\}. \tag{21}
 \end{aligned}$$

The vector coefficients $\underline{b}_m^+$ and $\underline{b}_m$ in Eq. (20) have components along each coordinate axis:

$$\underline{b}_m^+ = b_{mx}^+ \underline{e}_x + b_{my}^+ \underline{e}_y + b_{mz}^+ \underline{e}_z; \quad \underline{b}_m = b_{mx} \underline{e}_x + b_{my} \underline{e}_y + b_{mz} \underline{e}_z.$$

All coefficients in Eq. (20) except for b_{mz}^+ and b_{mz} are chosen to be fixed over each domain G_{ni} . The coefficients b_{mz}^+ and b_{mz} are fixed over each G'_{ni} . This choice is made so as to yield a three-point difference representation of the axial diffusion. The subscripts "ni" designate the coefficients in these domains. For example,

$$a_{mni} = a_m(x, y, z) \text{ for } (x, y, z) \in G_{ni}.$$

The energy-group index has been suppressed thus far, and the index g will be used for energy dependence. Thus, the flux for group g is

$$\phi^g(x, y, z) = \sum_{m_i} a_{nigm} \phi_m^g(x, y, z) \in G_{ni}. \tag{22}$$

$$\left(\text{We replace } m(z) \text{ by } m_i \text{ for } z \in \left[\left(z_i - \frac{h_{i-1}}{2} \right), \left(z_i + \frac{h_i}{2} \right) \right] \right).$$

If we choose to replace ϕ_m^+ by ϕ_m throughout this analysis, we reduce the computational effort by a considerable amount. Relative merits of various alternatives for base trial function may best be evaluated by numerical studies.

The stationarity equations for the function of Eq. (5) with trial functions of Eq. (20) yield a system of linear equations in the free parameters. These equations are not difficult to derive, but the algebra is tedious and the equations involve many terms. The details may be found in Ref. 6.

For each value of i , we may solve the stationarity equations for $\{b_{mi}\}$ and $\{c_{mi}\}$ in terms of the $\{a_{mi}\}$ as in Section III. Stationarity

with respect to $\{\delta a_{mi}^+\}$ then yields nodal difference equations of the form

$$\Lambda_i a_i + L_{zi} a_i - L_{zi+1} a_{i+1} - L_{zi-1} a_{i-1} + P_i a_i = 0, \quad (23)$$

where a_i is a vector with components

$$a_{nm_i g}, \quad \begin{aligned} n &= 1, 2, \dots, N; \\ m_i &= 1, 2, \dots, M_i; \\ g &= 1, 2, \dots, G. \end{aligned}$$

The matrices of order $N \times M \times G$ in Eq. (23) are

$$\begin{aligned} L_z & \text{ (from axial leakage);} \\ P_i & \text{ (from radial leakage);} \\ \Lambda_i & \text{, the non-diffusion contribution.} \end{aligned}$$

The elements in these matrices are given in Ref. 6.

V. APPLICATION TO THE DEPLETION PROBLEM

In this section we present a variational procedure for analyzing the depletion equations, and show that the procedure can be coupled in a convenient manner (in that many integrals that have to be evaluated for the depletion equations have to be evaluated anyway) to the multichannel synthesis procedure presented in Section IV. The coupling of these procedures may therefore prove to be quite useful in life studies.

A. The Depletion Equations

We define the isotopic density vector as

$$\underline{N}(r, t) = \begin{bmatrix} N^1(r, t) \\ N^2(r, t) \\ \vdots \\ N^i(r, t) \\ \vdots \\ N^I(r, t) \end{bmatrix}, \quad (24)$$

where i is the isotope index and r is a generalized space coordinate. Over each depletion step, we assume known constant fluxes:

$$\phi(r, t) = \sum_m \alpha_m(r, t_0) \phi_m(r); \quad t_0 \leq t \leq t_1. \quad (25)$$

Time intervals are chosen sufficiently small to allow this hypothesis with acceptable loss of accuracy.

We obtain from 2-D life-studies for various reactor elevations and control rod configurations a set of isotope distributions:

$\underline{N}_j(r)$; $j = 1, 2, \dots, J$. The index 1 denotes the initial composition, so that $\underline{N}(r, 0) = \underline{N}_1(r)$.

Having computed fluxes at time t_0 , we wish to estimate $\underline{N}(r, t_1)$, and for this purpose we use the approximation

$$\underline{N}(r, t) = \sum_{j=1}^J \beta_j(r, t) \underline{N}_j(r); \quad t_0 \leq t \leq t_1. \quad (26)$$

We choose β_j to be constant over each depletion region consisting of a specified axial segment of a channel:

$$\beta_j(r, t) = \beta_{jn}(d, t). \quad (27)$$

For each depletion region, we have an equation of the form

$$\frac{d \left(\sum_{j=1}^J \beta_{jn}(d, t) \underline{N}_j(r) \right)}{dt} = -A(r, t_0) \sum_j \beta_{jn}(d, t) \underline{N}_j(r); \quad t_0 \leq t \leq t_1. \quad (28)$$

The assumption of constant flux over the time step is evidenced by the constant-coefficient matrix $A(r, t_0)$ rather than $A(r, t)$.

To evaluate the free parameters $\beta_{jn}(d, t)$, we require adjoint isotope distributions, which we denote by the set of row vectors $\{\underline{N}_j^+\}$. In order to ascertain the form of these adjoints, we first develop the variational formalism by means of which the β_{jn} will be determined.

Consider the functional (utilizing boundary terms as in Ref. 5)

$$\begin{aligned} F[\underline{N}^+, \underline{N}] = & \int_{t_0}^{t_1} \left\{ \frac{1}{2} \left(\underline{N}^+ \cdot \frac{\partial \underline{N}}{\partial t} - \frac{\partial \underline{N}}{\partial t} \cdot \underline{N} \right) + \underline{N}^+ \cdot A \underline{N} \right\} dt \\ & - \frac{1}{2} \left[\underline{N}^+(t_1) \cdot \underline{N}(t_1) + \underline{N}^+(t_0) \cdot \underline{N}(t_0) \right]. \end{aligned} \quad (29)$$

The variation in F resulting from a change in $\underline{N}^+$ is obtained by noting that

$$\int_{t_0}^{t_1} \left(-\frac{\partial \underline{N}^+}{\partial t} \cdot \underline{N} \right) dt = -\underline{N}^+(t_1) \cdot \underline{N}(t_1) + \underline{N}^+(t_0) \cdot \underline{N}(t_0) + \int_{t_0}^{t_1} \underline{N}^+ \cdot \frac{\partial \underline{N}}{\partial t} dt,$$

so that

$$F[\delta \underline{N}^+, \underline{N}] = \int_{t_0}^{t_1} \delta \underline{N}^+ \cdot \left(\frac{\partial \underline{N}}{\partial t} + A \underline{N} \right) dt - \delta \underline{N}^+(t_1) \cdot \underline{N}(t_1). \quad (30)$$

If $\delta \underline{N}^+(t_1) = 0$ and $\underline{N}$ satisfies the equation

$$\frac{\partial \underline{N}}{\partial t} + A \underline{N} = 0, \quad (31)$$

then F is stationary with respect to changes in $\underline{N}^+$.

Similarly, we find that

$$F[\underline{N}^+, \delta \underline{N}] = \int_{t_0}^{t_1} \left(\frac{\partial \underline{N}^+}{\partial t} - \underline{N}^+ A \right) \cdot \delta \underline{N} dt - \underline{N}^+(t_0) \cdot \delta \underline{N}(t_0),$$

or that the functional is stationary with respect to perturbations in $\underline{N}$ when $\delta \underline{N}(t_0) = 0$ and $\underline{N}^+$ satisfies the equation

$$\frac{\partial \underline{N}^+}{\partial t} - \underline{N}^+ A = 0. \quad (32)$$

We thus see that the initial-value problem of finding the isotopic densities which satisfy Eq. (31) is adjoint to the final-value problem for $\underline{N}^+$ given by Eq. (32). The matrix A is not symmetric, so the adjoint problem is not the same as the direct problem with time reversed. We now attempt to find out how to choose adjoint trial functions.

The solution to Eq. (31) is

$$\underline{N}(r, t) = \exp \left[- \int_0^t A(r, t) dt \right] \underline{N}(r, 0), \quad (33)$$

and for any small time interval over which $A(r, t) = A(r, t_0)$ we have

$$\underline{N}(r, t) = e^{-A(r, t_0)(t - t_0)} \underline{N}(r, t_0). \quad (34)$$

Isotopic depletion is such that the eigenvalues of A are distinct, and

$$A = J^{-1} \Lambda J, \quad (35)$$

where Λ is a positive diagonal matrix and J is real. We obtain from (34) and (35),

$$\underline{N}(r, t) = J^{-1}(r, t_0) e^{-\Lambda(t-t_0)} J(r, t_0) \underline{N}(r, t_0)$$

and

$$\left[J(r, t_0) \underline{N}(r, t) \right] = e^{-\Lambda(t-t_0)} \left[J(r, t_0) \underline{N}(r, t_0) \right]. \quad (36)$$

The solution to Eq. (32) is

$$\underline{N}^+(r, t) = \underline{N}^+(r, t_1) e^{-\int_t^{t_1} A(r, t) dt},$$

and for any small time interval over which $A(r, t) = A(r, t_0)$ we have

$$\underline{N}^+(r, t) = \underline{N}^+(r, t_1) e^{-A(r, t_0)(t_1-t)}, \quad (37)$$

and

$$\underline{N}^+(r, t) = \underline{N}^+(r, t_1) J^{-1}(r, t_0) e^{-\Lambda(t_1-t)} J(r, t_0),$$

or

$$\left[\underline{N}^+(r, t) J^{-1}(r, t_0) \right] = \left[\underline{N}^+(r, t_1) J^{-1}(r, t_0) \right] e^{-\Lambda(t_1-t)}. \quad (38)$$

We observe from Eq. (36) and (38) that $(\underline{N}^+ J^{-1})^T$ and $J \underline{N}$ are the same except for time reversal, if we use the boundary condition

$$\left[\underline{N}^+(r, t_1) J^{-1}(r, t_0) \right]^T = \left[J(r, t_0) \underline{N}(r, t_0) \right],$$

where the transpose is required on the left-hand side to convert the adjoint row vector into a column vector. We obtain from the above equation

$$\underline{N}^+(r, t_1-t) = \left[J^T(r, t_0) J(r, t_0) \underline{N}(r, t) \right]^T. \quad (39)$$

In other words, the functions $J \underline{N}$ and $(\underline{N}^+ J^{-1})^T$ are the same except for time reversal. We therefore define the adjoint base trial function

$$\underline{N}_j^+(r) = \left[J_j^T(r) J_j(r) \underline{N}_j(r) \right]^T. \quad (40)$$

B. Depletion Matrices

The adjoint trial function for $t \in (t_0, t_1)$ is

$$\underline{N}^+(r, t) = \sum_{j=1}^J \beta_j^+(r, t) \underline{N}_j^+(r). \quad (41)$$

If we assume that the direct and adjoint solutions at t_1 are well represented by approximations of this form, then we may fix

$$\beta_j^+(r, t_1) = \beta_j(r, t_0),$$

so that in Eq. (30) $\delta \underline{N}^+(r, t_1) = 0$, and stationarity of the integrand of the functional yields the set of equations

$$\int dr \underline{N}_k^+(r) \cdot \left(\frac{\partial \underline{N}(r, t)}{\partial t} + A(r, t_0) \underline{N}(r, t) \right) = 0. \quad (42)$$

By substituting Eq. (26) into Eq. (42) and integrating over the depletion region in Eq. (27) over which

$$\beta_j^+(r, t) \text{ and } \beta_j(r, t)$$

do not vary with r , we obtain

$$\sum_{j=1}^J \left[\left(\int_{r \in n, d} \underline{N}_k^+(r) \cdot \underline{N}_j(r) dr \right) \frac{\partial \beta_{jn}(d, t)}{\partial t} + \left(\int_{r \in n, d} \underline{N}_k^+(r) \cdot A(r, t_0) \underline{N}_j(r) dr \right) \beta_{jn}(d, t) \right] = 0; \quad k = 1, 2, \dots, J; \quad t_0 \leq t \leq t_1. \quad (43)$$

We define matrices ρ_{nd} and $\theta_{nd}(t_0)$ of order $J \times J$ by:

$$\rho_{nd} \equiv [\rho_{kj}]_{nd}; \quad \rho_{kj} = \int_{r \in n, d} \underline{N}_k^+(r) \cdot \underline{N}_j(r) dr \quad (44)$$

and

$$\theta_{nd}(t_0) \equiv [\theta_{kj}(t_0)]_{nd}; \quad \theta_{kj}^{nd}(t_0) = \int_{r \in n, d} \underline{N}_k^+(r) \cdot A(r, t_0) \underline{N}_j(r) dr. \quad (45)$$

We define the vector

$$\underline{\beta}_{\text{nd}} \equiv \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_J \end{bmatrix}_{\text{nd}} \quad (46)$$

Then the system of simultaneous Eqs. (43) becomes

$$\rho_{\text{nd}} \frac{\partial \underline{\beta}_{\text{nd}}(t)}{\partial t} + \theta_{\text{nd}}(t_0) \underline{\beta}_{\text{nd}}(t) = 0; \quad t_0 \leq t \leq t_1. \quad (47)$$

Equation (47) may be solved for $\underline{\beta}_{\text{nd}}$ at t_1 :

$$\underline{\beta}_{\text{nd}}(t_1) = \exp\left(-\rho_{\text{nd}}^{-1} \theta_{\text{nd}}(t_0)(t_1 - t_0)\right) \underline{\beta}_{\text{nd}}(t_0). \quad (48)$$

We note that the matrix ρ_{nd}^{-1} is not time-dependent and is computed initially from elements defined in Eq. (44). The matrix $\theta_{\text{nd}}(t_0)$ must be computed at the beginning of each depletion step. Elements of θ_{nd} and of Λ in Eq. (23) are closely related so that the variational depletion equations and the flux synthesis equations dovetail together. This is not unexpected in view of the consistent nature of the various approximations.

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COMMENTS ON COMPUTING

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Significances of Automation and Computing

Having had little to do with the computer simulation of nuclear reactions since I left the Los Alamos Scientific Laboratory in 1952, I found it most enlightening to listen to the speakers at this Symposium and learn of the advances made. Dr. Schaefer referred to the computer god in his address, implying it to be a golden calf, while a later speaker seemed to suggest that a computer god was better than many others. Those of you who have done such excellent work with computers may well resent handwavers like myself. Yet it seems to me of importance that your work be interpreted on a wider scale to see how it fits in with other conceivable applications of computers and, more generally, of automation. In this paper, I attempt a necessarily restricted gesture in this direction.

In a general sense the significance of the use of computers in any area is that it produces more energy than it consumes. The same may be said of many tools, and I consider systems of automation complexes of tools, which, properly used, should improve the lot of mankind. Some foolish people, especially those who consider themselves artistes, will decry technology although they use the printing press, the typewriter, radio, and television to do so. Seemingly, they do not realize that they are largely molded by the media generated by the toolmakers. So it is with automation. People will live different, if not better, lives because of automation.

One of the currently exciting and significant developments in the application of computers is their use to aid in medical diagnosis. This amounts to an attempt to make available to more doctors the results of observations and systematic research which they would otherwise either not learn about until later or perhaps not at all. In this sense computers will help to amplify the usefulness of research--to save our history. I think that this development will force a change in the education of doctors.

In this connection I observe that any glow of pride in accomplishments should not reach the point that we begin to claim complete knowledge or effectiveness. There is no complete medical history of any one individual for a period of even one week. Medical science rests on the division

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of people into subclasses each of which has the same state of well-being insofar as current knowledge is concerned. It is only possible to treat an individual as a member of a class; what computers may enable is the refinement of these classes as to diagnosis and treatment.

At The University of Wisconsin I proposed that we emulate the move toward use of computers in medicine by a pilot study of the usefulness of computers for advising students. Currently the adviser meets the student and, in discussion, decides the state of his academic conditions. This is diagnosis. The ensuing advice is treatment. The major difference in practice between advising and medical treatment is that the medical doctor has been trained, if not completely, at least at some length to do his job. The faculty adviser has not been trained or tested or licensed. Moreover, he is usually irresponsible in his attitude toward this task.

When a student appears in my office for advice, I warn him or her about the state of my ignorance. "In the few minutes I shall spend with you," I might say, "I will learn almost nothing about you. I do not know the precise requirements for graduation, so you will have to attempt to decipher the catalogue yourself. I will, however, sign any program you want to select, and I grant you authority to sign it for me if you do not wish to return. Beyond that I am willing to discuss your choices if you wish and to give whatever benefit there might be of my experience." You might say that this is a poor attitude. I agree. Every adviser I know of has some kind of poor attitude, the worst of which, I believe, is the presumption of knowledge where there is little. I do not intend to become a good adviser since that would occupy all my time. After a student accepts advice and subsequently fails, does the faculty adviser concern himself about the possibility that he gave poor advice, the better to advise another time? No! Does he pitch in to rectify his errors? No!

Here is a situation, then, which cries for automation, since the chance for improvement seems assured. However, universities are so enmeshed with the mass production of automata that the energy to improve the assembly line is often lacking. The easiest place to use computers for advice is the beginning graduate level, since the student usually has some explicit area of interest and the number of choices before him is comparatively small. One student I heard of was assigned a mathematics professor as an adviser. "I want to take statistics," said the student. "What is statistics?" answered the adviser. "You should study mathematics." While this might be good advice, the chances are that simple ignorance and pride on the part of the adviser were being displayed. Could we do worse by machine? Not without trying. The destruction of energy by poor advice must be enormous.

Concerning our education systems in general I might note that there are many who mouth words about freedom, liberty, and independence in connection with schooling. Education is primarily a form of thought and

action control, its objective is to produce partial automata--people who respond in an acceptably determined manner to most situations--people who have good habits. What freedom is accorded the child in school? Did he choose to go? Did he elect the courses, select the teacher, the materials? No! Society is determined to mold that presumably plastic material into an acceptable adult whether he or she chooses or not. By the time choices become available, the student is supposed to make most of them according to pattern, and the success of education may be measured largely by the automatic responses induced.

In closing this section let me observe that I have selected two examples of computer applications from very difficult areas. In neither medical diagnoses and treatment nor in advising is there a really well-developed theory which allows us to calculate decisions. These applications are a matter of collecting, collating, appraising, and storing information provided by people and making them available at the right time and place. In both areas people might be very much helped, but it is difficult to see how unemployment or other ills concomitant with automation would ensue. These ills are real, here and now, but they are primarily in the inertia of our social structure in comparison to the rapid change brought about by automation.

Mathematics and Computing

Mathematical models and mathematical systems are applied in many aspects of computing. Attempts to do mathematics by computers raise intriguing questions. Some persons have claimed that all mathematics could be done by computers, suggesting that the work of most mathematicians might be automated. Mathematicians, especially those who do not understand computing, often display their ignorance in answering such foolish statements. In this section I will discuss some aspects of these questions as well as point out the effect computers may well have on mathematics.

Someone once said that a million monkeys trained to use typewriters would sooner or later produce the complete works of Shakespeare. It is true that even one illiterate person might sit at a typewriter and type out a play. So it is with computing and mathematics. If the chain of symbols used in writing a theorem, a proof, or a definition indeed contains the item, then I can conceivably produce a comparable chain in the printer of the computer. Therefore, there is nothing which may be encoded in an alphabet which cannot be produced via computers. The central problem of computer usage in doing mathematical work is not, therefore, a problem of physical possibility; it is a question of feasibility. Is it feasible to produce mathematics by computers? Answers to the question are therefore time and machine dependent. It is easy to say that more and more mathematics will be done with the help of machines as time goes on. The kind of

mathematical work for which computers are now best adapted are precise manipulations of symbols with precise recall of formulas.

For example, it is now possible, using a computer to get the 50th derivative of a function which no ordinary mathematician would even care to attempt. In her Ph.D. thesis, Sister Mary Kenneth Keller recently showed that using a computer to establish a formula for the n th derivatives of a function is within reach for some functions. Future developments, not far off, will permit computers to generate formulas too lengthy and complicated for man to read, to say nothing of verifying them.

Professor D. L. Lehmer has used with colleagues a computer to establish a theorem in number theory which he states is inaccessible to direct human proof. This example is what we should expect to see. The computer, like other tools, amplifies our capacity to do work. Does Professor Lehmer believe that the number theory has been degraded? On the contrary, he may well be proud of accomplishment. What has also been demonstrated, then, is that certain information will be made available that was impossible before computers. Astronomers benefit by telescopes, cameras, and spectrosopes; biologists by microscopes, centrifuges; and so on. Why shouldn't mathematicians have some tools besides chalk and pencil?

There are mathematicians, of course, who feel that computing is very specialized and is of little use to them. What they may fail to see is that by making demands on certain types of mathematics, computers will force change in mathematical activity. As a matter of fact, computers have made changes in mathematical emphasis--witness the linear programming, dynamic programming, automata theory, control theory, numerical approximation being developed by mathematicians appreciative of the use of computers.

I do not wish to dwell on those aspects which would be obvious by classifying mathematicians by interests today as compared to 1950; I wish instead to bring up another feature. The presence of computing demands more general mathematics!

If I consider the applicability of mathematics to discourse concerning activities and objects of interest, I find that there are two kinds of reasons why mathematics may not apply. One is that while an available mathematical model is adjudged adequate to embrace the phenomena, the theory fails to provide the desired information. For example, a system of differential equations with appropriate side conditions may theoretically imply what is needed. Perhaps the theory will directly state that the solution exists and is unique, but perhaps it will be impossible now to find out if the solution is bounded.

The second cause of inapplicability of mathematics is that the scope of mathematical systems does not embrace the phenomenon in question. In other words, mathematics may fail partially because it lacks generality! You may find this statement rather unpalatable. Haven't mathematicians exceeded the bounds of good taste or of reasonableness with their pursuit of abstraction? What about set theory, abstract algebra, topology, measure theory, and infinite-dimensional spaces? Despite these and many others, I say mathematics is insufficiently general to describe many phenomena. Moreover, I say that if we are to implement effectively the doing of higher-level mathematical labor by machine, we need a theory which systematizes mathematical theories.

I have been frequently distressed in my work to find that concepts which I was told were of primary importance, by my mathematics teachers and my colleagues, would not apply in computing or numerical analysis. For example, let me take the topological concepts of neighborhood, limit point, continuity, and connectedness. Why is it that these do not apply to computer language and operation? The answer is that they are too restricted in scope by the usual framework in which they appear in mathematics.

In the time you might wish to spend I cannot give details, but I wish to survey briefly the results of my study of continuity in intuitive terms. In topology and analysis it would be nonsense generally to speak of a continuous transformation from one set to another if both were finite (i.e., contained a finite number of elements). In computing, however, there is a transition from one state to another state, both of which may be considered finite sets. Why should not "continuity" apply to such transformations?

Since 1951 I have repeatedly returned to the consideration of continuity. I have generalized the concept from topology repeatedly, each time feeling not too satisfied. On the fifth stage of generality beyond topology I got a definition I can use in computing, but it is still less general than that given in the dictionaries!

A transformation is continuous with respect to the properties or relations it preserves; this is roughly what I have concluded. For an example embracing continuity and approximation let me suppose that I have a translation of a story of de Maupassant from French into English. The translation is an approximation to the original. If you say the translation is good, then I say you have said that the mapping (on translating) was continuous because it preserved the important features. If someone else says the translation is inadequate, then the mapping is not continuous--to him. These considerations are important, of course, in the attempted computer translation of languages. However, my theory does not embrace the above common language generality. Algebraic homomorphisms are included as are relation-preserving maps.

In the system I have been studying, which I call extended topology, I have found that most concepts generalize and, pleasantly enough, so also do many results. In order to be of optimal use in computing, it is necessary that extended topology also include the possibility of applying to itself even as a language is used in discussing a language.

If you should worry about finite sets, let me discuss that notion. In order to avoid dealing with the tremendous amount of information present in physical realization of surfaces, it was necessary to discard it and have the comparatively information-free planes, lines, and so on, of Euclidean geometry. The interpretation of a plane as an infinite set of points is very practical. However, no one has ever written but a few words about planes. If I am to do mathematical work with a computer, I again use only the finite number of finite states available. My theory must apply to those, and to languages, since these are our primary modes of communication.

Let me give a few overtones of continuity. What is there about you which is unchanged in an interval of one year? It is what the transformation of time has not changed. It is what is continuous in the time mapping. Invariance and continuity are two sides of the same coin! Why do we prize our names? Is it because these are invariant in time and hence give us something to attach to ourselves?

The scientists search for laws which do not change in time, the religious man searches for unchanging truths and/or beings, and so on. The "mapping" from the universe to a physical theory is continuous if it preserves the essential features. Einstein made the mapping more continuous by his relativity theory.

In conclusion, let me draw another analogy. A computer may be likened to a very fast-writing pen, with a long piece of paper and a precision memory. If we can but learn well how to write, we will be able to use our intelligence much more fruitfully. I predict that within 20 years most of the best mathematicians will be using computers necessarily.

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SESSION III

LINKED CALCULATIONS

Tuesday, May 18, 1965

CHAIRMAN: B. H. Mount
Bettis Atomic Power Laboratory

CO-CHAIRMAN: Peter Struch
Reactor Centrum--The Netherlands

SCIENTIFIC SECRETARIES: Dorothy Bingaman
Bert Toppel
Argonne National Laboratory

USE OF DIGITAL PROGRAMS IN REACTOR PLANT DESIGNS

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(Paper presented by H. E. Stevens, Jr.)

Introduction

Physicists and engineers commonly have been confronted with the task of integrating several technologies into efficient, balanced designs of nuclear power systems which operate ever nearer to the materials limits, yet maintain an exceedingly high degree of reliable performance. Detailed digital programs have already been developed for most of the individual technologies but the manual integration of these digital programs has stifled progress, limited the degree of perfection, and required extensive managerial coordination of design personnel.

This situation demands an integration and a mechanization of the analytical methods. Three avenues of approach to the problem are available:

1. By accumulating the output of one program as input to a succeeding program, these programs can be iterated until all reactor and plant variables have been stabilized.
2. Each of these specific programs can be successively chain loaded into the computer, thus eliminating the need for the transmission of data from one to the next.
3. A new, single program can be designed which would use the features of each of the detailed programs, in a less detailed sense. The individual specific programs can be retained and used to correct, update, or improve the master program.

The first approach (see Fig. 1) is the least desirable of the three, in that the manual handling and transmission of data from one program to the next introduce great chance for human error. It would require the most man-hours of effort per problem and result in unreasonable time delays before completion.

*Operated by General Electric Company for U.S. Atomic Energy Commission.

Fig. 1. Concept No. 1

At the present time, it does not appear that the second method (see Fig. 2) can be ultimately automated to the extent where the master program and each of the specific programs could exist in "chain-loaded" form, since a large degree of human judgment is involved in deciding when to look at certain areas of the overall design in more detail. Furthermore, so many different technical disciplines are involved in the engineering design and analysis of an overall reactor plant system that the technical maintenance of such a huge program would not be feasible.

The master program (see Fig. 3), which recognizes the features of all of the specific programs in a limited form but combines all of the reactor and power plant variables into one overall control program, is clearly the best approach. Such a program has been developed and, when used in conjunction with the existing detailed programs, can be shown to be a successful tool in the design and evaluation of an entire reactor and power plant. It is the purpose of this paper to describe this master program and show how the mechanization and technical integration have been accomplished.

Relationship of Master and Satellite Programs

The master program and satellite programs complement, calibrate, and extend each other (see Fig. 4). The master program is a transient program which provides the interdependency, often called "feedback," of integral models of several of the specialized programs. The specialized programs, which are mostly quasi-steady-state or open loop, provide greater detail within a component and provide a standard for calibrating and determining the adequacy of the integral model. An example of some of these specialized programs follows.

A pressurizer transient analysis program is used to study, in detail, the behavior of a coolant-system pressure controller under various steady-state and transient conditions. For a given set of operating conditions, this program calculates and edits pressure, mass, energy, and volume changes as a function of time. This type of program can be used to set and modify the design coefficients of the pressurizing device in the master program.

A program to study the interaction between the pressurizing device and the primary coolant system is used to study the behavior of the coolant system for various conditions. This program can also be used to study and evaluate any void models developed for the coolant system.

The heat exchangers (boilers) which perform the coupling between the reactor and the power plant are analyzed in detail by several programs. One program evaluates the steady-state two-phase circulation ratio and drum levels for various steam rates. This program can be used as a design tool for optimum sizing in preliminary design studies and for performance calculations once the design has been established.

Fig. 2. Concept No. 2

Fig. 3. Concept No. 3

Fig. 4. Relationship of Master and Satellite Programs

Another program is used to calculate the steady-state and transient water level in a boiler using mass, momentum, energy, and volume equations.

An automatic feedwater-control system is also provided for in the calculations.

The evaluation of the steady-state performance of a power plant for single or balanced multiloop operation can be handled by a single program when several specific types of plant operation are considered. Primary loop temperatures, loop flows, secondary steam temperatures, and secondary side pressures can be calculated for the various operating conditions.

Flow and temperature conditions in any network of flow paths and junctions can also be calculated in a separate program. The flow paths can be within a reactor, primary system, secondary system, or any component being studied in detail. A pressure drop can be calculated for each flow path by means of one-dimensional hydraulic equations, and flow and heat balances can be performed for each junction. This program uses an initial estimate of flows with a given heat distribution and iterates to a solution.

The temperature and power-level transients of a reactor resulting from fast reactivity insertions or removals are calculated by an open-loop program which studies one typical channel of the reactor in detail. Reactivity insertions and removals, as studied by this program, involve motions of control elements, temperature changes at the reactor inlet, and in-core temperature changes resulting from the temperature feedback effect. Since this is an open-loop program, no feedback from the secondary system is considered.

The number of axial and radial nodes in the fuel element and coolant channel can be variable, depending upon the detail required in the study.

A detailed study of reactor thermal and hydraulic behavior can be performed with an open-loop reactor transient analysis program. This program is designed to evaluate reactor behavior for the following types of transients:

1. variations in flow;
2. removal or insertion of reactivity;
3. changes in temperature at the reactor inlet;
4. variations in system pressure;
5. any combination of the above.

In addition to the study of reactor behavior, a safeguards analysis (reactor safety) is provided at each time step during the transient. This

evaluation is based on the behavior of one or more hot channels. In this program, the reactor core is represented by one nominal channel and several hot channels. Single or multipass cores can be analyzed, and several radial nodes can be used in the fuel-element model to permit an accurate representation of the fuel-element temperature distribution during the transient.

Calculations are based on known nominal inlet temperature and flows for the channel and the total pressure drop across this channel as a controlling item. Nominal and hot-channel axial flow and enthalpy profiles as well as reactor power are determined as a function of time.

This program can be used in conjunction with the master program to check the thermal and hydraulic equations representing core regions and to verify hot-channel performance with more accurate energy, momentum, and continuity equations.

The programs which can be used to adjust pressure drop and channel flow obtain operating parameters from the master program and then perform the calculations. The new information is then used in the master program to study the effects on the entire system. These programs emphasize core detail over physics and transient thermal-hydraulic capabilities.

Related studies involving the master program can be performed with two shielding programs to optimize the positions of nuclear sensing devices in the primary shield of the reactor by means of physics information from the large neutron-diffusion programs, and flow and temperature data within the reactor from the master program, the shielding programs determine the attenuated neutron flux at various points outside the reactor pressure vessel. Optimum placement of the detection and sensing devices, such as ion chambers, can be determined for various reactor operating conditions throughout the life of the core.

The resulting neutron attenuations calculated in these programs can then be used in the master program to evaluate new indicated power levels.

Physics data for the master program are supplied by the large neutron-diffusion programs used in the nuclear design of the reactor core. These programs can mock-up the core as a 2-dimensional grid of calculation points (up to 20,000 points for an xy plane or 6000 points on a rz plane). Three-dimensional information can be obtained by synthesizing programs which splice various xy planes, using rz information, into a 3-dimensional simulation of the core.

From these nuclear design programs, the master program can obtain core power distributions, reactivity coefficients, core coupling coefficients, and lifetime variations of all of the above.

Description and Use of the Master Program

By now the reader must have some insight to the composition and development problems of a single master computer program. It must be big enough to calculate the performance of a whole reactor and power plant; small enough to run fast at low cost; flexible enough to keep up with progress; simple enough for engineers to use with confidence; detailed enough for the most ardent specialist; concise enough to yield information with a minimum amount of output; reliable enough that one dropped bit won't ruin the whole night's production.

The master computer program achieves flexibility in three ways. For the first, a wide variety of plant models can be handled. By this means, it is not only possible to study several distinct systems, but a single system can be mocked up in ways which emphasize the features of immediate interest. Tomorrow, when attention is directed at another problem, the model will be changed to focus on the new area. The second type of flexibility comes from the use of many options. These range all the way from minor changes in the amount of information to be printed as output, to insertions or eliminations of whole sections of the calculation. The adroit combination of new models with unusual options, and perhaps a small patch or two, has enabled ingenious engineers to study a wide variety of conditions. Much work has been done on short studies of special features, where brevity of the task would not warrant a new program, and it has indeed been fortunate that the versatility was available. New features can be added and obsolete ones deleted.

In addition, a number of special calculations can be activated at the user's option. For example, a channel which is suspected of running abnormally hot can be modeled in greater detail than usual and extra calculations performed for it. Several of these "hot" channels can be included in a single run. As another example, several different protective systems can be built into the program with rather elaborate detail.

A master program of such large scope will be complex and unwieldy unless a determined effort is made to make it manageable. Such an effort goes on continuously and has produced a number of novel features. The first of these was not just a modification of the transient program, but was a completely new program virtually identical which computes only steady states. By eliminating all the calculations of time-varying parameters, it is possible to compute a great many steady-state conditions in the time needed for a single transient. Consequently, parameter surveys can become normal production. A second purpose is to get starting values for the transient program. While the transient program will zero in, of course, on initial conditions all by itself, this is a waste of machine time when the steady-state program is around. The program architects have taken great care to make these programs compatible with each other, with a corresponding easing of the strain on the user. For example, the input decks for

the two programs are identical insofar as the inherent differences of the calculations will permit.

The second user-oriented feature is a restart capability. At any time during the course of a solution, the transient program can be asked to write its data onto a tape; several such writeouts can be made during a single run. At some later time, the program can be told to read these data and continue with the solution. However, when the problem is restarted, the user may make numerous changes, and in this way a single base run may be used as the springboard to several subsidiary runs. For example, if an engineer wants to see the effect of an abnormal transient, he runs the normal transient, writing for restart at four or five places along the way, and he then calls for the abnormal occurrence (equipment failure) and restarts from each place. In this way, he can find out where the worst time for the abnormal equipment operation is, with only a single running of the base transient.

How much output should the master program generate? A single run can easily produce several thousand 11- by 13-in. pages, but this practice is not recommended. Excessive output means more than just wasted paper, wasted machine time, and wasted storage space. It means the engineer has to wade through mountains of data to find the few numbers he wants, and it means he will have a hard time assimilating the big picture. The program has three kinds of output. The first is a "short form," which prints only the major plant variables and is complete on one page. The "long form" adds two or three pages of detail to the short form. The frequency of printing both forms is under the user's control. Commonly, however, both of these edits are almost completely suppressed in favor of the third output type, which is graphical. Eight or ten curves are drawn on a sheet, and up to 8 such sheets can be plotted. A curve sheet for even a moderately long problem can be printed on two pages, so a complete transient, with enough detail to satisfy almost everybody, can be edited in fewer than 25 pages.

In order to describe the analytical model adequately, a large input deck is required. The large number of cards becomes inconvenient to transport to and from the computer, and the possibility of having a card out of place is quite high. To solve this problem, models are read onto a model tape as soon as they are created. The user calls for the model he wants by a single card, and once the model on the tape has been checked out, there need be no more fear of its becoming garbled. The input deck then consists largely of title cards, option cards, and initial operating conditions, such as power, temperature, and flow.

A program with the power of the master program would lose much of its effectiveness if it cost too much to use. High cost can come from many sources, including expensive input preparation, errors requiring reruns, and long searches of voluminous data to find the significant facts.

Some of the action taken to reduce costs in these areas has already been described. Another major source of cost is the running time on the computer. Where time is worth several hundred dollars an hour, each minute is important.

One of the common causes of excess machine time is the indiscriminate use of magnetic tape as auxiliary storage. Reading data from core to tape and back again can be made to increase the running time by an order of magnitude with hardly any effort at all. In the master program the calculation is completely core contained. Tape is used only for input, output, and restarts, and by taking advantage of the curve-drawing feature even the output is held to a minimum. It has been possible to stay within core by careful programming to hold down the number of large arrays that have to be stored.

Another way to increase the machine time in a sequential calculation like the master program is to use microscopic time steps. It is obvious that using a time step of a thousandth of a second when a hundredth would do will raise the cost an order of magnitude. It should also be clear that the use of a hundredth of a second when a tenth would do can be just as expensive. It is well known that the time-step limit is governed by the fastest frequency or the shortest time constant in the system, and that a larger time step leads to calculational instability. Mathematical techniques which surmount this are used throughout the master program, so that time steps many times larger than the shortest time constant give both stability and accuracy.

Quite a number of less noticeable time savers are built into the master program. Conventional (but slow) subroutines, such as logarithm and exponential, are used very sparingly. All permanent mathematical relations, such as the density of water as a function of pressure and enthalpy, are fitted with very simple but sufficiently accurate expressions. Engineering approximations to the characteristics of the plant are sprinkled generously throughout the program. They range from a simplified version of the two-phase pressure-drop correlation to a four-node representation of a steam generator, and they conserve machine capacity as well as running time. The net result is that a typical full-scale transient calculation only takes 3 or 4 times real time, and there have been instances where real time was bettered.

In fact, the program is so fast that it is customary for the problems of a number of engineers using the same model to be stacked one after another and run as a single batch. This will minimize the number of times that the program and model tapes must be read. One bad card in such a stack, or one machine failure, could wreck all subsequent jobs. To circumvent this, each run in a stack is treated as an independent case. Should failure occur within a case, a routine is provided for recovery of the failed case by the operator. Otherwise, it is skipped and the machine moves on to the next one in the stack.

Application of Master Program Outputs to Reactor Plant Design and Performance Criteria (see Fig. 5)

The master program can solve a broad spectrum of reactor engineering transients. These include such problems as up and down power transients, control-element runaway, cold startup, and loss and recovery of flow. It is intended to answer questions on overall plant performance, such as locating the limits of capability of the system, evaluating the adequacy of safeguards, and determining which operating conditions are most severe. It is not intended to answer detailed questions on the design of components; instead, it generates data on coolant flow, temperature, pressure, reactor power, steam flow, control-element motion, excess reactivity, and other variables, which can be used as input to other more specific programs. Several examples follow.

All reactor channels are studied in detail to assure that satisfactory design margins are maintained to limiting thermal criteria and flow oscillations for all time intervals during specified limiting transient operational modes. The effects of channel geometry, power distribution, flow rate, pressure, and void distribution on limiting thermal criteria as determined from extensive analytical and experimental studies are compared to the master program outputs at critical time steps by use of detailed thermal and hydraulic programs.

Thermal test data are compared directly to hot-channel operating conditions to provide positive assurance of adequate design margins. Peak, central fuel-element temperature is determined for steady-state and transient conditions, and checks the margin to maximum allowable temperatures and time at maximum temperatures. Allowances are made for effects of crude deposits and corrosion products on pressure drop and heat transfer rates from hot-channel surfaces. Changes are made in fuel conductivity with depletion of fuel.

Flow oscillations in reactor channels may be studied by use of other programs. The margin to inception of flow oscillations in the hotter reactor channels is determined from a system of linearized continuity, momentum, and energy equations, together with perturbation theory to show the sensitivity of the oscillation margin to changes in channel geometry and flux distributions. The amplitude and frequencies of local channel-flow responses during power and flow transients are determined for limiting operational transients. Suitable design adjustments may be made in channel-flow restrictions and geometry to limit the oscillation amplitude or prevent oscillation inception as the designer requires. Time-variant reactor pressure drop and local channel power distributions from the master program are used as inputs for the oscillation analyses.

Fig. 5. Application of Master Program

Upper and lower pressure outputs from the master program are compared to relief valve settings to assure that adequate margins exist for all modes of operation without opening of relief valves.

Variables which determine the extent of moisture carryover from the steam generator to the turbine are compared to their limit values to show that carryover is maintained below safe design values for all transients. Similar programs are utilized to determine the extent of "hideout" of chemicals in the steam-generator regions.

Margins to flow inception in the steam generator are determined from linearized perturbation programs.

Conclusion

In conclusion, the master computer program described above has been used and upgraded over a considerable period of time.

A measure of the importance of the computer program is the amount of information obtained per block of computer time.

Using the concept of a master program, supported by individual studies on detailed specific programs, the mechanical, thermal, and hydraulic features of a reactor, primary system, and associated power plant can be evaluated for design and performance purposes at a fraction of the cost, in machine time, of performing the nuclear design.

METHODS FOR THE INTERPRETATION AND PREDICTION OF REACTOR POWER DISTRIBUTIONS WITH AN APPLICATION TO FUEL CYCLE CALCULATIONS

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SUMMARY AND CONCLUSION

Methods for the solution of the two-dimensional diffusion equations are discussed. The most elaborate method is an extension of the source-sink method to finite fuel channels, but this is reformulated in terms of the conventional finite-difference equations plus some extra terms. Results of sufficient accuracy for many purposes are, however, obtained in AGR situations from the third method, which solves the conventional finite-difference equations using one in-channel mesh point per lattice. As an application of this last method a program for studying fuel cycles in AGR is described.

INTRODUCTION

In the design of an AGR reactor, temperature limitations are placed both on the fuel and on its cladding material. Thus, if the reactor is to be designed to avoid violating these conditions, accurate estimates of the power distribution are required at all times during the life of the reactor. In all practical systems of calculation the normal breakdown of the calculation into two parts is made. The cell neutron spectra are first obtained from a lattice cell calculation with a reflective outer cell boundary. Few-group data for use in the reactor calculation are then formed by condensing reaction rates over the cell spectra.

In this paper we consider three methods of making these reactor calculations and discuss the application of the simplest of them to fuel-cycle studies. The most accurate method considered is the direct solution of the neutron-diffusion equations in the moderator with boundary conditions at the channel wall representing thermalization and absorption within the channel. The second method is an approximation to the fully heterogeneous method, in which the equations are converted to finite-difference form with one mesh point per channel and direct coupling between all mesh points. The third method is the conventional finite-difference solution, again using one mesh point per channel, but with coupling only to immediately adjacent channels.

Comparisons are then presented between calculational and experimental results for AGR situations, including the Windscale AGR commissioning core and small HERO cores. The first and second methods are shown to give answers which are virtually identical in a particular case, but the third method gives results which are satisfactory for many purposes when using only two groups of neutrons.

As an application of this latter method a two-dimensional fuel-cycle program is described. Appropriate channel-averaged data may be deduced from an (r, z) version and used in the (x, y) code. Radial and axial power shapes are thus deduced independently. The power shape is determined at each time step, and burnup proceeds with updating of the lattice data and re-evaluation of the power shape until fuel changes are necessary. The code may be used to study various schemes of fuel management, and many refuelling options are available. In one, automatic power shaping as well as criticality may be simulated by the movement of discrete absorbers, and the selection of channels for refuelling or shuffling is made by a variety of criteria.

Results from this code are presented for a typical AGR system, and the advantage in lifetime of a frequent change of fuel is demonstrated.

LATTICE CALCULATION

The ARGOSY⁽¹⁾ method of making lattice calculations was used in most of the calculation reported in this paper. The aim of this method is to use basic nuclear data and to represent physical effects as accurately as possible consistent with a rapid computation.

The normal cylindricalisation of the cell is made, and the calculation recognizes three different energy bands. In the thermal group (below 4 eV) reaction rates are determined by SPECTROX,⁽²⁾ using the generalised heavy gas (or HOROWITZ) approximation to treat thermalisation. Events in the fuel channel are treated by collision probabilities, and the spatial flux shape in the moderator is assumed to be of one-group form. With these approximations the equations are simplified to provide only mean values of fuel and moderator spectra, and reaction rates.

Resonance integrals (representing the range from 4 eV to 10 keV) are stored within the programme and interpolated as desired. In the fast group (above 10 keV) three subgroups are considered, and a collision-probability approach is again used to obtain a spectrum and permit condensation to one fast group.

Various options are available for controlling the three-group spectrum to represent a critical cell. The program, written for an IBM 7090, also provides data for controllers and reflector regions, and performs a point burnup calculation.

When data were required in more than three groups, a more generalised transport-theory treatment (TRACER⁽³⁾) was used.

BASIC THEORY

The key assumptions which one must make to render the calculation of the two-dimensional flux distribution in a heterogeneous reactor at all feasible are (i) that diffusion theory is used in the moderator with suitable "averaged" boundary conditions representing absorption, production, moderation, and scattering of neutrons within the fuel channels, and (ii) that the moderator cross sections and diffusion characteristics are constant throughout the entire moderator (except possibly for annular zones with uniform properties).

The early work of, for example, Feinsberg⁽⁴⁾ and Galanin⁽⁵⁾ simplified the problem by assuming a uniform infinite moderator. The fuel channels were replaced as far as fission was concerned by line sources which produced neutrons at a unique energy which "slowed down" according to a Fermi-age law.

The present work differs in that multigroup treatment is used in place of continuous slowing down, and boundary conditions at the actual channel walls are used in all groups. The work is divided into three sections: (a) the derivation of the heterogeneous equations as a set of simultaneous equations for the channel fluxes, (b) a reformulation of these equations of which the dominant terms are of conventional "finite differences" homogeneous type and "correction" terms which depend on more distant mesh points representing the heterogeneity effects, and (c) a discussion on the merits of various finite-difference schemes for the solution of heterogeneous reactors.

THE HETEROGENEOUS MULTIGROUP EQUATION

These equations form the basis of an IBM 7090 computer programme MAGPIE,⁽⁶⁾ which has been used for some time now in the interpretation of small, nonuniform cores such as HERO.

(i) Moderator Equation

One downscatter only is assumed, but since the theory is easily generalised, the moderator equations will be written in matrix form:

$$D\nabla^2\phi - \Sigma\phi = 0, \quad (1)$$

where ϕ is $\text{col}\{\phi_1, \phi_2, \dots, \phi_N\}$, D is $\text{diag}\{D_1, D_2, \dots, D_N\}$, and $\Sigma = \{\Sigma_{ij}\}$ is such that $\Sigma_{ii} = \Sigma_{\text{rem},i}$, $\Sigma_{ij} = -\Sigma_{i \leftarrow j}$. One can define a new flux Q by the transformation

$$\left. \begin{aligned} \underline{Q} &= C \underline{\phi} \\ \nabla^2 \underline{Q} &= \lambda \underline{Q} \end{aligned} \right\}, \quad (2)$$

where $\lambda = \text{diag}\{\lambda_1, \lambda_2, \dots, \lambda_N\}$, C being a square matrix whose rows are the eigenvectors of $(D^{-1}\Sigma)^T$ and $\lambda_1, \lambda_2, \dots$, the corresponding eigenvalues. Thus each component Q_j satisfies a one-group equation:

$$\nabla^2 Q_j = \kappa_j^2 Q_j \quad (\kappa_j^2 = \lambda_j). \quad (3)$$

In terms of $\underline{Q}$ it can be shown that in a cylindricalised cell of radius R the mean value of $\underline{Q}$ over the moderator is given by

$$\bar{Q}_m = \bar{Q}^\rho + X\rho \left(\frac{\partial Q}{\partial n} \right)_\rho, \quad (4)$$

where $(\partial Q / \partial n)_\rho$ is the mean gradient of $\underline{Q}$ at channel surface $r = \rho$, $\bar{Q}_\rho$ is the mean value of $\underline{Q}$ there, and $\underline{X} = \text{diag}\{X_1, X_2, \dots, X_N\}$, with

$$X_j = \frac{K_0(\kappa_j \rho) I_1(\kappa_j R) + I_0(\kappa_j \rho) K_1(\kappa_j R)}{\kappa_j \rho \{K_1(\kappa_j \rho) I_1(\kappa_j R) - I_1(\kappa_j \rho) K_1(\kappa_j R)\}} - \frac{2}{\kappa_j^2 (R^2 - \rho^2)}, \quad (5)$$

and it has been assumed that there is zero current at $r = R$.

Thus, in terms of the original flux $\underline{\phi}$, we may write

$$\bar{\phi}_m = \bar{\phi}^\rho + CXC_\rho^{-1} \left(\frac{\partial \phi}{\partial n} \right)_\rho. \quad (6)$$

(ii) Boundary Conditions

Assume that the flux near a channel is given by an expression

$$\phi_j(r) = \phi_j^{(0)}(r) + \phi_j^{(1)}(r) \cos(\phi - \alpha) + \text{higher angular terms}. \quad (7)$$

Then the boundary conditions are

Source-sink condition:

$$\left(\frac{\partial \phi_i^{(0)}}{\partial r} \right)_\rho = \sum_i \left(\alpha_{ij} + \frac{1}{k_{\text{eff}}} \beta_{ij} \right) \phi_j^{(0)}(\rho); \quad (8)$$

Dipole condition:

$$\left(\frac{\partial \phi_i^{(1)}}{\partial r} \right)_\rho = \lambda_i \phi_i^{(1)}(\rho), \quad (9)$$

where

$$\left. \begin{aligned} \alpha_{ii} &= \Sigma_{\text{rem},i}^{\text{ch}} V_{\text{ch}} \bar{\phi}_i^{\text{ch}} / 2\pi \rho D_m^i \phi_i^{(0)}; \\ \alpha_{ij} &= -\Sigma_{i \rightarrow j}^{\text{ch}} V_{\text{ch}} \bar{\phi}_j^{\text{ch}} / 2\pi \rho D_m^i \phi_j^{(0)}; \\ \beta_{ij} &= -\beta_i (\nu \Sigma_f)_j^{\text{ch}} V_{\text{ch}} \bar{\phi}_j^{\text{ch}} / 2\pi \rho D_m^i \phi_j^{(0)} \end{aligned} \right\}, \quad (10)$$

and the subscript ch denotes volume average within the channel and $\phi_j^{(0)}$ in the above formula is the $\bar{\phi}_j^{\rho}$ determined from Eq. (6) using the ARGOSY values of $\bar{\phi}_j^{\text{m}}$ and $(\partial \phi_j / \partial n)_{\rho}$. This ensures that the correct reaction rates in the moderator and fuel will be present in the diffusion-theory cell model. In fact, the detailed moderator fine structure is also accurate to within one or two per cent in typical AGR situations. The above method is appropriate for regular lattice geometry in which a definite lattice cell can be identified. An approximate formula for the λ_i (deduced by a comparison of the leakage terms in the critical equation for a periodic flux $e^{i\mathbf{B} \cdot \mathbf{r}}$ based on the heterogeneous equations which follow later, with the conventional homogeneous leakage terms) involves moderator and radial diffusion coefficients; thus

$$\lambda_i = \rho \left(\frac{1 - b_i}{1 + b_i} \right); \quad b_i = \frac{V_{\text{cell}}}{V_{\text{ch}}} \cdot \frac{(D_i^{\text{R}} - D_i^{\text{m}})}{(D_i^{\text{R}} + D_i^{\text{m}})}. \quad (11)$$

(iii) Formal Solution

For a uniform cylindrical moderator of radius R, the general solution for an arbitrary array of channels with centres at $\mathbf{r}_k$, containing three arbitrary constants at each channel consistent with the source and dipole boundary conditions, is

$$\left. \begin{aligned} Q_i(\mathbf{r}) &= \sum_{\mathbf{r}_k} A_k^i K_0(\kappa_i |\mathbf{r} - \mathbf{r}_k|) + (C_k^i \cos \theta_k + S_k^i \sin \theta_k) K_1(\kappa_i |\mathbf{r} - \mathbf{r}_k|) \\ &\quad + \sum_{n=0}^{\infty} (E_n^i \cos n\phi + F_n^i \sin n\phi) I_n(\kappa_i r), \end{aligned} \right\} \quad (12)$$

where r and ϕ are polar coordinates of $\mathbf{r}$ relative to the centre of the core, and θ_k denotes the angular coordinate of $\mathbf{r}$ relative to the centre of channel at $\mathbf{r}_k$ and the direction $\mathbf{r}_k$. E_n^i and F_n^i are given by the equations

$$\left. \begin{aligned}
E_n^i &= -\delta_n \frac{K_n(\kappa_i R)}{I_n(\kappa_i R)} \sum_{\underline{r}_k} \left\{ A_k^i I_n(\kappa_i r_k) \cos n\phi_k + \mathcal{C}_k^i \cos n\phi_k I_n(\kappa_i r_k) \right. \\
&\quad \left. - n \mathcal{S}_k^i \frac{I_n(\kappa_i r_k)}{\kappa_i r_k} \sin n\phi_k \right\} \\
F_n^i &= -\delta_n \frac{K_n(\kappa_i R)}{I_n(\kappa_i R)} \sum_{\underline{r}_k} \left\{ A_k^i I_n(\kappa_i r_k) \sin n\phi_k + \mathcal{C}_k^i \sin n\phi_k I_n(\kappa_i r_k) \right. \\
&\quad \left. + n \mathcal{S}_k^i \frac{I_n(\kappa_i r_k)}{\kappa_i r_k} \cos n\phi_k \right\}
\end{aligned} \right\}. \quad (13)$$

δ_n = Kronecker delta.

Thus in the neighbourhood of the channel centre $\underline{r}_p$ we have

$$Q_i(\underline{r}_p + \underline{\rho}) = A_p^i K_0(\kappa_i \rho) + B_p^i I_0(\kappa_i \rho) + \{(\mathcal{C}_p^i + C_p^i) \cos \theta_p + (\mathcal{S}_p^i + S_p^i) \sin \theta_p\} K_i(\kappa_i \rho) + \dots \quad (14)$$

where B_p^i , C_p^i , and S_p^i are certain lattice summations involving the A_k^i , etc., with $\underline{r}_k \neq \underline{r}_p$. The boundary conditions on $\phi^{(0)}$ and $\phi^{(1)}$ then lead to the final equations:

$$\left. \begin{aligned}
\sum_j c_{ij} A_p^j / I_0(\kappa_j \rho_p) &= \sum_j \mathcal{C}_{ij}^p \{A_p^j K_0(\kappa_j \rho_p) + B_p^j I_0(\kappa_j \rho_p)\}; \\
\sum_j c_{ij} \kappa_{ij}^p \begin{pmatrix} \mathcal{C}_p^i \\ \mathcal{S}_p^i \end{pmatrix} &= - \sum_j c_{ij} \mathcal{S}_{ij}^p \begin{pmatrix} C_p^i \\ S_p^i \end{pmatrix}; \\
e_{ij}^p &= \kappa_j \rho_p \frac{I_1(\kappa_j \rho_p)}{I_0(\kappa_j \rho_p)} - \rho \sum_k c_{jk} \gamma_{ik}^p; \\
\kappa_{ij}^p &= (1 + \lambda_i^p / \rho_p) \begin{pmatrix} K_1(\kappa_j \rho_p) \\ I_1(\kappa_j \rho_p) \end{pmatrix} + \frac{\lambda_i^p}{\rho_p} \kappa_j \rho_p \begin{pmatrix} K_0(\kappa_j \rho) \\ -I_0(\kappa_j \rho) \end{pmatrix} \\
c_{ij} &= (C^{-1})_{ij} \\
\gamma_{ij} &= \alpha_{ij} + \beta_{ij} / k_{\text{eff}}
\end{aligned} \right\}. \quad (15)$$

The above equations have been programmed on the IBM 7090 computer for solution by an iterative process which sweeps through the groups, with inner iterations round the rods in turn, and outer iterations on the fission source. Because of the time-consuming nature of such fully heterogeneous solutions, it is desirable to have a method of solution which takes into account the main features of the heterogeneous equations, while remaining competitive with finite-difference methods; such a method is described in the next section.

MODIFIED FINITE-DIFFERENCE METHOD FOR SOLVING HETEROGENEOUS EQUATIONS

Several authors have shown that solutions of the form $e^{iB_1 r_k}$, $J_0(Br_k)$ are possible for large uniform heterogeneous arrays and that the critical equation is very close to the "equivalent" homogeneous reactor. This suggests that, since the above solutions satisfy $\nabla^2 \phi + B^2 \phi = 0$, a second-order difference-equation of diffusion type might form the dominant terms in a re-formulation of Eqs. (15) obtained by combining the equations for the channel with those at its nearest neighbours. This was first demonstrated to be possible in Ref. 7, and some improvements are reported here.

Derivation of the Modified Equation for a Triangular Lattice

Neglecting dipole terms and terms due to the finite reflector, we may write the equation for $\bar{Q}_j^\rho$ in the form

$$\bar{Q}_j^\rho = A_p^j K_0(\kappa_j \rho) + B_p^j I_0(\kappa_j \rho); \quad (16)$$

$$B_p^j = \sum_{k \neq p}^* A_k^j K_0(\kappa_j |r_p - r_k|) + \sum_{\underline{k}}^{**} A_k^j \left\{ \sum_{n=0}^{\infty} \delta_n I_n(\kappa_j r_p) K_n(\kappa_j r_k) \cos n(\theta - \theta_k) \right\}, \quad (17)$$

where $\sum^*$ and $\sum^{**}$ refer to summations over channels included and excluded, respectively, in the "star" consisting of a given channel 0, the local origin of coordinate, and its six neighbours numbered 1-6 as in the figure below.

Equations (16) and (17) may be further rewritten as

$$\bar{Q}_j^p = \chi_j^p + \psi_j^p,$$

with

$$\left. \begin{aligned} \chi_j^p &= A_p^j K_0(\kappa_j \rho) + I_0(\kappa_j \rho) \sum_{\underline{k} \neq p}^* A_k^j K_0(\kappa_j r_k) \\ \psi_j^p &= \sum_{n=0}^{\infty} (a_n^j \cos n\theta_p + b_n^j \sin n\theta_p) I_n(\kappa_j r_p) \\ a_n^j &= \delta_n \sum_{\underline{k}}^{**} A_k^j K_n(\kappa_j r_k) \cos n\theta_k \\ b_n^j &= \delta_n \sum_{\underline{k}}^{**} A_k^j K_n(\kappa_j r_k) \sin n\theta_k \end{aligned} \right\} \quad (18)$$

If one now defines an operator Δ_0^2 such that

$$\Delta_0^2 F = \frac{2}{3c^2} \left\{ \sum_{k=1}^6 F_k - 6F_0 \right\}, \quad (19)$$

it is easy to show that

$$c^2(\Delta_0^2 \psi_j - \kappa_j^{*2} \psi_j^0) = 4 \sum_{m=1}^{\infty} a_{6m}^j I_{6m}(\kappa_j c); \quad (20)$$

$$c^2(\Delta_0^2 \chi_j - \kappa_j^{*2} \chi_j^0) = c^2 K_j \Delta_0^2 A_j + 4L_j A_j^0, \quad (21)$$

where

$$\kappa_j^{*2} c^2 = 4\{I_0(\kappa_j c) - 1\},$$

$$K_j = K_0(\kappa_j \rho) + I_0(\kappa_j \rho) \left[2K_0(\kappa_j c \sqrt{3}) + K_0(2\kappa_j c) - 4K_0(\kappa_j c) - \frac{3}{2} \kappa_j^{*2} c^2 K_0(\kappa_j c) \right]; \quad (22)$$

$$L_j = \left\{ \begin{aligned} & [K_0(2\kappa_j c) + 2K_0(\kappa_j c \sqrt{3}) - 3K_0(\kappa_j c)] I_0(\kappa_j c) \\ & - \frac{3}{2} \kappa_j^{*2} c^2 \left\{ \frac{1}{6} K_0(\kappa_j \rho) + I_0(\kappa_j \rho) K_0(\kappa_j c) \right\} \end{aligned} \right\}. \quad (23)$$

Combining the Eqs. (20) and (21) for χ_j and ψ_j , one obtains

$$c^2 (\Delta_0^2 \bar{Q}_j - \kappa_j^{*2} \bar{Q}_j^0) = c^2 K_j \Delta_0^2 A_j + 4L_j A_j^0 + 8I_6(\kappa_j c) \sum_k^{**} A_k^j K_6(\kappa_j r_k) \cos 6\theta_k + \dots, \quad (24)$$

and since formally

$$A_k^j = A_0^j + (\underline{r}_k \cdot \underline{\nabla})_0 A^j + \frac{1}{2!} (\underline{r}_k \cdot \underline{\nabla})_0^2 A^j + A_k^{j'}, \quad (25)$$

for a slowly varying reactor and suitable definition of the operators $(\underline{r}_k \cdot \underline{\nabla})$, $(\underline{r}_k \cdot \underline{\nabla})^2$, we have

$$c^2 (\Delta_0^2 \bar{Q}_j^0 - \kappa_j^{*2} \bar{Q}_j^0) = c^2 \left\{ \begin{aligned} & \left(K_j + 2I_6(\kappa_j c) \sum_{\infty}^{**} (r_k^2/c^2) K_6(\kappa_j r_k) \cos 6\theta_k + \dots \right) \Delta_0^2 A_j \\ & + 4 \left(L_j + 2I_6(\kappa_j c) \sum_{\infty}^{**} K_6(\kappa_j r_k) \cos 6\theta_k + \dots \right) A_j^0 + I_j' \end{aligned} \right\}, \quad (26)$$

where

$$I_j' = 8I_6(\kappa_j c) \sum_k^{**} A_k^{j'} K_6(\kappa_j r_k) \cos 6\theta_k + \dots \quad (27)$$

Now it was shown in Ref. 7 that the coefficient of A_j^0 in Eq. (26) is to a very good approximation equal to

$$-\kappa_j^{*2} c^2 \left\{ K_0(\kappa_j \rho) + I_0(\kappa_j \rho) \frac{K_1(\kappa_j R)}{I_1(\kappa_j R)} \right\}, \quad (28)$$

where R is the equivalent cell radius $\left[\text{more exactly } \frac{K_1(\kappa_j R)}{I_1(\kappa_j R)} \text{ should be } \sum_{r_k \neq 0} K_0(\kappa_j r_k) \right]$. Similarly, the coefficient of $\Delta_0^2 A_j$ can be replaced approximately by

$$K_0(\kappa_j \rho) + I_0(\kappa_j \rho) \left\{ \frac{K_1(\kappa_j R)}{I_1(\kappa_j R)} - \frac{2}{\kappa_j^2 R^2} \right\} = \omega_j, \quad (\omega_j \sim 0.4). \quad (29)$$

After some tedious algebra Eq. (26) can be written in the significant form

$$V_c \Delta_0^2 \bar{Q}_j^m - \kappa_j^2 V_m \bar{Q}_j^m - 2\pi\rho \left(\frac{\partial \bar{Q}_j}{\partial n} \right)_\rho = \Delta q_j, \quad (30)$$

where Δq_j is a correction term of the form

$$\Delta q_j = \frac{\kappa_j^2}{\kappa_j^{*2} c^2} I_j' + e_j \bar{Q}_j^m + f_j \left(\frac{\partial \bar{Q}_j}{\partial n} \right)_\rho + \Delta_0^2 \left(g_j \bar{Q}_j^m + h_j \frac{\partial \bar{Q}_j}{\partial n} - \omega_j A_j \right), \quad (31)$$

with suitable definitions of e_j , f_j , g_j , and h_j , which are corrections due to finite channel size and finite difference errors, and where $\bar{Q}_j^m$ has the same definition as that used in the cell calculation for the determination of α_{ij} and β_{ij} of Eqs. (5-10), i.e.,

$$\bar{Q}_j^m = \bar{Q}_j^p + \rho X_j \left(\frac{\partial \bar{Q}_j}{\partial n} \right)_\rho.$$

Thus, insofar as $\bar{Q}_j^m$ as defined above is a good approximation to the mean value of Q_j over the moderator of a finite reactor lattice cell, Eq. (30) can be identified with the equation obtained by integrating the moderator Eq. (3) over the moderator of a lattice cell, i.e.,

$$\int_{\text{boundary}}^{\text{cell}} \frac{\partial Q_j}{\partial n} ds - \kappa_j^2 V_m \bar{Q}_j^m - 2\pi\rho \left(\frac{\partial \bar{Q}_j}{\partial n} \right)_\rho = 0, \quad (32)$$

where $\partial/\partial n$ denotes differentiation along the direction from the channel into the moderator. Thus, neglecting Δq_j , it has been shown that the leakage from the cell of a "slowly" varying reactor is equal to $D_j^m V_c \Delta_0^2 \bar{Q}_j^m$, assuming that

$$\bar{Q}_j^m = \bar{Q}_j^p + \rho X_j \left(\frac{\partial \bar{Q}_j}{\partial n} \right)_\rho,$$

which justifies the conventional finite-difference approximation to leakage in the case of a heterogeneous lattice only for mesh points placed at channel centres, with the prescription that the flux at the "mesh point" be interpreted as the mean moderator flux.

If one now multiplies Eq. (30) by the matrix C^{-1} followed by D^m , one obtains for ϕ

$$V_c D_i^m \Delta^2 \bar{\phi}_i^m - \sum_{\text{rem}, i}^m V_m \bar{\phi}_i^m + \sum_{i \leftarrow i-1} V_m \bar{\phi}_{i-1}^m - 2\pi\rho D_m' \left(\frac{\partial \bar{\phi}_i}{\partial n} \right)_\rho = D_i^m \sum_j c_{ij} \Delta q_j, \quad (33)$$

where, as in Eq. (6),

$$\bar{\phi}^m = \bar{\phi}^P + CXC^{-1}\rho\left(\frac{\partial\bar{\phi}}{\partial n}\right)_\rho. \quad (34)$$

Finally,

$$D_i^m \Delta^2 \bar{\phi}_i^m - \sum_{\text{rem},i}^{\text{cell}} \bar{\phi}_i^m + \sum_{i \leftarrow i-1}^{\text{cell}} \bar{\phi}_{i-1}^m + \frac{\beta i}{k_{\text{eff}}} \sum (\nu \Sigma_f)_j^{\text{cell}} \bar{\phi}_j^m = R_i, \quad (35)$$

with standard definitions of cell-averaged cross sections normalised to mean moderator flux.

Equation (35) with the leakage term replaced by the conventional expression

$$\frac{2}{3c^2} \sum_{k=1}^6 \frac{2D_{Rk}^i D_{R0}^i}{D_{Rk}^i + D_{R0}^i} (\bar{\phi}_{ki}^m - \bar{\phi}_{0i}^m) \quad (36)$$

forms the basis of a code RAVEN for an IBM 7090 computer, and very good agreement with the fully heterogeneous code MAGPIE has been obtained with much smaller computing times.

CONVENTIONAL FINITE-DIFFERENCE TREATMENT

The use of standard finite-difference methods in the calculation of flux distributions in heterogeneous systems is normally based on the assumption that various zones of the reactor can be replaced by equivalent homogeneous multiplying media in each zone and the diffusion equations for the "homogenised" zonalised reactor, solved as accurately as possible with a mesh which may bear no relation to the actual reactor lattice, especially near control rods where it may be necessary to use a very fine mesh. The results of the previous section show that it is unnecessary, and may give erroneous results, to use a mesh bearing no relation to the heterogeneous lattice geometry and that the best results should be obtained with mesh points at channel centres. Thus TRIFID, the uncorrected version of RAVEN, has been in use for some time with in-channel mesh points in the interpretation of triangular lattices, such as the Windscale AGR and HERO, and has been demonstrated to give good results.

EXPERIMENTAL COMPARISONS

We now turn to a comparison with experiment of results obtained by the methods of the previous section. The first measurements we shall consider were made on the HERO reactor--a zero-energy reactor,

graphite-moderated with a triangular lattice pitch of 10.75 in. Before quoting experimental results it is, however, convenient to discuss the effect of the number of neutron groups on the flux shape calculated for an idealised version of this core.

A group structure with a total of 14 groups including 10 below 4.5 eV was first considered. A 5-group structure was then used with 3 groups below 4.5 eV and finally the 3 thermal groups were condensed to give a 3-group structure. Table I shows the manganese (largely $1/V$) reaction rate along a radius normalised to the 14-group value.

Table I
EFFECT OF NUMBER OF GROUPS ON RADIAL FLUX SHAPE

No. of Groups	Centre of Core	One Pitch	Two Pitches	Three Pitches	Four Pitches (Edge Channel)
14	1	1	1	1	1
5	1.006	1.006	1.005	1.002	0.984
3	1.013	1.012	1.011	1.005	0.963

We see that the $1/V$ flux at the core edge is reduced by some 4% by the use of 3 groups instead of 14. Not all the edge channels were as exposed to the reflector as the one above, and the average error in edge channels was about 3%. Table II demonstrates that the fast and resonance group can be condensed together without greatly affecting the flux shape, so this error should also apply to a two-group scheme. In practice this error may be significantly reduced by allowing for leakage effects in the lattice calculations, but corrected data of this type have not been used in this paper.

Table II
COMPARISON BETWEEN THEORY AND EXPERIMENT FOR HERO CORE

Channel No.	1749	1949	2050	2149	2250	2349	2351	2450	ρ
Experiment	5830 ± 152	5523 ± 40	5083 ± 33	4908 ± 12	4227 ± 9	4119 ± 17	3817 ± 31	3791 ± 13	0.00674 ± 0.00040
MAGPIE 3-GRP	-0.53	0.99	1.24	0.47	2.17	0.15	-2.49	-2.90	0.00551
MAGPIE 2-GRP	-1.13	0.36	0.77	0.24	2.29	0.46	-1.31	-1.90	0.00616
TRIFID 3-GRP	0.14	1.61	1.85	1.28	2.67	-0.17	-3.85	-5.59	0.00582
TRIFID 2-GRP	-0.31	1.23	1.63	1.16	2.90	0.15	-3.30	-5.12	0.00809
CRAM 3-GRP COARSE	-1.51	0.04	0.43	0.06	2.03	1.09	-0.92	-0.95	0.00741
CRAM 3-GRP FINE	-2.06	-0.51	0.04	-0.39	1.82	1.48	0.13	0.63	0.00937
CRAM 2-GRP COARSE	-1.78	-0.20	0.37	0.08	2.43	1.29	-0.65	-1.08	0.00937
CRAM 2-GRP FINE	-2.30	-0.69	-0.06	-0.31	2.27	1.68	0.29	0.32	0.07009

The comparison of experimental and theoretical values of manganese reaction rates for the uniform 55-channel core fuelled with 1.8% ^{235}U oxide clusters is presented in Table II for the eight different channel positions in the core. Theoretical values are presented as percentage (theory-experiment) errors. CRAM is a rectangular-mesh finite difference code, and with the coarse mesh four mesh areas, 13.65 x 11.82 cm, represented one hexagonal cell. The mesh was doubled in both directions to give the fine mesh.

The two-group scheme has the fast and resonance ARGOSY groups condensed into one group. The two- and three-group results are only slightly different, showing that the use of only one group above 4 eV introduces less error than the use of only one group below 4 eV.

We conclude that MAGPIE (method a) gives the best results, as expected from theoretical consideration, since the main error, about 3% near the reflector, is of the order expected from a 2- or 3-group calculation. Results from RAVEN (method b) are very close to those from MAGPIE. Those from TRIFID (method c) are also reasonably good since the error of 5 to $5\frac{1}{2}\%$ near the reflector is only 2 to $2\frac{1}{2}\%$ higher than expected due to the group structure.

The results from the rectangular mesh code CRAM are, in fact, in best agreement with experiment, but the agreement is regarded as fortuitous, with the error in mesh representation cancelling the error from the group structure.

Figure 2 shows results from a three-group TRIFID calculation on a more heterogeneous HERO core containing fuel with 1.8% ^{235}U , fuel with 0.25% plutonium, in uranium of 0.9% ^{235}U , and vacancies. In Fig. 2(a) the available values of manganese reaction rate are plotted against distance from the core centre, and in 2(b) the ratio of calculation to measurement is also shown. We see from Fig. 2(a) that the plutonium-fuelled channels have manganese reaction rates about six per cent higher than uranium channels on the same core radius. The TRIFID code is, however, able to predict these channel-to-channel variations satisfactorily, as shown in Fig. 2(b). The weakness of TRIFID and the uncorrected lattice data at the reflector-core interface are again highlighted in Fig. 2(b).

Figure 1 shows the comparison between TRIFID and measurement of manganese reaction rates in the Windscale AGR commissioning core, which again has a triangular lattice. Channels not containing fuel are indicated, and the core is seen to be highly heterogeneous. Nevertheless, the root-mean square of the error is only 2.5%, which can be regarded as very satisfactory. We conclude that the simple finite-difference method with one mesh point per channel is adequate for purposes of reactor survey.

Fig. 1. Comparison of TRIFID and Experiment on WAGR Commissioning Core

FUEL-CYCLE APPLICATION

Method (c) above has been applied to fuel-cycle calculations in the ODYSSEUS program developed by A. N. Buckler from the ZADOC program of F. R. Allen.

Two broad types of fuel cycle are possible. The first type, in which a large part of the core is changed at one time, we call "batch charge." The second type, in which one channel, or perhaps a few, are changed at one time, we call "continuous charge." Adoption of the batch system leads to significant engineering advantages in an AGR design, but at the cost of a reduced core lifetime and of controlling significantly greater amounts of reactivity than is required for normal operation.

The relative merits of various fuel cycles may be assessed in the equilibrium conditions by reactor calculations using smeared data, coupled with supercell calculations. It still needs to be demonstrated, however, that an equilibrium condition can be reached, and it is also important to evaluate the power produced by a reactor during the approach to equilibrium.

The ODYSSEUS program was designed primarily to investigate this approach with continuous charge systems, although it can be used to investigate a batch system also. Lattice data are stored within the program as a function of irradiation for various fissile materials, and nonfissile materials are also permitted. Control to critical is represented either as an eigenvalue or neutron source, or as a factor θ on the thermal absorption cross sections in specified mesh positions.

The diffusion equation is solved, the power distribution evaluated, and the decision taken whether to advance the core irradiation a time-step or to refuel one or more channels. The process is then repeated until a criterion for stopping the calculation is satisfied.

OPTIONS IN THE USE OF ODYSSEUS

Numerous refuelling options are available. The simplest is one in which channels are refuelled in a specified order, refuelling taking place whenever the reactivity (or θ value) falls below a specified value. The use of this option in the design of a good fuel cycle has proved laborious, and the aim has been to make the program itself choose the channels when refuelling is required.

Relatively simple options have proved unsuccessful. For example, if the channels of lowest reactivity are loaded with new fuel whenever extra reactivity is needed, new fuel elements tend to accumulate in neighbouring channels. It is clear from this that power level is more useful than reactivity in determining the need for refuelling; and this conclusion led to the box feature in ODYSSEUS.

BOX FEATURE

The channels are divided into groups of three kinds which are known as boxes:

- (i) donor boxes: provide partly irradiated fuel to receiver boxes and receive new fuel in its place;
- (ii) receiver boxes: receive fuel from donor boxes and discharge fuel from the reactor;
- (iii) passive boxes: receive new fuel and discharge fuel from the reactor.

Each box has a target power, which may vary with time, and the box with the least power relative to its target is identified for refuelling. If this is a donor or receiver box, a box of the other type is also identified on a power criterion to enable a radial shuffle to take place. The problem of specifying the particular channel for refuelling within a box remains, and the solution which appears most promising at present is as follows. The channels within each box are divided into one or more rings which are visited in turn, the channel with least absolute power fuel within the ring being refuelled.

A careful balance between the total number of channels in receiver and donor boxes is required to allow a successful fuel cycle to emerge. Care and experience in the choice of target power are also important, since the form factor at any time is influenced by the previous history of the core.

FLUX SHAPING BY CONTROLLERS

The aim of the box feature in ODYSSEUS is to use the refuelling process to shape the flux into a desired form. This process can be carried still further by using the controllers also to shape the flux. The factors θ on the absorption cross section now take different values θ_k for the absorbers in different boxes to equate the box powers to their targets. Refuelling is then initiated if the lowest θ_k is less than a specified number, and occurs in that box. This option has presented considerable convergence problems and requires large amounts of machine time. Development work is, however, continuing, as this option is regarded as simulating most closely the practical situation.

RESULTS

Figure 2 shows the radial form factor for a typical large AGR using lattice data from Ref. 8. In the cycle considered, the initial charge was mostly of twice natural enrichment with a few channels of feed enrichment at three times natural enrichment. Each fuel element undergoes at most a single radial shuffle, but all fuel entering the central region after the initial loading had been irradiated for a short time in the outer region.

Fig. 2. Manganese Reactions in
HERO Plutonium Core

Figure 3 shows typical values of radial form factor obtained by trial and error specifying the sequence of changes in advance. The calculations ceased when the central half of the core contained only fuel of feed enrichment. The spiky nature of the curve illustrates the difficulty of obtaining good results from the program operating in this simple mode. In fact, two iterations were made to obtain the present curve, and experience has shown that with further work a smoother curve could be obtained. It is hoped that when the more elaborate versions are fully operational, smoother curves will be obtained with much less effort. Figure 3 also shows the form factor obtained when the fuel was loaded in three equal batches, instead of two or three channels at a time. There is some reduction in form factor with this bulk approach, but 20% less lifetime is obtained from the core during this first part of its life.

Fig. 3. Variation of Radial Form Factor for a Typical AGR

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THE AUTOMATION OF REACTOR DESIGN CALCULATIONS AT THE KNOLLS ATOMIC POWER LABORATORY

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(Paper presented by W. H. Turner)

INTRODUCTION

The trend toward automation of reactor design calculations at KAPL has closely paralleled the growth in the Laboratory's digital computer capability. For convenience of discussion, this growth is shown in Fig. 1 as occurring in three eras, an IBM 704 era that is now history, a Philco 2000 era that is now in its twilight, and a CDC 6600/6800 era that will dawn late this year. Although the Laboratory went through a pre-704 era on CPCs, 650s, and off-site UNIVACs, the total reactor design effort did not reach a coherence that warranted a serious attempt to plan a unified automated system until late 704 days. The remaining sections of this paper describe in some detail the three eras referred to above--past, present, and, to the extent that our crystal ball is reliable, the future.

THE 704 ERA

This $3\frac{1}{2}$ -yr period marked the emergence of a number of isolated one-, two-, and three-dimensional diffusion codes for various geometries. No attempt was made to standardize input and output conventions, and any communication between these codes was done strictly through human intervention. Even related calculations using the same code--life studies, for example--required a good deal of manual card shuffling in between time steps and in between model adjustments in search of criticality. Single-channel three-dimensional synthesis calculations were performed manually by converting two-dimensional output data into input data for a separate integration routine whose punched output had to be combined with other data to feed a final one-dimensional code which performed the ultimate axial synthesis. Temperature coefficients were calculable with a perturbation code, provided flux and adjoint results were prepared from separate prior runs. Also the perturbation code, originally written for conventional xy and rz geometry only, never did keep pace with later developments, such as xy geometry with diagonal material interfaces or periodic symmetry conditions, or triangular mesh geometry. Although several codes might use the same basic group constant routine, each would have its own separate copy as part of its system tape, creating untold maintenance problems and constant worries about consistency.

*Operated for the Atomic Energy Commission by the General Electric Company, Schenectady, New York.

Era	Time	Relative Machine Speed (x704)	Machine Characteristics	Primary Languages	Typical Usage
IBM-704	4/57-9/60	1	36 bit binary word, 32K core memory +10 unbuffered 22.5KC tapes	Machine Language, small amount of FORTRAN	Separate use of 1D and 2D problems with considerable manual data handling necessary for life studies, perturbation calculations, and one-channel synthesis calculations.
Philco 2000 Model 211	4/60-6/63	6	48 bit binary word, 32K core memory +16 4-way multiplexed 90 KC tapes	Machine Language, FORTRAN II	KARE system provides automatic criticality search and time-step sequencing for life studies, plus automatic perturbation and multi-channel 3D synthesis calculations.
Philco Model 212	6/63 Present	24		FORTRAN IV	
CDC 6600	10/65-5/67	200	60 bit binary word, 64K core memory + 512K extended core storage with 25 nsec streaming rate + 40 million words of 1250KC disk storage +80 million words of on-line Datacell storage	FORTRAN IV and FORTRAN 66	Further automation of more complex problems, on-line master cross section libraries serve many NOVA system modules, extensive use of man-machine interaction techniques in parallel with background batch processing.
6800	5/67 ?	1000			

Fig. 1. The Trend Toward Automation of Reactor Problems

A flexible thermal-energy Monte Carlo program was developed in this period, but although this program was converted from the 704 to the Philco 2000, it has remained disjoint from other programs in both eras.

THE PHILCO 2000 ERA

As a result of experience gained in the 704 era, it was decided that an integrated series of programs be planned for the Philco 2000 rather than piecemeal conversion of 704 programs. If a system of computer programs is to be useful for such an approach, certain features are required:

1. The system must contain programs which can solve the reactor model in sufficient detail in any desired variable.
2. The results of each calculation must be readily available to subsequent steps in the process.
3. The system should be adaptable to many different simplification processes, since each design calculation has its own unique requirements.

4. Each component program should be consistent with all other programs when this is reasonable. For example, all group-constant routines should use the same collection of basic nuclear data.

The KARE system consists of a collection of machine-language programs written for the Philco 2000. Each program depends on the other programs of the system and will not function alone. KARE is hand-tooled to deal with rather specific classes of problems. However, for a problem in one of these classes, KARE is fully automatic.

The KARE system will perform life studies of one-, two-, and three-dimensional reactor models. All required calculations proceed automatically according to the following pattern:

1. Calculate few-group constants for use as elements of diffusion, absorption, and fission matrices, D , A , and F .

2. Solve

$$-\nabla D \nabla \phi + A \phi = \lambda F \phi$$

for ϕ , the few-group neutron flux vector, and λ , the fundamental eigenvalue; or solve

$$-\nabla D \nabla \phi_{\gamma} + A \phi_{\gamma} = S$$

for ϕ_{γ} , the few-group gamma ray flux vector, using a point-wise source S generated from a previously calculated neutron flux.

3. If non-critical, adjust the model and return to 1.
4. Deplete the model and prepare input for the next time step. Return to Step 1.

Group constants for up to four neutron groups or five gamma-ray groups are available from KARE programs. The thermal-neutron group may be represented as two "overlapping" groups, each with a different trial spectrum. This representation, with variational computation of combining coefficients, gives an inexpensive, but accurate calculation of the effect of spatial variation of the thermal spectrum.

The two-dimensional geometries available are:

1. x, y with axes at 90° ;

2. x, y with axes at 120° (uses a uniformly spaced triangular mesh);
3. rz ;
4. $r\theta$.

Up to 20,000 points may be used in these geometries.

The set of program segments that comprises KARE is shown schematically in Fig. 2.

Fig. 2. The KARE Program

KARE was begun in late 1959. Although an initial version of the system was operating shortly after the Philco 2000-211 was delivered in April 1960, the system is essentially an "unfinished symphony" whose system tape has been growing at the rate of one inch per day since that time. The system now contains approximately 100,000 machine-language instructions plus a few FORTRAN-compiled segments; this represents

about 50 man-years of effort. (If we consider segments that became obsolete and were replaced, this averages out to better than eight debugged instructions per man per day. Since other large-scale multiprogrammer efforts have been known to dip as low as two instructions per man per day, this is considered to be a favorable output rate. Nevertheless, the increased leverage of FORTRAN programming over assembly language had better be at least four to one if the replacement for KARE is to achieve comparable status in a reasonable time. Early returns on the conversion now in progress indicate that this can be achieved.) Approximately 300 hr of KARE calculations are now being performed per month on the Philco 2000-212.*

Some of the key features in KARE that automate design studies are described below.

Fig. 3. A Model with 90° Rotational Symmetry

1. Key data are passed from time step to time step via a "history tape." To minimize machine time, the history tape will supply any two-dimensional problem with a source and flux guess from the problem of the same type last performed in the study, usually from the preceding time step.

2. xy and triangular mesh geometry contain rotational symmetry options for 90° periodicity and 120° periodicity, respectively (see Fig. 3). When it becomes necessary to perform a midlife calculation which is not 90° periodic, an input option allows automatic x 4 expansion of the basic quarter-core model with

subsequent modification to any desired quadrant. KARE will then revert to the quarter-core model until another nonperiodic problem is requested later in life.

3. Gamma heating and perturbation calculations for any time in reactor life can be specified for completion in one pass at the machine.

4. Several two-dimensional studies can be stacked on a history tape for immediately subsequent multichannel synthesis calculations (see Fig. 4).

*The internal speed of the Philco 2000-212 is about twice that of an IBM 7094 II. A field modification now in progress will decrease its floating-point multiply time from 6 to 2 μ sec, raising the average instruction rate above that of a STRETCH.

Fig. 4
Multichannel Synthesis

The preceding description is incomplete, but it does give some of the highlights of KARE. The advantages of such a system are ease of use and efficiency of operation. Its drawbacks, which led us to a somewhat modified approach to automated reactor calculations are:

1. It is often difficult to apply this large system to a simple problem.
2. Many aspects of reactor theory are not incorporated in KARE. These include Monte Carlo, higher-order approximations to the transport equation, and multigroup treatment.
3. The KARE system has grown to be very difficult to extend, due to the extreme dependence of each program on other programs in the system.

In an attempt to retain the advantages of KARE's automation and, hopefully, to regain some of the flexibility lost in the process of producing it, a successor system called NOVA is being planned for the era described in the next section.

THE CDC 600/6800 ERA

The NOVA system will consist of a collection of FORTRAN programs, called modules, each of which functions as a separate entity. Many modules will serve the same purpose, but differ in speed and accuracy. Within NOVA, such modules may be used interchangeably, depending on the specific application.

All modules have access to a common set of mass storage devices, called the DATAPOOL. The individual modules take their input from the DATAPOOL, and store their results there. Thus, when a series of modules is run, each may use, as input, the results of all previous modules. After a brief look at the total system, we shall return to the DATAPOOL.

The user of NOVA will specify the series of modules he desires to execute, designating the source of input to each. The modules will then be executed in the order indicated. Certain standard sequences of modules may be specified by single-word requests.

NOVA modules fall into one of several broad categories:

1. group-constant calculations, which compute D, A, and F matrices for 2;

2. solution of

$$-\nabla D \nabla \phi + A \phi = \lambda F \phi \text{ for } \phi \text{ and } \lambda$$

or

$$-\nabla D \nabla \phi + A \phi = S \text{ for } \phi$$

for G groups on a finite difference mesh, where λ is the fundamental eigenvalue, D, A, and F are arbitrary matrices of order G, and ϕ and S are vectors with G components. D, A, F, and S are assumed given;

3. other approximations to the transport equation which do not fit into the formalism of 2. A Monte Carlo spatial calculation is one example;

4. calculations based on the availability of one or more type 2 or 3 calculations. These include depletion, perturbation theory, and certain transient techniques;

5. service programs which generate libraries, process customer-supplied input, perform editing and integrating functions, adjust reactor parameters, etc.

Several different approaches to the same general program will be available in each category.

At the present time, no true three-dimensional calculation is planned for Category 2. Instead, a variational multichannel synthesis program to be described in another paper (by E. L. Wachspress) will be included.

With a large and growing system like NOVA, problems of co-ordination of, and communication among, modules are of fundamental importance. Our approach was to consider the general module in isolation. Figure 5 shows the basic idea. A module takes data from storage, processes the data, and produces additional data, which is stored. If we treat all storage mechanisms as one unit, we get the concept of the DATAPOOL. The CDC 6600/6800 DATAPOOL will consist of the devices shown in Fig. 6.

Figure 5
NOVA Data Paths

Device	Word Capacity	Access Time	Transfer Rate (words/sec)
Extended Core Storage	0.5×10^6	$1.6 \mu\text{sec}$	40×10^6
Disk Storage	32×10^6	30-100 msec	0.6×10^6
Datacells	80×10^6	0.2-0.6 sec	5500

Fig. 6. Storage Devices Available for DATAPOOL

There will also be two magnetic-tape units supplementing the above devices, but these are not expected to be used very often. The eighty-million words of Datacell storage will allow a high percentage of frequently used data files to be kept on-line at all times. Since the Data-cell storage is removable in four-million word chunks, less frequently used data can be placed on-line as needed.

We require that all information to be stored in the DATAPOOL be organized into formally defined collections, called files. Each basic type of file is named and described by a page or two in a loose-leaf NOVA Dictionary. Some such files are flux, the D, A, and F matrices, and

number densities of isotopes. Thus, when a module is to be produced, the storage format of all, or most, input and output files is already well-defined.

A DATAPOOL Monitor exists as a subroutine within the operating system. All file storage and retrieval are done via this Monitor. The modules use Hollerith names to refer to the files, the Monitor assuming complete responsibility for locating the named file within the DATAPOOL. This causes a great simplification in the problem of intermodule communication. The Monitor maintains a permanent directory of all files currently stored in the DATAPOOL. This allows data stored by module A at time t to be used by module B at time $t + \Delta t$, where Δt may be from microseconds to months in length.

With such a simple communication system, the coordination of modules becomes a matter of course, performed by a subroutine called the Director. On completion of its function, each module exits to the Director, which selects and gives control to the next module. In essence, ordered lists of module names are stored in the DATAPOOL. The Director simply selects the desired list and calls the modules in the indicated order.

These lists of modules are called paths. Many standard paths exist, and each has a single word name. The user may supply his own path, and NOVA will follow it if it is feasible.

A path is feasible if the input files for each module are available within the DATAPOOL when control is given to that module. We plan to extend the Director to test a nonstandard path for feasibility, but, this has not yet been done. There is a minimum need for such a test, since restarting is quite simple with the DATAPOOL Monitor. The faulty path may be modified and the Director instructed to begin the modified list at any indicated point.

Figure 7 may help to visualize the operation of NOVA. Diagram 1 occurs at the beginning of the NOVA run. The Director has control, and calls the desired path from the DATAPOOL.

In Diagram 2, the first module of the path is being taken from the DATAPOOL.

In Diagram 3, control has been passed to the module, which is processing data.

In Diagram 4, the module has completed its function and has returned control to the Director.

In Diagram 5, the next module of the path is being readied for execution.

Fig. 7. The NOVA System Logical Flow

There are many advantages to the NOVA type of system. A few of the most interesting will be described.

Whenever a new module is added to the system, its results are immediately available to all other modules. This will allow the system to be extended indefinitely without extensive revamping.

Indeed, the user may add his own FORTRAN program to the system to manipulate the input and output of the standard NOVA modules.

Consistency is achieved simply by having all modules use a common set of basic data. This will be particularly rewarding in the field of cross sections.

The use of single code words to specify standard paths retains the simplicity of use of special-purpose systems. The ability to specify any feasible series should allow NOVA to be applied to an extremely broad range of procedures.

Discussion of Paper
Presented by Mr. Turner

MR. RAVETS (Westinghouse Astronuclear): It is very rare that a programmer or physicist take advantage of critical experiments which exist. We still realize the shortcomings of the approximation to be made to the solution of the Boltzmann equation and the inherent errors that exist in cross-section data. In a system of this nature I don't see where you are taking advantage of critical experiments: 1) to normalize, or 2), to decide what model to use in the next step. This is a very serious problem, I think, in many of these types of systems.

MR. TURNER: We have done some thinking, as yet unsuccessful, and I would certainly appreciate any thoughts for integration of such knowledge. So far we have had to put the man back in each time we wanted to take advantage of critical facility experiments.

MR. RAVETS: It is still an identical problem; if a man can do it, in essence the machine can. You can build in normalization procedures and selection procedures.

MR. TURNER: A great deal of such information does come in. These group-constant modules work from an approved library of pointwise group constants. This approved library is modified as based on human experience, automatically, but the human experience itself has to be fed into the machine in some form. Perhaps we haven't thought enough about how to get a general way to feed in the human experience.

MR. SEGAL (Atomic Power Development Associates, Inc.): This is a very beautiful system, very logical and definitely reflecting the current trend of the, I wouldn't like to say computer god, but you are going to have an administrative problem. In other words, the user will become more insulated from the actual equations and the actual specifications which are in these codes. For instance, suppose a user runs a NOVA problem one year and he says to you next year "I think there may be a mistake. Could you tell me exactly what processes you were using last year in such and such a part?" Now this system is going to be updated; it is going to be very fluid; it is going to be changing. Are you going to be in a position to answer this sort of question?

MR. TURNER: Traditionally this question has always embarrassed people in my position, and I am afraid it probably still will, but that is my responsibility. I must see to it that we have adequate documentation. We will have basic paths through the NOVA system that will be clearly defined. I would hope that a man would be able to put in a one-word request and get a definite selection of modules in a given order from NOVA as it exists right then. There will be approved modules in NOVA in the same sense that there are approved cross-section libraries available to the group-constant routines. If he has run a standard path through NOVA and I have

done my job right, I should be able to reconstruct for him what was done as he followed that standard path. If he wrote his own path, one only hopes that his output has some traces of what the path actually consisted of.

MR. EMON (Texas A&M): What thought has been given to all this automation? A small mistake in the input ties up quite a bit of machine time. I know there are obvious things, like dumps and so on, that normally one gets when you divide by zero or something obvious along this line. One might put in just an order-of-magnitude sort of an input when you first start a design project so that you would catch things of order-of-magnitude difference in the number densities and things like this, and not waste a lot of machine time. If it is all automated one may have gone through half an hour of machine time which is wasted. What sort of thought has been given along this line as an initial check sort of thing?

MR. TURNER: Two things. First, to get input into the DATAPOOL, you must go via a module called the input processor. We don't expect humans to live with the basic data forms that the computer has to live with. We don't expect a human to have to make up, for instance, a number-density file. Perhaps he would much rather put in his input in masses, volumes, and that sort of thing, and allow the computer to do the basic translation. Now, there will be a good bit of error checking in the input processor itself. I would also hope that when one is early in the process of making up a model, he would tend to run an abbreviated series of NOVA modules simply far enough to look at his first set of group constants before continuing a life study that might run quite a long time. We will make certain tools like that available to the user, but it will always be up to the user to make use of them. Our experience is that that's not always the case.

MR. SANGREN (Computer Applications): One thing that bothers me is that you use one iterative process for all of the possible matrices that you have. I suggest one further step and allow the generality of using different iterative processes, depending upon what the D, the A, and the F matrices turn out to be.

MR. TURNER: That is our intent. The first module that goes on the shelf will be the most general one we can produce. Then, for specific cases, in calendar time, these will be added to the library as the specific cases come up. Undoubtedly very early in the game we'll have one for the diffusion equation. I want, first, a module that will handle what we can conceive of trying rather than trying to get all the special cases at once. With that generalized module, we'll reduce the calendar time enormously to run a set like this because we don't have to produce the specialized one to handle the particular case.

MR. OLSEN (The Martin Company): The trend in the computer seems to be to multiprocessing and I wonder if you can make use of that.

MR. TURNER: Yes, we hope to. We are getting, I think, six remote consoles a few months after delivery. I would hope that then we can have a background of large NOVA problems chugging along and a foreground of physicists interrogating the DATAPOOL to ask what the eigenvalue was at the fifth time-step of such and such a study, or what was the worst power. There will be modules whose purpose is strictly to go in and read files from the DATAPOOL, analyze them, and type out abbreviated responses.

MR. OLSEN: Can you change the input while it is running? Can you interrupt and change an input variable if the results are not as expected?

MR. TURNER: With these big computers I'm not at all sure you know where it is, even if you are standing there beside the computer. Maybe what must be done is to interrupt and see if things are okay; perhaps a module list may be derived that will interrupt itself and let you look at it. If we can tell what's going on, we will certainly try to take advantage of it and allow manual interrupts. But these things are so fast and so complicated, especially in a multiprogramming environment, that I don't think it will be that way.

A SYSTEM FOR NUCLEAR REACTOR DEPLETION COMPUTATION

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(Paper Presented by R. J. Breen)

I. INTRODUCTION

Digital computer programs are presently available which will yield solutions to few-group diffusion-theory problems in 50,000 or more spatial mesh points in two dimensions in x-y, r-z, or hexagonal geometry⁽¹⁾ and up to three million spatial points in three dimensions.⁽²⁾ Most geometrical configurations can be described accurately with the present spatial programs.

In contrast, depletion programs used to date have been quite limited in the range of problems they can handle. Most depletion programs contain the depletion equations for a small, specific set of nuclides. The few-group cross sections assigned to these nuclides are assumed either to be constant or to vary in prescribed functional forms. The depletion framework has usually reflected the specific reactor type for which it was written. In order to solve the more general problems of interest today, it is necessary to improve our capabilities in the depletion portion of the diffusion-depletion process.

The purpose of this paper is to describe a new depletion system called HARMONY,⁽³⁾ which has been developed to be used with few-group diffusion-theory programs. This system has the desired flexibility for covering a much wider range of depletion problems. It allows, in effect, the user to formulate his own depletion program to meet his needs. Rather than tailoring his reactor description to meet the requirements of a particular depletion program, the user is able to tailor the depletion system to describe the reactor.

A general depletion system is of little interest if it is difficult to use or out of proportion to the computing costs required. A practical system requires a careful balance between the generality desired and the cost of evaluation, with particular attention to the ease of input and availability of output in a proper form. This balance has been achieved in this system with four basic components:

- 1) a general solution to the depletion equations;
- 2) the representation of the time behavior of cross sections with interpolating tables;

*Work performed under the auspices of the U. S. Atomic Energy Commission.

- 3) availability of basic output for further processing;
- 4) the dynamic allocation of computer storage.

Although no one of these features is novel, their combination in a single system yields a greatly increased capability at reasonable expense.

II. DEPLETION CHAINS

Most depletion programs written in the past have contained depletion equations for a fixed set of nuclides. For example, the CANDLE and TURBO⁽⁴⁾ programs treated 13 depletable nuclides: specifically, U^{235} and U^{236} ; 4 nuclides in the U^{238} chain; Sm^{149} and Xe^{135} with their precursors; plus three more nuclides to represent burnable poisons and the effect of the remaining fission products. Increase of the number of depletable nuclides was not practical within the program framework. Any attempt to treat nuclides other than those listed above required replacement of some of the existing nuclides with those of interest, plus modification of the depletion chains to obtain the desired coupling between nuclides. For instance, a reactor containing thorium could be represented only by ignoring any U^{238} that was present. No capability existed to represent several of the more important fission products explicitly.

This new depletion system has overcome the limitations of the depletion chains of past depletion programs by 1) not imposing an explicit limit on the number of depletable nuclides that may be represented, and 2) allowing the user to specify the equations to be solved by the program for each nuclide.

A. Chain Description

Fig. 1. Linear Chains

The equations defining the time-dependence of the nuclides in HARMONY are patterned after those used by T. R. England.⁽⁵⁾ The concentration of a particular nuclide may depend on more than one immediate parent as well as its own radioactive decay, neutron absorption rate, and yield from fission. A complete schematic of all coupling mechanisms between the precursors which feed and transform each nuclide may appear to be quite complicated (see Fig. 1 for a relatively simple example). The algorithm currently used in this program to solve the associated differential equations requires couplings in which nuclei are fed by a single parent. However, provided that a nuclide concentration is

independent of the concentration of any of its progeny, it is always possible to resolve more complicated couplings into a set of linear chains.

In the example of Fig. 1, two linear chains are required. In the first chain, the solutions for the first three nuclides give the final values for the concentrations, while the values for nuclides 4 and 5 are only partial concentrations. In the second chain, the solution for nuclides 1 and 2 duplicate those of the first chain (this is indicated by the -1) while the concentrations of nuclides 4 and 5 must be added to the previous values to obtain final concentrations (this is indicated by the +1).

The concentration of the i^{th} nuclide in a linear chain is determined by the equation

$$\frac{dN_i}{dt} = \bar{Y}_i + \alpha_i \beta_{i-1} N_{i-1} - (\lambda_i + A_i) N_i, \quad (1)$$

where

$$\bar{Y}_i = \sum_k \gamma_{ik} \overline{NF}_k, \text{ the average direct fission yield; the summation } k \text{ extends over all fissile nuclides;}$$

$$\gamma_{ik} = \text{yield fraction/fission of nuclide } k;$$

$$\overline{NF}_k = \frac{1}{2} [N_k(t_0) F_k(t_0) + N_k(t_1) F_k(t_1)];$$

$$t_1 - t_0 \text{ is the time interval for which solution to Eq. (1) is obtained (the subinterval discussed later);}$$

$$F_k(t) = \sum_g \sigma_k^{f,g}(t) G_k^{f,g}(t) \Phi_g(t_0);$$

$$\sigma_k^{f,g}(t) = \text{fission cross section for nuclide } k \text{ in group } g;$$

$$\Phi_g(t_0) = \text{flux for group } g \text{ normalized to a specified power at } t_0;$$

$$G_k^{f,g}(t) = \text{self-shielding factor for fission cross section, group } g, \text{ nuclide } k;$$

$$\lambda = \text{decay constant;}$$

$$A_i = \text{total absorption rate at } t = t_0, \text{ similar to } F \text{ except that } \sigma^a \text{ is used;}$$

$\beta_{i-1} = \lambda_{i-1}, C_{i-1}, \text{ or } (\lambda_{i-1} + C_{i-1}),^*$ depending on the coupling from precursor $i-1$;

$C_{i-1} = A_{i-1}(t_0) - F_{i-1}(t_0)$, capture rate at $t = t_0$;

α_i = input quantity; this term will usually be unity.

An equation of the form

$$\frac{dN}{dt} = \bar{Y} \quad (2)$$

is available for special purposes. It must be used for a one-nuclide chain and can be used to represent lumped fission products. If the chain has no yield term, the equation has the form $dN/dt = 0$ and can be used as a dummy chain to represent a nondepleting nuclide.

The preparation of a chain description is somewhat time-consuming and must be done with great care. Once the description has been prepared for a particular chain, though, it need not be repeated from one problem to another. The input format allows the same cards to be used for all problems in which that chain is desired.

B. Solution of Depletion Equations

The solution method of England⁽⁵⁾ was selected because of the control of rounding errors using only single precision calculation. The set of equations to be solved are

$$\frac{dN_i}{dt} = \bar{Y}_i + \delta_{i-1}N_{i-1} - \gamma_i N_i; \quad i = 1, \dots, I. \quad (3)$$

The term $\bar{Y}_i$ and coefficients $\delta_{i-1} = \alpha_i \beta_{i-1}$ and $\gamma_i = \lambda_i + A_i$ are assumed constant insofar as the solution of Eq. (3) is concerned.

The general solution for the n^{th} nuclide in a chain at time t_1 ($t_1 = t_0 + \Delta t$) is

$$N_n(t_1) = \sum_{m=1}^n \delta_n^{-1} \prod_{k=m}^n \delta_k \left\{ \bar{Y}_m \left[\frac{1}{\prod_{\ell=m}^n \gamma_\ell} - \sum_{j=m}^n \frac{\exp(-\gamma_j \Delta t)}{\gamma_j \prod_{\substack{\ell=m \\ \ell \neq j}}^n (\gamma_\ell - \gamma_j)} \right] + N_m(t_0) \left[\sum_{j=m}^n \frac{\exp(-\gamma_j \Delta t)}{\prod_{\substack{\ell=m \\ \ell \neq j}}^n (\gamma_\ell - \gamma_j)} \right] \right\}, \quad (4)$$

*The $\lambda_{i-1} + C_{i-1}$ coupling is not a real physical phenomenon but may be useful in approximating a more complicated chain.

provided $\gamma_i \neq \gamma_j$ for $i \neq j$ and $\gamma_i \neq 0$. The interpretation of Eq. (4) is that nuclide $m(m < n)$ feeds n indirectly by feeding $m + 1$, which feeds into $m + 2$, etc. These contributions defined by the outer summation are further resolved into the contribution from the yield source of m (first set of brackets), and the contribution from the accumulation of m present at time t_0 (second set of brackets).

From this physical interpretation of the terms of Eq. (4) it is clear that for small Δt or for large differences of $n - m$ such partial contributions must tend to zero; that is, terms in the two sets of brackets must become small. Because of the finite number of significant digits carried in the computation (say N), it is also clear that the summation cannot be calculated correctly if it is smaller than $\bar{B} \cdot 10^{-N}$, where $\bar{B}$ is the maximum of the bracketed terms. Thus, when the inequality

$$|[B_m + \dots + B_n]/\bar{B}| \geq 10^{-N} \quad (5)$$

is not satisfied for some $m = \mu$ and $n = \nu$, this contribution and contributions from all nuclides further removed from n are ignored, that is, the outer summation for the bracketed terms is changed to be from $m = \mu + 1$ to n for $n = \nu, \nu + 1, \dots, I$. For the Philco-2000 computer $N = 9$ is used. The above criterion is applied automatically, and no indication is given in the output when it is triggered.

Small terms in the second bracketed expression could also cause trouble. In this case the program examines

$$|\gamma_i \Delta t| \geq 10^{-M} \quad (6)$$

and

$$|(\gamma_i - \gamma_j) \Delta t| \geq 10^{-M}, \quad (7)$$

again with $M = 9$ with the Philco-2000. The inequality (6) is tested for each i in the chain. If the inequality does not hold, γ_i is replaced by $10^{-M}/\Delta t$, and a comment in the output indicates that at a certain point in the mesh, the decay constant of the i^{th} nuclide in the k^{th} chain has been modified by $[(10^{-M}/\Delta t) - \gamma_i]$. Similarly, the second criterion is then applied to each i in the chain for each $j > i$.

C. Time Intervals

Three time intervals are involved in the depletion calculations. The largest time interval is that between spatial calculations, i.e., within this time interval, say from T_0 to T_1 , each of the group fluxes is assumed not to vary in shape.

The second time interval is called a renormalization interval and is a subdivision of the interval between spatial calculations. Experience has shown that the thermal-group flux level changes more rapidly with depletion than does the shape of the flux in any of the groups. The renormalization interval is used to keep the depletion calculation close to constant power by a renormalization of the thermal flux level. For example, in a highly enriched uranium core the thermal flux will increase from one renormalization interval to the next to account for the decrease in Σ^f .

The renormalization interval Δt may be further subdivided into subintervals of equal length, $\Delta t' = \Delta t/n$. This third time interval allows the cross sections and self-shielding factors to vary in time. Equation (3) is then solved for each subinterval. Since the cross sections are evaluated at the beginning of each subinterval and remain constant for the subinterval, they are treated as step functions.

D. Chain Lists and Their Assignments

Once the chain descriptions have been established, there must be a mechanism for determining which nuclides will appear together in a composition. This is done in two steps by (1) giving several lists of chains and then (2) associating one of these chain lists with each depleting composition.

A chain list is merely a list of chain numbers of those chains which are to be grouped together. Through the chain list assignment, each composition is given a chain list number. Thus, a list of permissible nuclides is assigned to each composition.

III. CROSS-SECTION DATA

The advantage of the few-group rather than the multigroup formulation of the diffusion equations lies, of course, in the economy achieved. This is particularly important when two or three spatial dimensions are involved. The basic assumption, of course, is that appropriate cross sections for each of the few groups can be defined. In practice, it is assumed that the cross sections are uniform within any region in which the materials properties are uniform.

The simplest representation of cross sections is that used in the original CANDLE and TURBO programs. One set of microscopic cross sections was assumed to apply throughout the problem; this corresponds to an assumption that the reactor spectrum within a group was spatially independent. The macroscopic cross sections were calculated from

$$\Sigma = \sum_i N_i \sigma_i \quad (8)$$

and varied from one region to another through inventory changes only.

The need for improved accuracy in the analysis of long-lived reactors has resulted in extensions of this simple representation. What is generally required is the ability to represent (through the microscopic cross section) changes of the spectrum within a group both spatially and, as depletion occurs, with time. This need has been realized to date by representing the microscopic cross sections as functionally dependent on the concentrations of the nuclides in the region. The functional form used in each case has been chosen to best represent the cross-section variation of the particular nuclide in an anticipated environment. For instance, self-shielding factors have been represented as a hyperbolic function of a nuclide concentration; the cross sections used to represent lumped burnable poisons have been represented as a fifth-degree polynomial in the poison concentration; the epithermal absorption cross sections of U^{235} , U^{238} , Pu^{239} , and Pu^{240} have been represented as a bilinear fit to the U^{235} and U^{238} concentrations.

The capability of having the program user specify an arbitrary set of nuclides and depletion equations puts even a greater demand on the representation of few-group cross sections in depletion programs. A suitable solution to the problem has been developed by use of n-dimensional interpolation tables. This approach clearly will allow the desired generality. At first sight, however, it would appear to result in a prohibitive data-storage problem. Fortunately, by recognizing features of the physical problem, the generality of the n-dimensional tables can be retained while the number of table entries required is severely reduced.

Few-group cross sections are required in two segments of the diffusion-depletion calculations, macroscopic quantities for the spatial solution, and microscopic cross sections for the depletion. Macroscopic cross sections are computed in this system from the equation

$$\Sigma^{t,g} = \Sigma_0^{t,g} + \sum_i N_i G_i^{t,g} \sigma_i^{t,g}; \quad Dg = (3\Sigma^{tr,g})^{-1}, \quad (9)$$

where t = type (absorption, removal, etc.), g = group, i = nuclide index, N = nuclide concentration, and G = shielding factor. Both Σ_0 and σ may be composition dependent and, in addition, the user may specify some or all of Σ_0 , σ , and G to have a dependence on up to three nuclide concentrations, i.e., Σ_0 , σ , and G may vary spatially from point to point as they are interpolated from spatial nonuniform nuclide concentrations.

The microscopic cross sections used in computing $\Sigma^{t,g}$ are only those assigned to depletable nuclides. For a given composition, the depletable nuclides are those in the chain list assigned to that composition. The contribution of the nondepletable nuclides in that composition to $\Sigma^{t,g}$ must be included in the $\Sigma_0^{t,g}$ term.

The cross-section data are input in one of three basic table forms. A table of fixed values (not time-dependent) of the macroscopic cross sections $\Sigma_0^t g$ may be specified. This table is complete in that values of $\Sigma_0^t g$ are to be specified for all types t and all groups g . A Σ_0 table completely specifies the few-group cross sections for a nondepletable composition.

The second type of table [called the $\sigma(i,g)$ table] is used to specify fixed values of microscopic cross sections for the depletable nuclides. One $\sigma(i,g)$ table specifies all types (σ^{tr} , σ^a , σ^r , σ^f , ν , κ) for group g of nuclide i . The reason for identifying the $\sigma(i,g)$ tables separately for each group is that in one group the microscopic cross sections for nuclide i may differ from one composition to another, whereas for another group the same $\sigma(i,g)$ table may be used in several compositions.

The third type of table (interpolating table) allows any of the parameters Σ_0^t , $G_1^t g$, or $\sigma_1^t g$ to vary with time. This time dependence is accomplished by allowing the cross section to depend on up to three nuclide concentrations N_j in an n -dimensional table, e.g., $\sigma = \sigma(N_1, N_2, \dots)$. It is recognized, however, that the nuclide concentrations are not truly independent variables. As one of the nuclide concentrations, say N_1 , changes with depletion, there is a most probable combination of $N_2, N_3 \dots$ for each value of N_1 , representative of the average found in the composition. This combination defines the principal diagonal of the table.

Fig. 2. Example of a Two-dimensional Interpolation Table

An example of the principal diagonal is shown in Fig. 2 for a two-dimensional table. The principal independent variable is assumed to be N_1 . The combinations of N_1 and N_2 indicated by the X entries in Fig. 2 represent results that may have been obtained from a point depletion of the material or from a spatial average of a previous diffusion-depletion problem. Although the combinations of concentrations given by the diagonal elements are typical, other combinations will occur which reflect the variation in group-flux ratios occurring spatially in the region. Entries

off the diagonal provide a means for representing deviations from the principal diagonal, as shown by the circles in Fig. 2.

It is assumed that the number of off-diagonal locations that will have entries will be much less than the total number of locations available. The ability to describe the dependence of the functions with tables that are not full is important in the storage of the cross-section data.

For each combination of independent variables indicated by the entries in the two-dimensional table of Fig. 2, a value of the dependent variable [e.g., $\sigma(N_1, N_2)$] is available. Let us assume that a cross section is desired for the combinations of N_1 and N_2 indicated by the triangle. $\sigma(\Delta)$ is obtained as follows. A one-dimensional interpolation is performed for σ vs N_1 , the principal independent variable, to obtain $\sigma(\square)$. A similar interpolation is performed from the diagonal values of N_1 to obtain the value of N_2 corresponding to N_1 at the $\square$ point. The off-diagonal entries closest to the Δ point are now used to correct $\sigma(\square)$ to $\sigma(\Delta)$. The slopes between X_4 and O_3 and between X_6 and O_4 are found; then an interpolation of these slopes vs N_1 is performed to get the slope corresponding to the N_1 at the Δ point. This slope is used to correct $\sigma(\square)$ to $\sigma(\Delta)$.

The interpolation procedure also recognizes that the same combinations of independent variables may be used for several cross-section interpolations. Several tables of cross sections may be assigned to a single mask of independent variables. This eases the storage requirements and also makes the interpolation more efficient. For a particular depletion block, a formula is generated involving only the independent variables for which the function is to be determined. The formula is then evaluated for each function that applies to that mask, thus considerably reducing the computing time.

The assignment of cross-section tables by composition is performed by table set. A table set is a collection of the three types of tables described above and may include one Σ_0 table, several $\sigma(i, g)$ tables, and several interpolating tables. The use of the table set allows a simple identification of a collection of tables which are usually found together. A straightforward input of cross-section tables would involve the construction of a unique table set for each composition. Each table set would contain a Σ_0 table and a $\sigma(i, g)$ table for each group for each depletable nuclide. If some of the cross sections were desired to be time-dependent, additional interpolating tables would also be assigned to the table set.

The more complicated problems will generally require a large number of tables. However, the program is limited in the total number of data items which can be retained. In order to run large problems which would otherwise exceed the storage capacity there must be some procedure for reducing the total number of tables used. This is done by allowing a table to be used in more than one composition. For example, the user may decide that $\sigma(i, g)$ tables from several table sets are essentially the same and, after choosing one of these, may discard the others.

IV. OUTPUT

The output data from this program are available in two forms: (1) hard-copy printing and (2) data files. The printed data are optional and include mesh-dependent data (flux, power, nuclide concentrations) as well as integrals and averages of quantities computed by the system. The output of this program may be used for further engineering analysis of the reactor and power plant. This may be accomplished with the data files stored on magnetic tape to which access may be made by other programs.

No attempt is made in the program to make available all of the combinations of integral data of possible interest to the user. Rather, basic integral data (absorption rates, fission rates, average nuclide concentrations, etc.) are placed on file, and the user may process the data with other programs in the computer system to satisfy specific needs. In both the filed and edited data, integrals and averages may be obtained over arbitrary regions and sets of regions, independent of the material regions.

V. STORAGE ALLOCATION

One of the more difficult problems to solve in programming a system of this kind in which very few constraints are imposed is that of storage allocation, both fast and external. For example, there are no fixed limits to the number of nuclides that may be represented, the amount of editing requested, the number of mesh blocks to be depleted, nor to the number of energy groups of fluxes allowed. This requires the program to make judicious decisions as to assignment of data to balance core-storage availability and external storage use with random access requirements. For instance, when integral data (by region) are required, the number of regions may be too large for the amount of core storage available. The program senses the situation in which the data would overflow core storage and reduces the number of regions (with an appropriate comment in the output) so that overflow does not occur. The program uses no fixed storage layout, but "trades-off" each variable against all others. Thus the limitations imposed on problem size are not as to the size of any one parameter, but on the total amount of storage required. For example, a large number of fission products may be represented explicitly at a cost of more core storage due to an increase in the number of nuclides, but this may imply a reduction in the number of time-dependent cross sections that may be represented in order to fit within the total storage available.

VI. APPLICATION

There is no doubt that the use of this system in its full generality and capability is expensive. However, the program is so written that a trade-off of accuracy, completeness, and running time can be made fairly easily.

For example, in early-design survey work, the user may use representations of nuclides and cross sections that are appropriate to the accuracy required at a relatively low cost. However, if the user in some final design studies wishes to use a more sophisticated treatment of nuclides and/or cross sections, the capability is readily available at a reasonable increase in cost.

The cost of this system is not easy to ascertain because of the many parameters involved. Time dependence of cross sections may be obtained at many different costs depending on the complexity of the interpolating tables used. For example, one-dimensional interpolations are less expensive by an order of magnitude than two-dimensional interpolations. Also, the running time of the depletion is not necessarily directly proportional to the number of nuclides present. The time to deplete depends, again, on the complexity and number of interpolations that have to be performed, and also on the specific descriptions of the chains present. For example, it is much more costly to evaluate a ten-nuclide chain than to evaluate five two-nuclide chains.

The HARMONY depletion system has been implemented in the five-group, two dimensional PDQ 5, 6 spatial programs, replacing the TURBO depletion system used in the past. Some examples of the variety of problem types for which HARMONY is being used are given below.

A. Detailed Representation of Fission Products

The older depletion models⁽⁴⁾ allowed fission product poisoning to be represented in an approximate fashion with two fictitious nuclides. The fission yields and cross sections for these nuclides are obtained from a fit to an infinite-medium depletion calculation⁽⁵⁾ in which 179 fission product nuclides are represented explicitly.

One of the analysis groups used HARMONY to perform a series of calculations to test the validity of the fitting process being used. With the HARMONY system in PDQ-5, thirty-two fission product nuclides were represented explicitly along with seven fuel nuclides. Four groups of neutron energy were used in a 15,000-point problem, which was explicitly depleted in 4500 depletion areas. (No renormalization or subintervals were used.)

The total running time for these problems was approximately one hour with the Philco-2000. Of this hour, the time required to evaluate the macroscopic cross sections for the spatial calculation from the microscopic data was about 5 min. Full mesh depletion required about 10 min.

B. Study of Long-lifetime Reactors

The extensive depletion of long-lived reactors results in a significant change in inventory between the beginning and end of life. The few-group

cross sections are affected not only through the direct change in concentration of the different materials, but also through the effect of a change in the spectrum on the microscopic cross sections. These changes in microscopic cross sections may be as large as 50% as a result of extensive depletion.

An example of extensive use of tabulation in HARMONY is found in the study of such a reactor. In the study, six different material compositions which were depleted were investigated. In each composition an average of 10 two-dimensional tables and 15 one-dimensional tables were used. The two-dimensional tables had 10 diagonal entries and 9 off-diagonal entries. The one-dimensional tables averaged 8 entries. The total running time per time step for a 4000-point problem was approximately 0.5 hr. Of this time, 0.3 hr was used in calculating the macroscopic cross sections and obtaining the spatial solution, while ~0.15 hr was used in performing the depletion calculation (no renormalization was done). This example demonstrates the use of the system to obtain an accurate cross-section representation while still keeping the relative costs in balance.

C. Beginning-of-life Surveys

Another example of the use of the interpolating tables in HARMONY is their use in survey calculations with PDQ-5. Of interest in these calculations is the effect of metal-to-water ratio, k_{∞} , optical thickness of lumped boron, fuel loading, enrichment, etc., on the multiplication and power distributions of a reactor. The procedure used is to tabulate the few-group macroscopic cross sections vs one or more of these parameters. The parameter is represented in the program as a nuclide of concentration N_p and zero cross section. Then, as each value of the parameter is desired, it is entered in the program for N_p , the macroscopic cross sections are interpolated, and the desired problem solved.

D. Temperature-feedback Calculations

The iteration between power shape and temperature effects requires calculation of the macroscopic cross sections for spatial iteration n based on the density and temperature distributions obtained from iteration $n - 1$. The cross-section representation used in HARMONY is well-suited to represent the desired cross-section changes when the thermal-hydraulics equations are added to a spatial-depletion program. In one application, fictitious nuclide concentrations are defined as $N_{\rho} = \Delta N_{H_2O}$, $N_{TM} = T_M - T_{MO}$, and $N_{TF} = \sqrt{T_F} - \sqrt{T_{FO}}$. The quantities ΔN_{H_2O} , $T_M - T_{MO}$, and $\sqrt{T_F} - \sqrt{T_{FO}}$ are deviations from nominal of the coolant density, coolant temperature, and fuel temperature. These are calculated for each thermal-hydraulics region of a problem each time the thermal-hydraulics equations are solved.

In the HARMONY system these fictitious nuclides can be used as independent variables for the group cross sections, allowing any of the cross sections to be functions of moderator density, moderator temperature, or fuel temperature. An approach more economical in table storage and evaluation cost is to assign cross sections to the T-H variables themselves. In practice, a combination of the two representations is required to yield a good representation of temperature-feedback effects in a depletion problem.

E. Replacement

Still another use for which the system is well-suited is the replacement of a depletable portion of the reactor with new material. This problem turns up in practice when a power or test reactor is used as an irradiation facility. The assignment of depletion chains by composition allows the new material to contain nuclides that did not exist in the original reactor. After the substitution has been made, the new material can be depleted in the environment of a partially depleted reactor.

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Discussion of Paper
Presented by Mr. Breen

MR. GRIGGS (Windscale): Did I understand you to say that you solved the burnup equations analytically rather than numerically?

MR. BREEN: We do have the analytical solution for the linear chains in the program.

MR. GRIGGS: It seems to me that this might lead to great complication when you are coupling this with the facility to write your own depletion chains. How do you manage to write the analytic solution if the user is writing the chains? How do you know what the analytic solution is of the chains which you are going to specify?

MR. BREEN: Basically we use the equation

$$\frac{dN_i}{dt} = \bar{Y}_i + \delta_{i-1}N_{i-1} - \gamma_i N_i.$$

MR. GRIGGS: Is this a sufficiently general equation to cope with what your user might need?

MR. BREEN: Yes, very definitely. The fact that he must resolve a complicated chain into a linear chain means that all chains look the same.

MR. GRIGGS: We found in the ARGOSY program that some of the chains were very long if you were starting with uranium-238 and going to plutonium-241. In looking at the fission products, we saved a lot of computer time by using Runge-Kutta integration techniques. I was wondering if you had compared the two.

MR. BREEN: No, we were looking for a general capability. The fission products are treated separately. They are not shown as a continuous chain along with the fuel nuclides. We represent the fuel nuclides and the fission product chains with different sets of equations and couple them through the yield term - the $\bar{Y}$ term - so we don't end up with 50 element chains or anything like that.

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EXPERIENCE WITH UNUSUAL TECHNIQUES USED IN ORNL DEPLETION CODES*

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Introduction

Calculation of the long-time behavior of a reactor core is possible only after gross simplifications have been made to fundamental equations. The number and nature of these simplifications raise questions as to the reliability of results. The decrease in computing cost and increase in capacity of digital computers allow expanded treatment of the depletion problem, but the effort and cost required to develop computer programs cause effective tools to lag behind computer capability.

The purposes of this presentation are to discuss unusual techniques used in core-depletion codes developed at ORNL, to examine results of representative calculations, and to examine effects of some of the approximations usually employed. Special techniques have been used to derive iterative procedures, and a form of direct iteration has been found practical to solve the neutron-flux problem for a desired eigenvalue by necessary adjustment of nuclide concentrations. Use of a general, explicit calculation of nuclide concentrations with flux exposure has proven successful. In this, chain relationships are specified as input data, and thereby control is exercised over the treatment used in each case.

The techniques under discussion are used in the IBM-7090 codes TONG,⁽¹⁾ EQUIPOISE BURNOUT,⁽²⁾ and ASSAULT.⁽³⁾ These codes are, respectively, a point spectrum calculation, a two-group, two-dimensional diffusion-theory calculation, and a multigroup, two-dimensional diffusion-theory calculation, as indicated by the descriptions in Table 1. These programs have been used successfully for the analysis of many different core concepts using the techniques described.

Table 1
DESCRIPTION OF DEPLETION CODE TREATMENT
(Complete group-to-group scattering allowed)

Code	Geometric Dimensions	Neutron Groups	Direct Search	Nuclide Cross-section Sets	Number of Nuclides	Normal Use	Example of IBM-7090 Time (hr)
TONG (multizone)	0	30	Fuel, poison	75	1,000	Many cycles, long history for large cores	1
EQUIPOISE BURNOUT	2	2	Fuel poison	100	8,000	Well-behaved cores	2
ASSAULT	2	~20	Poison, source	200	12,000	Cores with complex neutron spectra	7

Notes

TONG--Depletion problem in the fast memory, except that tape is used to supply microscopic transfer cross sections
EQUIPOISE BURNOUT--Eigenvalue problem with search is in the fast memory
ASSAULT--Uses the iterative procedure of EXTERMINATOR,⁽⁴⁾ involving machine language buffering of data and line relaxation

*Research sponsored by the U. S. Atomic Energy Commission under contract with the Union Carbide Corporation.

Practical Observations about Iterative Techniques

The method conventionally used to solve the finite-difference, neutron-flux eigenvalue problem consists of iteration of the flux through the space-energy mesh to satisfy a fixed fission source. The source is then recalculated and the process continued. The single-point eigenvalue problem without upscatter will be solved by code TONG in one downward pass through the energy mesh.

The thermal-flux problem converges more rapidly if the source is renormalized to the new fluxes or the fluxes renormalized to the source. Many situations have been found for which the source can be moved toward the fluxes faster than the iterated fluxes will move toward the source. The EQUIPOISE method⁽⁵⁾ uses latest sources; it has been found that most problems are solved as fast by this method as they are by the inner-outer iterative technique, and faster if upscattering is involved.

A point of concern is that the techniques currently being used do not fulfill the presently known theoretical requirements for assuring a convergent process. A problem must be driven to reduce calculating time, and the Liebmann over-relaxation process is commonly employed, as shown in Eq. (1):

$$\phi_{n+1} = \phi_n + \beta(\phi^* - \phi_n). \quad (1)$$

Here β is the over-relaxation coefficient, n represents the iteration number, and ϕ^* is the newly calculated flux. Theory predicts an optimum value of β for a noneigenvalue problem which depends on the particular iteration procedure used. This optimum value also applies to the eigenvalue problem when nearly converged, since, when the eigenvalue of the problem has been obtained to several significant figures, the iterative problem becomes, in effect, a noneigenvalue problem. Experience with calculations has shown that a large value of β is desirable in the early stages of a problem. Solution with code ASSAULT of an eigenvalue problem started with a flat source required a value of β greater than 1.6 to obtain convergence in a reasonable number of iterations. For succeeding calculations during reactor depletion, with good source guesses available, an optimum value of 1.2 was found.

Whereas Eq. (1) allows negative values, it has been found desirable to modify the over-relaxation process to restrict ϕ_{n+1} to positive values. This point is discussed in greater detail by Tobias in a paper presented at this conference.⁽⁶⁾

Extrapolation of point-flux values is especially desirable for eigenvalue problems in which a good initial flux guess is available and may allow more elaborate treatments within the limitations on computer time that can

be justified. The technique employed is that of Richardson.⁽⁷⁾ If the flux values are moving in a well-defined mode such that the absolute error is well behaved, then

$$\phi_{\infty} - \phi_n \cong A u^n, \quad u < 1. \quad (2)$$

Here, A is a constant and u is a measure of relative change, given by

$$u = \frac{\phi_n - \phi_{n-1}}{\phi_{n-1} - \phi_{n-2}}. \quad (3)$$

A well-behaved mode is indicated when u is relatively constant, and in this case extrapolation is employed in the form

$$\phi_{\infty} = \phi_n + \left(\frac{u}{1-u} \right) (\phi_n - \phi_{n-1}). \quad (4)$$

A suitable value of u must be estimated from a set of point-flux values, usually when only a few of all the values of both ϕ_n and ϕ_{n-1} are available. Experience is being relied on to indicate how best to determine u , whether or not some limiting maximum flux change is desirable, and how often extrapolation is desirable. The direct search method discussed below adds complications. Further work in this area is expected to improve the extrapolation procedure. Console control is used for problems requiring a large amount of machine time. In a representative calculation with code ASSAULT, less than 40 iterations were required to satisfy a specified convergence with extrapolation compared with about 100 iterations without it for a two-dimensional, five-fast and three-thermal group problem.

Direct Search

One method frequently used to determine the critical value of a selected reactor parameter involves solution of a succession of eigenvalue problems for successive estimates of the desired critical parameter. With an inner-outer iteration technique for solving each of the eigenvalue problems, a three-fold iteration scheme is required to determine the selected parameter. Considering that the EQUIPOISE method solves the eigenvalue problem in a single iterative process,⁽⁶⁾ it seemed reasonable that a single iterative scheme could be used for criticality search on poison or fuel concentration. The direct search method is the EQUIPOISE method, with the search nuclide concentration treated as the eigenvalue of the problem. Consider that a sweep has been made through the energy-space mesh. The summed neutron productions, absorptions, and external leakage are then calculated with the latest flux values. An unconverged eigenvalue, Λ^n , may be associated with this mesh sweep as required to satisfy a neutron balance,

Eigenvalue x Productions = Absorptions + Leakage, or

$$\Lambda^n P^n = A^n + L^n. \quad (5)$$

If this eigenvalue is within the convergence criterion specified (and other criteria are also satisfied), the problem is solved. Otherwise, the total contribution to Eq. (5) from the search nuclide is calculated:

$$\delta_N(\Lambda^n P^n - A^n) = \sum_{\text{Volume}} \Delta V N^n \sum_{\text{Energy}} \phi^n (\Lambda^n \nu \sigma_f - \sigma_a), \quad (6)$$

where

Λ^n is the specified eigenvalue,

$\Delta V N$ is the total volume times the nuclide concentration, and

$\nu \sigma_f$ and σ_a are the microscopic production and absorption cross sections.

If a small change in N produces a proportional change in δ_N , a first approximation, then the required change in N is estimated by

$$\frac{\Delta N}{N} = \frac{A^n + L^n - \Lambda^n P^n}{\sum_{\text{Volume}} \Delta V N^n \sum_{\text{Energy}} \phi^n (\Lambda^n \nu \sigma_f - \sigma_a)}. \quad (7)$$

The iterative process is then continued with this change introduced. Since only production and absorption terms are considered, a moderator search is not possible. However, small changes in macroscopic cross sections may be included.

Code TONG employs this scheme with several variations. Several nuclide concentrations may be considered to vary in proportion to either existing or initial concentrations. Several may be increasing while another decreases (inverse search). In code ASSAULT, we only consider the absorption contributions in the denominator of Eq. (7) in a macroscopic sense. More elaborate weighting of reaction rates than used in Eq. (7) could be obtained with adjoint fluxes, but would not be practical in this scheme of direct iteration.

Whereas any real physical reactor problem has an eigenvalue, there are situations for which it is impossible to satisfy a desired eigenvalue by changing certain nuclide concentrations. By means of the above direct search, such impossible situations will usually be discovered in only a few iterations.

To illustrate an application of the direct search, consider that a small, high-energy neutron source is located in a subcritical core. The steady-state flux distribution is to be determined. One procedure might be to iterate the flux values from some initial set. The alternative procedure would be a direct search on the required source strength, with renormalization after convergence. Application of the first approach to such a problem concerning the EGCR core did not produce a solution after many iterations, while application of the direct search required relatively few iterations.

An initial fuel-search calculation with the code TONG might normally require fifteen sweeps through the energy mesh, but only about five iterations are required for succeeding poison search problems even when several thermal groups are considered. A representative, ordinary eigenvalue problem containing 2376 "inside" energy-space points was solved in 0.050 hr of machine time by the code EQUIPOISE BURNOUT; a direct search on poison required 0.084 hr and a direct search on fuel required 0.100 hr. The direct search problem is solved in about the same number of iterations as the ordinary eigenvalue problem, but requires more computing time since constants for the point neutron balance equations must be recalculated. Nevertheless, the computing time is considerably less than would be required in a conventional, three-fold iteration scheme.

Results of Calculations

A comparison of results of code ASSAULT calculations is possible from the presentation in Table 2. In this code the direct search takes no more time for a mesh sweep than the usual eigenvalue problem. Little effect is found from significant relaxation of convergence criteria. Application of a two-dimensional code to a one-dimensional problem is not very efficient. These results are considered representative of what would be obtained with consideration of two dimensions; the machine time which would be required to make this study considering two dimensions could not be justified. The capability to deplete a critical core is considered very important.

Table 2
EFFECT OF RELAXING CONVERGENCE CRITERIA ON LIFE CALCULATED^a
FOR A 1000-MW PRESSURIZED WATER CORE

Case	Depletion Time Steps	Number of Iterations		Maximum Relative Flux Change at End of Eigenvalue Problems		Depletion Life (hr)	IBM-7090 Machine Time (hr)
		Total	Initial Eigenvalue Problem	First Problem	Last Problem		
Nonpoisoned (Eigenvalue "Floated")							
KK-1 ^b	13	582	72	6.3-05 ^c	9.0-05	14,714	0.78
KK-2	13	116	20	2.3-02	5.0-03	14,690	0.46
KK-3	13	46	10	0.49	0.017	14,740	0.43 ^d
Direct, Uniform Control Poison Search (Boron, Shielded Thermally)							
KL-1 ^b	13	551	72	8.0-05	7.6-05	15,490	0.79 ^d
KL-2	13	116	20	2.4-02	3.1-03	15,455	0.46
KL-3	13	46	10	0.48	0.026	15,325	0.41

^aDepletion code ASSAULT, one space dimension, nine neutron energy groups including one thermal, 3.068% enrichment

^bSpecified convergence criterion

$$\text{Max} \left| \frac{\phi_n - \phi_{n-1}}{\phi_n} \right| < 0.0001$$

^c6.3-05 = 6.3×10^{-5}

^dFirst problem charged some extra set-up time

By means of the TONG program, calculations were made of the fuel-cycle cost of a 1000-MWe pressurized water reactor, averaged over a 30-yr life. An initial excess reactivity was specified as well as that following refueling; one-third of the core was refueled each time control rod poison had been removed. A basic, fine-energy-group library of cross sections and a particular set of economic ground rules were used. Results of these calculations are displayed in Table 3 and in Fig. 1, showing the dependence of the results on the number of neutron energy groups employed. Relative results are of interest. Not only does the two-group treatment give relatively good results, but it also finds the position of minimum fuel-cycle cost. It may be seen that the inclusion of several thermal groups is as important as the inclusion of several fast groups for this particular water-moderated core. The nine-group calculation employing outer-iteration on nuclide concentration and recalculation of macroscopic transfer cross sections required 170% more computing time for the depletion problem than was required when the direct search method was used. A number of such comparisons may be made by examining the results in Table 3.

Table 3
EFFECT OF NEUTRON GROUPS TREATED
(Three-zone PWR Point Depletion Calculation)

Start-cycle Excess Reactivity	Feed Enrichment (%)								Equilibrium Exposure (MWDt/T)				IBM-7090 Machine Time (hr)	Lines of Machine Edit
	30-yr Average				Equilibrium									
	1 24 (1 14)	1 26 (1 16)	1 27 (1 17)	1 29 (1 19)	1 14	1 16	1 17	1 19	1 14	1 16	1 17	1 19		
Neutron Groups, Total ^a (Fast, Thermal)														
2(1, 1)	2 402	2 835	3 082	3 660	2 424	2 894	3 169	3 829	23,870	30,060	33,480	41,220	0 47 ^b	26,692
9(8, 1)	2 391	2 842	3 104	3 729	2 410	2 898	3 191	3 916	23,800	30,220	33,860	42,350	0 53	28,276
17(16, 1)	2 390	2 840	3 104	3 729	2 412	2 901	3 194	3 922	23,880	30,330	33,980	42,510	0 80	30,204
25(24, 1)	2 393	2 845	3 108	3 735	2 416	2 906	3 200	3 931	23 950	30,430	34,090	42,670	1 05	32,623
28(24, 4)	2 339	2 815	3 101	3 814	2 355	2 869	3 188	4 026	23,600	30,490	34,510	44,430	1 09	36,104
30(24, 6)	2 337	2 815	3 103	3 819	2 353	2 870	3 190	4 032	23,560	30,500	34,530	44,490	1 20	36,105
9(8, 1) ^c	2 388	2 838	3 099	3 745	2 407	2 894	3 185	3 911	23 770	30,180	33,800	42,302	1 22	28,733
9(8, 1) ^d	2 368	2 803	3 055	3 650	2 386	2 854	3 133	3 856	22,890	28,880	32,250	40,050	0 48	23,891
Fuel-cycle Cost (mills / kWhre)														
	30-yr History				Equilibrium									
2(1, 1)	1 6300	1 6154	1 6222	1 6563	1 6167	1 6126	1 6278	1 6905						
9(8, 1)	1 6254	1 6093	1 6162	1 6554	1 6117	1 6062	1 6220	1 6908						
17(16, 1)	1 6228	1 6070	1 6141	1 6533	1 6094	1 6043	1 6204	1 6895						
25(24, 1)	1 6218	1 6061	1 6131	1 6524	1 6086	1 6037	1 6198	1 6891						
28(24, 4)	1 6121	1 5919	1 5988	1 6454	1 6010	1 5917	1 6086	1 6896						
30(24, 6)	1 6117	1 5910	1 5980	1 6452	1 6002	1 5903	1 6074	1 6891						
9(8, 1) ^c	1 6257	1 6094	1 6161	1 6551	1 6121	1 6062	1 6218	1 6904						
9(8, 1) ^d	1 6706	1 6541	1 6602	1 6963	1 6539	1 6470	1 6615	1 7238						
28(24, 4)	1 6270	1 6065	1 6135	1 6602	1 6163	1 6064	1 6235	1 7041	(Semi-annual instead of quarterly accounting)					
28(24, 4)	1 6118	1 5924	1 5995	1 6464	("Jersey Central" declining load factor normalized, quarterly accounting)									

^aThermal cutoff 1.86 eV, 0.13 hr required to prepare 9-group cross sections

^bCould be reduced considerably with a two-group program, time is dependent on information obtained in edit

^cOuter iteration on nuclide concentrations macroscopic transfer cross sections recalculated

^dSimple eigenvalue calculations, k floated (not made critical), direct search used each refueling

Fig. 1. Dependence of Equilibrium Fuel-cycle Cost on Neutron Groups Treated

These results should not be projected directly to space-dependent problems. Experience gained from two-group calculations has shown that the fast-group properties, particularly downscatter, change significantly with position. Only by accounting for this position dependence can reliable eigenvalue results be obtained. When appreciable internal leakage occurs, such as between fuel and fertile zones, multigroup calculations are considered necessary; this is particularly true if such leakage is time dependent.

For a small maritime core, the dependence of calculated life on the length of time steps and the number of fuel-depletion zones was determined with the EQUIPOISE BURNOUT program. The results shown in Table 4 indicate the calculated life to be insensitive to the particular parameters considered; it is noteworthy that here the finite-difference approximations in both space and time yielded an over-estimate of core life.

Table 4

DEPENDENCE OF CALCULATED LIFETIME ON NUMBER OF
FUEL DEPLETION ZONES AND NUMBER OF TIME STEPS

Case	Number of Fuel Depletion Zones ^a	Number of Time Steps	Calculated Reactivity Lifetime (hr)
1-A	9	15	12,954
2-A	18	15	12,852
3-A	18	23	12,811

^aIdentical geometric meshes for a small, enriched uranium, water-moderated core.

Numerical Significance

Usual digital-machine calculations are adequate, accurate to within the probable error of data. However, when two nearly identical numbers are subtracted, serious problems have been encountered in solving equations which appear to present no difficulty. Only by careful arrangement of equations and programing can such problems be minimized.

The explicit solution to the chain equations which describe nuclide behavior as a function of flux exposure involves terms such as

$$e^x - e^y = e^x(1 - e^{y-x}).$$

If $y - x$ is small, then the quantity inside the parentheses may be obtained accurately only by expansion, preferably in a form which allows fast calculation:

$$(1 - e^{-x}) \simeq x(1 - 0.5 x(1 - 0.33 \dots x(1 - 0.25 x(1 - 0.2 x(1 - 0.16 \dots x))))). \quad (8)$$

Even with care in programming there is a limit to the number of nuclides which can reliably be handled in a chain. A situation was examined with nuclide concentrations calculated for a fixed period of exposure to a constant flux. Several short intervals were used rather than one, and the apparent accuracy of final concentrations is indicated in Table 5. Improved results would be expected if short-lived Th^{233} were not included. In most situations the primary source is located within five nuclides back, so the problem is not as serious as might be interpreted from the results shown.

Table 5

APPARENT ACCURACY OF THE EXPLICIT CHAIN CALCULATION
(Significant figures in results)

Nuclide in Chain		Number of Equal Time Steps				
Name	Number	5	10	20	50	99
Th ²³²	1 ^a	7	6	6	6	6
Th ²³³	2	6	6	6	6	5
Pa ²³³ ^b	3	6	7	6	6	6
U ²³³	4	6	6	6	5	5
U ²³⁴	5	6	6	6	5	5
U ²³⁵	6	6	5	6	5	5
U ²³⁶	7	3	3	3	3	3
Np ²³⁷	8	3	3	2	2	2
Pu ²³⁸	9	1	1	1	1	1
Sink	10	1	1	1	1	1

^aOnly first nuclide had an initial concentration and was depleted 10%.

^bU²³⁴ production resulting from Pa²³³ capture, followed by Pa²³⁴ decay, was explicitly included.

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Discussion of Paper
Presented by Mr. Vondy

MR. ROY (Babcock and Wilcox): I am interested in the dependence of the number of thermal groups that were used in the calculation as shown in the figure with the initial fuel enrichment. Were the calculations done for a uranium-238 cycle reactor?

MR. VONDY: Yes, it was with 238 recycle. Plutonium would be the big factor and have a big effect.

MR. ROY: Would you need a large number of thermal groups for the thorium cycle?

MR. VONDY: We have some indication that it is desirable to treat some thermal groups. This is a very complicated problem. If one starts with a set of cross sections that are weighted over a cell, then one does pick up some shift in the cell cross sections if a multi-thermal-group treatment is allowed, and I think this is desirable. How important it is, I don't know.

MR. WACHSPRESS (Knolls Atomic Power Laboratory): Your iterative techniques apparently are justified by numerical experience. There is very little mathematical support for the convergence, as you pointed out, and you have mentioned that the theory for this is very difficult to establish. I would like to point out that the theory is very well-developed for homogeneous reactors. With one material region, a very specific theory, and a theory which explains what is going on for the iterative methods that we use at KAPL, for example, can be developed. I think it would be profitable to look at your equations for a homogeneous reactor, and to examine the convergence rates and the relationship of the effect of your beta on convergence, actually going through a theoretical analysis.

MR. OLSEN (The Martin Company): Kaplan and Henry are publishing a paper, I believe in Nuclear Science and Engineering, discussing, among other things, the discrepancy between a total core reactivity and that measured with the poison by rod bumping. I wonder if perhaps this might be related to the discrepancy that was observed in your results.

MR. VONDY: I believe you are referring to the difference in the depletion time calculated in the two different ways. No, when you deplete with just solving eigenvalue problems and use the associated fluxes you are not depleting with a critical set of fluxes. This leads to a distortion of the depletion problem; it's just a poor calculation. One likes to deplete a critical core.

TRANSMUTATION LOGIC FOR S_n TRANSPORT ANALYSIS

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ABSTRACT

The machine analysis of high-exposure spectral-shift breeder reactors has been extended to span bilinearly coupled multi-energy neutron transport theory and nuclide-transmutation theory. Scaled-matrix power-series evaluation of the matrix-exponential fine structure of the transmutation fields proves to be far superior to both chain-tracing and matrix-diagonalization methods, in range, reliability, speed, and simplicity of logic relevant to the occurrence of complex eigenvalues and coalescent eigenvalues.

MOTIVATION

The vast range and multiplicity of isotope mean lifetimes, the complex energy-angle-temperature dependence of nuclear reactions, the spectral-exposure and power-transfer advantages of heterogeneous multi-cellular structure, the dual seven-dimensional span of the neutron and adjoint phase space of transport theory, and the intricate bilinear interaction between multi-energy neutrons and several hundred isotopic species, all combine to place reliable nuclear-design optimization of high-exposure spectral-shift breeder reactors among the most fundamentally profound analysis problems of reactor physics.

The comparable importance of irregular fine-structure and gross-structure effects in all variables creates severe difficulties of numerical representation and delicately sensitive need for optimally balanced distribution of analysis effort, even for linearly coupled fields. The full effects of bilinear field coupling extend into the dark depths of undeveloped mathematics, but this much is known: analytic solutions for infinite-homogeneous-medium aspects of the problem include the entire family of monopole elliptic functions, which means that bilinear field coupling can generate a multiple-infinite-lattice maze of fine-structure singularities in the complex field, through which machine-integration methods based upon truncated polynomial expansions cannot reliably thread their way.

Machine-analysis penetration of such a pattern of imprecisely known complexity intrinsically requires basing the gross-structure digital representation upon analytic fine-structure functions spanning a convergent domain of completeness akin to that of Laplace-Fourier eigenfunctions.

Exploratory use of such a fine-structure representation for time-variant isotopic transmutation fields originated several years ago in physics development work at Hanford Laboratories (GE-HL program Dual Normal Modes). Theoretically predicted superiority in range, reliability, and speed has been verified empirically in advanced design work on high-exposure nuclear-fuel cycles by over 2 yr of automated comparison with former truncated polynomial representations. Several progressively more versatile versions of the analysis have been programmed for the IBM-7090 Electronic Data Processing System: GE-HL program ALCHEMY, a fast and reliable matrix-exponential transmutation loop developed for iterative use within more comprehensive analyses; GE-HL program ZODIAC, a merger with multi-energy diffusion theory; and GE-HL program S-XIII, a merger with multi-energy transport theory. The first and third of these last three are now available for cooperative exchange distribution.

MATRIX-EXPONENTIAL ISOTOPIIC TRANSMUTATION

With inclusion of both spontaneous and neutron-induced effects, the balance equation for isotopic transmutation underlying nuclear fuel-cycle design work takes the general form

$$\begin{aligned} \partial N_A(\underline{r},t)/\partial t = & Q_A(\underline{r},t) - N_A(\underline{r},t) \lambda_A + \sum_{A'} N_{A'}(\underline{r},t) \lambda_{A' \rightarrow A} \\ & + \int_0^\infty \left[-N_A(\underline{r},t) \sigma_{Aa}(E) + \sum_{A'} N_{A'}(\underline{r},t) \sigma_{A' \rightarrow A}(E) \right] \phi(\underline{r},E,t) dE, \end{aligned} \quad (1)$$

where $N_A(\underline{r},t)$ is the concentration (nuclei/volume) of isotope A at position $\underline{r}$ and time t ; λ_A is the inverse mean life (decay probability/time) of isotope A ; $\lambda_{A' \rightarrow A}$ is the partial inverse mean life (transmutation probability/time) for spontaneous decay of isotope A' into isotope A ; $\phi(\underline{r},E,t) dE$ is the neutron flux (neutrons/area/time) in neutron-energy increment dE ; $\sigma_{Aa}(E)$ is the neutron absorption cross section (total less scatter) of isotope A ; $\sigma_{A' \rightarrow A}(E)$ is the transmutation cross section for conversion of isotope A' to isotope A by all neutron reactions $[(n,\gamma), (n,f), (n,\beta), (n,\alpha), (n,p), (n,2n), \text{etc.}]$; and $Q_A(\underline{r},t)$ is a flexible source-sink representation (nuclei/volume/time) of reactor control rates, fuel-cycle input-output rates, flow divergence rates, and perturbation-theory refinements.

In advanced design work on fast reactors (for which spectral-shift effects vary quite slowly with time), there has evolved a useful range of applicability for a piecewise quasi-constant representation of the neutron energy spectrum $\phi(\underline{r},E,t)$. Such a representation also has potential usefulness for thermal and resonance reactors, subject to the limitation that

the analysis must be broken up into time segments more carefully selected to assure adequate piecewise quasi-constancy of spectral-shift effects.

Within such a time segment, the spectrum-integrated absorption and transmutation cross sections become constants, which can be combined cleanly with the spontaneous decay constants to form a composite transmutation-rate matrix $H_{A' \rightarrow A}(\underline{r})$ whose diagonal elements are the negative loss rates

$$H_{A \rightarrow A}(\underline{r}) \equiv -\lambda_A - \int_0^\infty \sigma_{Aa}(E) \phi(\underline{r}, E) dE, \quad (2a)$$

and whose off-diagonal elements are the positive production rates

$$H_{A' \rightarrow A}(\underline{r}) \equiv \lambda_{A' \rightarrow A} + \int_0^\infty \sigma_{A' \rightarrow A}(E) \phi(\underline{r}, E) dE. \quad (2b)$$

Expressed in terms of this asymmetric transmutation-rate matrix and a discrete Laplace transform representation of the flexible source-sink term, the transmutation balance Eq. (1) becomes

$$\partial N_A(\underline{r}, t) / \partial t = \sum_{A'} N_{A'}(\underline{r}, t) \cdot H_{A' \rightarrow A}(\underline{r}) + \sum_L Q_A(\underline{r}, L) e^{t\omega(\underline{r}, L)}; \quad (3)$$

or, in the more compact symbolism of matrix algebra, with N_A and Q_A viewed as components of row vectors N and Q , and with parametric position dependence suppressed, for brevity,

$$\partial N(t) / \partial t = N(t) \cdot H + \sum_L Q(L) e^{t\omega(L)}, \quad (4)$$

which integrates by inspection to the matrix-exponential solution

$$N(t) = N(0) \cdot e^{tH} + \sum_L Q(L) [e^{tH} - e^{t\omega(L)}] / [H - \omega(L)]. \quad (5)$$

The nuclide-transmutation outer loop of program S(Fig. 1) picks up the neutron flux $\phi(\underline{r}, E)$ from the criticality-controlled constant-power neutron-transport inner loop, processes all relevant input nuclear data in accordance with Eq. (2a, 2b), with inclusion of regional smearing flexibility, and numerically evaluates the matrix power-series representation of the analytic fine-structure solution (5), making exhaustive use of both scaling logic to control rate of series convergence and rounding logic to minimize accrual of truncation error.

Development work on program S began with this machine-analysis flow chart, which summarizes compactly and comprehensively both nuclear analysis method and capabilities. The dual adjoint (ϕ^*)-and-flux (ϕ) successive-free-flight transport loop revolves about the integrated action (S) principle. Loss operator L (leakage, collision, accumulation) may contain linear dependence upon eigenvalue H. Production operator P (fission, in-scatter) may contain linear or multiple-pole eigenvalue dependence. Transmutation logic (spectral-shift perturbation of matrix exponential) is optimal for high-exposure breeder cycles. Grasp the logic of this chart, and the rest of the method becomes deducible detail.

Fig. 1. Neutron- and-photon Transport and Nuclide Transmutation. Variational optimum formulation, plane-cylinder-sphere. General Electric Hanford Laboratories program S.

Output includes both the isotope concentrations (5) and their trends (4), for each region (or analysis point) in the reactor, with arbitrarily fine detail in exposure time, together with correspondingly detailed transport-perturbation-theory conversion to criticality fine structure.

At the end of each such quasi-constant-flux time segment, the final isotope concentrations (5) automatically feed on into the input of the next constant-power transport loop, as shown schematically in the flow chart of Fig. 1, to generate spectral-shift effects at the full level of detail of multi-energy transport theory. Physically realizable criticality controls, all at constant power, include any shape or size of deformation inducible by conformal variation of the metric tensor, and variation of the loading of any reactor material (burnable or inert).

NUMERICS

The machine-analysis symmetry of the general solution (5) can be improved considerably by the otherwise trivial rearrangement of terms

$$N(t) = N(0) + t \cdot N(0) \cdot H \cdot [e^{tH} - 1]/tH + \sum_L t e^{t\omega(L)} \cdot Q(L) \cdot [e^{tH-t\omega(L)} - 1]/[tH - t\omega(L)], \quad (6)$$

Structural similarity now makes it clear that the entire expression can be evaluated quite cleanly by repeated summation of the matrix exponential-integral power series

$$(e^Z - 1)/Z = \sum_{n=0}^{\infty} Z^n/(n+1)! = 1 + (Z/2!) + (Z^2/3!) + \dots, \quad (7)$$

with the matrix Z initialized as tH and modified to $tH - t\omega(L)$ on successive loop traverses.

Informative insight into the intricate numerical behavior of a matrix infinite series of this sort is obtainable by thinking in terms of a diagonalized representation of the matrix (if it exists), for then the matrix series becomes an uncoupled array of scalar series, with collective behavior deducible by scalar logic. Pursuing this thought makes it clear that a matrix infinite series will display satisfactory numerical behavior in machine analysis if and only if the following extremely stringent condition can be met: all the eigenvalues of the matrix must lie within the range of satisfactory numerical behavior for the analogous scalar infinite series.

A closely related observation relevant to devising a method of meeting such a stringent requirement is that the sum of the squares of the magnitudes of all the elements of a matrix is invariant under the unitary transformation group, and thus, for any diagonalizable matrix, is identifiable as the sum of the squares of the magnitudes of all its eigenvalues.

These considerations lead to evaluating the matrix exponential integral $(e^Z - 1)/Z$ by first scaling the matrix Z by the smallest integer power of two which will reduce the sum of the squares of the magnitudes of the elements of the scaled matrix $Z/2^N$ to less than unity, summing to solid convergence the numerically well-behaved scaled matrix series

$$\left[\left(e^{Z/2^N} \right) - 1 \right] / (Z/2^N) = \sum_{n=0}^{\infty} (Z/2^N)^n / (n+1)!, \quad (8)$$

and then unscaling this scaled sum by N -fold recursive traverse of the matrix identity sequence

$$e^Z = Z \cdot (e^Z - 1)/Z + 1; \quad (9a)$$

$$(e^{2Z} - 1)/2Z = [(e^Z + 1)/2][(e^Z - 1)/Z]. \quad (9b)$$

PERFORMANCE

Analysis versatility spans high-exposure spectral-shift breeders, with unrestricted inhomogeneity, with unrestricted exposure time, and with unrestricted transmutation intricacy (spontaneous and induced, endoergic and exoergic, decaying and multiplying, branching and cyclic) including energy-variant induced-yield fractions.

Memory demand is phenomenally low. The entire matrix-exponential isotopic transmutation block of Fig. 1, containing Eqs. (2a, 2b, 4, 5, 8, 9a, and 9b), together with regional smearing logic and control logic, occupies only 380 words of core storage.

Traverse time for the transmutation block varies as the cube of the number of isotopes, averages about 5 sec per exposure region per output-time-point for the fifteen-isotope representation in use by the Hanford advanced design group, and is independent of exposure time.

Cross checks for accuracy obtainable analytically for small full matrices, big degenerate matrices, and big rotation matrices all indicate that the scaling and rounding logic maintains firm six-figure numerical reliability even for the long exposure times of key interest in nuclear-fuel cycles.

The scaled-matrix power-series method of evaluating the matrix-exponential function displays unconditional numerical stability over the full range of machine numbers, positive and negative. As one unique consequence, the transmutation analysis can be run backwards in time quite freely. Correspondingly, it has evolved as standard practice, in running program S, to "thunderbolt" into the future in the overlapping zigzag pattern of a lightning flash, peering far ahead in the matrix-exponential cloudy-crystal-ball before taking each spectral-shift leap, and then glancing back into the spectral-shifted matrix-exponential past to generate intrinsic adequacy-evaluation information for each spectral-shift time segment.

Evaluative comparisons both with matrix-diagonalization methods (employed in program Dual Normal Modes) and with Bateman chain-tracing methods have proven the scaled-matrix power-series evaluation of the matrix-exponential fine structure of the transmutation fields (employed in program ALCHEMY and in program S) to be overwhelmingly superior in versatility, range, reliability, speed, memory economy, programming ease, numerical stability, and simplicity of logic relevant to the occurrence of complex eigenvalues and coalescent eigenvalues.

DEVELOPMENT POTENTIAL

The exploratory program ALCHEMY version of the analysis generates not only the matrix-exponential function, but also the entire family of matrix-generalized hypergeometric functions, such as matrix logarithms, matrix inverse trigonometric functions, matrix Bessel functions, matrix Legendre functions, matrix Tschebyscheff functions, matrix Hermite functions, matrix Laguerre functions, and matrix Jacobi functions. The logic of the ALCHEMY deck spans also complex matrix elements, Pauli spinor matrix elements, Hamilton quaternion matrix elements, Dirac 4-spinor matrix elements, and other hyperalgebraic matrix elements of unrestricted complexity, limited solely by memory demand and machine time. Numerical behavior and physical applications, within this vast unexplored domain of analytic tractability, remain to be investigated.

Background References

The variational-optimum transport-theory inner loop of program S, flow charted in Fig. 1, is described in detail in the following sequence of documents available both at USAEC depository libraries and from the USAEC Technical Information Service Extension, P. O. Box 62, Oak Ridge, Tennessee.

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MAFIA II
A ONE-DIMENSIONAL BURNUP CODE

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Summary

The report describes a one-dimensional burnup code written in Fortran II language for a 32-k-word computer.

The power distribution for up to 4 energy groups may be calculated while the neutron spectrum is recalculated at each time step in 68 fast and 96 thermal groups.

A facility for recharging or reshuffling the fuel in the reactor is included.

A saving in computing time can be achieved by representing the few-group cross sections as a function of the reactor lifetime by means of a polynomial fitting.

Preface

MAFIA-II has been developed because of the need for a code able to deal with both spatial effects of burnup and cross-section variations during life. The code had to cover various reactor types with different fuels.

It was necessary to treat cases for which the neutron spectrum is strongly distorted and has important variations during life as, for instance, with plutonium fuel in undermoderated reactors. For this reason and because of the need for comparing fuel cycles in different types of reactors, it was considered necessary not to use either simplified methods or few-group constants adjusted by experiment. Use of these would not allow the calculations to be easily extended to other reactor types or, for the same reactor, to different isotope contents during its life.

It was therefore decided to use a basic multigroup microscopic library from which few-group data can be produced at each time step during life. The fine structure of the flux in the cell could then be taken into account with previously calculated concentration-dependent self-shielding factors.

As considerable work had already been done in this field by General Atomics Division of General Dynamics Corp., a large use has been made of subroutines written in the codes FEVER,⁽¹⁾ GAM-I,⁽²⁾ and THERMALIZATION;⁽³⁾ the multigroup cross-section library also uses General Atomic data.

Introduction

MAFIA-II is a one-dimensional burnup code written in Fortran II language for a 32-k-word computer. The limitations may be expressed as: 150 meshpoints for the diffusion calculation, 20 burnup regions, and 25 isotopes per region. Calculations may be made in slab or cylinder geometry.

The basic multigroup library is used in a zero-dimensional neutron-spectrum calculation in which the actual reactor size appears only through energy-dependent bucklings and the cell structure through energy- and concentration-dependent self-shielding factors. The resonance absorption is treated as in the GAM-I code by the methods developed by L. W. Nordheim.

The neutron spectrum calculated in this way is used for producing averaged few-group (from 2 to 4) cross sections which allow a fast diffusion calculation giving the power distribution across the core. The few-group energy boundaries are given as input.

The burnup calculation is performed by treating separately a maximum of 20 core regions whose relative power is determined at each time step by the diffusion calculation.

Control poisons in various regions of the reactor can be automatically adjusted according to some specified sequence.

Reshuffling and recharging of fuel regions can be performed.

A simplified flow diagram is shown in Fig. 1.

The spectrum calculation

The calculation of the neutron spectrum is divided into two parts: the calculation of the fast spectrum, which uses a 68-group microscopic library, and the calculation of the thermal spectrum based on a 96-group library.

Each library is on a separate tape. The fast library is actually the General Atomic GAM-I library; the thermal library, especially prepared for MAFIA-II, contains cross section and scattering kernels for different isotopes and temperatures. Any scattering kernel produced with any model can be added to this tape, provided the 96-group structure of the code is used. No upscattering is considered above 2.0 eV, at which energy all kernels are truncated.

Fig. 1. MAFIA-II Simplified Flow Diagram

Out of these two tapes the code makes one short tape containing only the isotopes and kernels used in one particular calculation. The fast cross sections on this short tape are already modified for the Th²³² and U²³⁸ resonance calculation, which is done only at the beginning and never repeated during life.

The resonance integral of the plutonium thermal resonances can be changed during life by making use of concentration-dependent self-shielding factors.

Fine-group self-shielding factors given in the input can be applied to any isotope in the fast and thermal ranges. In addition, other concentration-dependent self-shielding can be applied in the thermal calculation to an energy range defined in the input, different for each plutonium isotope.

The formula used for the fitting of the self-shielding as a function of the concentration is

$$ss = \frac{1}{\sqrt{1 + Ax + Bx^2}},$$

where x is concentration and A and B are input data, previously determined, usually by means of a few DSN calculations. This formula proved in many cases to be better than the polynomial fitting which had been previously used.

The P_1 approximation is used for the fast-spectrum calculation, while P_0 has been considered sufficient for the thermal calculation.

The energy-dependent bucklings used in the spectrum calculation come from the previous diffusion calculation, so that they can be continuously changed during life. This is of particular importance for reactors which are strongly undermoderated at beginning of life; in this case the core has a high negative thermal buckling at beginning of life, whose absolute value strongly decreases at end of life.

An estimate of the initial bucklings is given in the input and, if required, the code can iterate on it between the spectrum and diffusion calculations, before starting with the burnup.

The spectrum calculation can be performed only once at beginning of life or can be repeated at each time step.

To allow for spectrum changes across the core, this can be divided into a maximum of 4 zones, and the zero-dimensional spectrum calculation can be repeated for each zone at each time step, producing 4 different sets of cross sections. By means of the fluxes from the diffusion calculation, different bucklings can be produced for each core zone. Usually, one core zone appears to be sufficient, and computing time increases considerably if more zones are used.

Some reflector regions can be specified, whose few-group cross sections are given as input and never recalculated.

The Calculation of Power Distribution and Effective Multiplication Factor

The diffusion calculation is performed with a maximum of 4 energy groups and with 150 meshpoints. Slowing down may occur only to the next adjacent group, no upscattering is considered, and the fission source may be in the highest group only. These limitations have to be considered when giving, in the input, the few-group energy boundaries.

The diffusion routine is a version of the code F-3⁽⁴⁾ as modified by Todt,⁽¹⁾ which solves the diffusion equations as difference equations in slab or cylindrical geometry.

Nuclides which have been specified in the input as control poisons can be automatically adjusted in various regions of the reactor according

to specified sequences until the effective multiplication factor reaches a given control point (usually 1.0).

The Burnup Calculation

The isotopic-depletion equations are solved by finite-difference approximation.⁽¹⁾ Each time step is subdivided in a given number of small time steps. At each big step the spectrum and diffusion calculations are repeated. At each small step only the flux amplitude is readjusted in order to keep the power constant.

In the present version, the burnup routine can handle up to 20 independent regions and up to 25 materials. The first 15 materials include the chains from Th²³² to U²³⁶, from U²³⁸ to Pu²⁴², a nonsaturating fission product aggregate, Xe¹³⁵, and Sm¹⁴⁹. The remaining 10 nuclides can be additional chains of fission products, burnable poisons, moderators, and structural materials. (A new version is being prepared, which will allow more than 25 materials.)

The calculation is continued until the reactivity drops below a specified control point, or until a given number of time steps, whichever occurs earlier.

Recharging and Reshuffling Subroutine

The reshuffling and recharging subroutine for the MAFIA-II code is kept as general as possible. For this purpose the reactor can be divided into reshuffling areas, each including one or more burnup regions. There can be up to 20 reshuffling areas, and each can include up to 20 burnup regions; the total number of burnup regions must not exceed 20. The regions composing a reshuffling area do not need to be adjacent.

Before each reshuffle the program calculates and prints the average atom densities for each area. Any area can be either recharged with a new composition specified in the input, or get the atom concentration of any other area, or remain unaltered. If an area gets the atomic concentrations of another area, the two volumes must be equal.

A reshuffle can take place after any specified number of time steps or when the reactivity drops below a specified control point. There can be any number of reshuffles during the core lifetime.

Because MAFIA is a one-dimensional code, it is not possible to treat two-dimensional variations of composition. This means that some recharging and reshuffling schemes cannot be followed with this code. For example, in radial geometry it can happen that after a recharge or reshuffle one gets azimuthal variations of composition: the same ring of

fuel elements can contain elements of different composition. One cannot homogenize the ring because in that case the individual composition of the elements is lost for the following reshuffles.

The possibility of defining reshuffling areas out of nonadjacent burnup regions can be used in these cases. In the above-mentioned example it is possible to simulate azimuthal variations by radial variations. The ring can be split into several radial regions, and each azimuthal zone of different fuel elements can be simulated by a reshuffling area consisting of alternative burnup regions.

In this way, as the regions can be made very small, the result of the diffusion calculation will be almost the same as if these zones were homogenized, but the composition of each group of fuel elements is kept separate during burnup.

This subroutine includes also the facility for iterating on the concentration of a material specified in the input, in order to adjust the reactivity to the beginning of life value. The iteration is performed in one or more reshuffling areas, as specified in the input. If the concentrations of the material used for the iteration are different in the areas specified, they are varied in such a way that their ratios remain constant.

Acceleration Option

The accurate representation of the spectrum during life has proved to be of the highest importance, especially in the case of plutonium-fueled, high-temperature graphite reactors.

In some cases the neutron spectrum varies so rapidly that it is necessary to repeat very often the zero-dimensional multigroup calculation, a consequence of which is a considerable increase in computing time. As it has been observed that the variation of the 4-group cross sections with irradiation can be well represented by a second-degree polynomial, an option has been included in the program which makes it possible to go once through the reactor life with two big time steps. The 4-group cross sections can then be represented as a function of irradiation by means of the initial and the two calculated values.

As the reactor composition as a function of irradiation is in this case not very accurate, it may be necessary to iterate once on this calculation. The polynomial fitting of the previous case can be used for obtaining the cross sections at each small time step, and two spectrum calculations can be performed again during life. These will be used to obtain a better representation of cross section. At this point it is possible to perform the final burnup calculation.

This will be as detailed as needed in the number of power-distribution calculations and control-poison adjustment during life, but will not need any spectrum calculation, as the 4-group constants will be calculated from the polynomial fitting at each small time step.

In many cases tested up to now this option has resulted in a considerable saving of computing time without loss in accuracy. The spectrum calculation is the most time-consuming part of the program because it requires a considerable amount of tape manipulation. Even if iteration of the procedure is needed, 4 spectrum calculations during life are sufficient in cases for which more than 12 were necessary for the same accuracy in the ordinary calculation.

This is, of course, useful only in cases in which spectral variations are expected to be considerable, so that one needs many spectrum calculations during life.

Additional Facilities

At each time step, fast and thermal spectra, power distribution, and reactivity are dumped on a tape which can later be used with an automatic data plotter. CALCOMP is at present used in ISPRA.

All data necessary for a restart are also dumped on a different tape so that it is possible to restart the problem after any number of time steps.

Computing Time

Computing time with the IBM-7090 depends upon the nature of the problem.

With 20 core regions, 86 meshpoints, 23 materials, and no control-poison search, typical running time has been of the order of 2.5 min per time step plus an additional 2.5 min at the beginning for starting the problem (making short tape, etc.).

Conclusion

The code has been used intensively for high-temperature graphite reactors and in a few cases for light and heavy water reactors, with uranium and with plutonium fuels.

Figure 2 shows the impressive spectral variations during life which can be found in an undermoderated high-temperature graphite reactor with plutonium fuel. Figure 3 shows the error in the curve of reactivity versus time which one would make by not recalculating the spectrum. Even with U-Th cycles spectral variations cannot be neglected in high-temperature graphite reactors (see Fig. 4).

Fig. 2. Thermal Spectrum with Plutonium Fuel

Fig. 3
Reactivity vs. Time

Fig. 4. Thermal Spectrum with Uranium Fuel

In a few calculations performed for uranium-fueled water reactors, the spectral changes have been found to be of very little significance, but with high plutonium concentrations the spectrum varies again strongly with life.

Acknowledgment

Thanks are due to Mr. G. S. Fassone for the help in debugging the code.

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MECHANISED HANDLING OF NUCLEAR DATA

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INTRODUCTION

Precise and detailed calculations are now a familiar part of the treatment of problems of reactor physics. Such calculations have become possible with the advent of high-speed digital computers having large memories, more advanced theoretical and numerical methods, and more accurate and extended nuclear data. In spite of the high cost of equipment to measure basic nuclear data and to effect complex computations, its use is economically attractive.

It is well-known, however, that basic nuclear data, i.e., essentially the information derived by measurement, are unsuitable for input to most neutronics codes, which generally require derived quantities such as group-averaged cross sections. The preparation of these derived quantities can be extremely laborious, and it is natural to utilize the power of the digital computer to reduce this expenditure of effort. A further advantage of this use of the computer is that the chance of an undetected human error at this stage is almost eliminated.

Many neutronics codes have associated libraries of group-averaged data, frequently in the form of one or more magnetic tapes. Nuclear data are drawn from these libraries on receipt of a relatively simple description of a problem in terms of materials, etc. The more sophisticated of these codes have many-group libraries and provide run-time facilities for data reduction to a number of groups which may be specified and which are considered to be adequate for the calculations in hand. Although arrangements such as these reduce the amount of card handling which need be performed when use is made of these neutronics codes, they do not reduce the considerable effort which is expended whenever additions to or modifications of such a library are required.

There is, therefore, a need to apply the computer to the processing of basic nuclear data to a form suitable for input to neutronics programmes. Without such a facility the use of the most recent nuclear data may be retarded or even inhibited. Further, since it is a common practice of the reactor physicist to compare two or more methods of calculation, it is necessary to ensure that precisely the same microscopic data are provided to the neutronics codes which perform these calculations, even though the nature and format of the derived quantities may vary from code to code.

It follows from the considerations of the previous paragraphs that an organization carrying out many large-scale neutronics calculations can benefit greatly, both in terms of reduced human effort and reduced time for the assimilation of the most recent data, if

- (a) there exists a library of properly assessed basic nuclear data;
- (b) these data are recorded in a form suitable for processing by one or more codes designed to prepare the derived quantities required for neutronics calculations; and
- (c) the above-mentioned code or codes exist and the results are in a form suitable for input to neutronics codes (it follows that it is desirable to restrict to a minimum the number of different input formats for neutronics codes).

THE UKAEA NUCLEAR DATA LIBRARY

The problems of mechanization and standardization outlined above have been treated in the UKAEA by the preparation of a standard library of basic nuclear data, together with a number of computer codes.

Historically, the first UK scheme of this sort was developed at AWRE, Aldermaston.⁽¹⁾ The present work, described by Story *et al.*,⁽²⁾ is the result of collaboration between Aldermaston and AEE, Winfrith, since 1961, and differs in that the nature of the recorded data has been modified and extended, in particular to allow a more refined treatment of the resonance and thermal energy ranges.

The evaluation of basic nuclear data is not discussed here. It will simply be noted that neutron cross sections in the range from 1 meV to 15 MeV for about 40 materials have been compiled by UKAEA workers and others. The data are punched on cards in a flexible and extendible format. A detailed discussion of data evaluation and formats is to be found in Ref. 3.

There are two main processing codes associated with the library: GALAXY,⁽⁴⁾ which generates multigroup cross sections, and DICE,⁽⁵⁾ which processes the basic information to a form suitable for Monte Carlo calculations. Both are written in FORTRAN.

In addition, there exists a set of ancillary codes which is vital to the proper functioning and checking of the library. These are also written in FORTRAN and are also briefly described in Ref. 3. The remainder of this paper is concerned with the detailed functions of one of the major processing codes, GALAXY.

GALAXY

The function of the code is to produce group-averaged data in a form suitable for use by neutronics codes, for instance, those based on the S_n and diffusion approximations to neutron transport theory. The code uses for input the basic nuclear cross-section data in the UKAEA library format, together with control information provided by the user. The group-averaged data produced by the output scheme are printed. In addition, special forms of the output are available for direct input to some of the standard multigroup neutronics codes, including STRAINT, a multigroup anisotropic scatter one-dimensional (sphere or slab) S_n code,⁽⁶⁾ and CRAM, a multigroup two-dimensional diffusion-theory code.⁽⁷⁾

It was recognized that generality would be a dominant characteristic of GALAXY if the code were to provide the majority of physicists with satisfactory facilities for transforming basic nuclear data into group-averaged cross sections. It was acknowledged, of course, that special requirements occasionally arise which could not be accommodated by GALAXY. The code specification and strategy, therefore, aimed at generality, and every effort has been made in the preparation of GALAXY to achieve this. Nevertheless, some restrictions have been imposed, most of which are of minor importance and can easily be relaxed. The only restriction to be noted here concerns the output scheme (see below), which is at present limited to a maximum of 40 groups.

Control data are specified for each of a number of mixtures in turn and include details of the weighting spectrum, proportion of constituent materials, and temperature. [Note: A "material" is an entity for which nuclear data are recorded in the library; it is normally a nuclide, but may be a mixture of nuclides (for instance, a naturally occurring element), or a chemical compound (for instance, BeO).] For each mixture, certain material-independent data are calculated, namely, the average reciprocal velocity, group widths in energy and lethargy units, the mean energy, and the energy corresponding to the mean lethargy. If the total cross section of the mixture is required for spectrum weighting, it is calculated at each of the aggregate of energy points at which the cross sections of the constituent materials are given. An option to form the reciprocally averaged transport cross section is also available.

The code calculates group-averaged partial cross sections for specified reactions and groups, for each material in turn. Any reaction for which data are in the library may be processed in this way. In addition, the group-averaged energy release rate per unit flux is calculated. For neutron-producing reactions, up to six coefficients of the group-averaged transfer cross sections expanded as a sum of Legendre polynomials in the cosine of the laboratory angle of deflection may be produced. At present,

routines exist which produce these moments for the following processes: elastic scattering by a static nucleus, thermal-neutron scattering in accordance with a scattering law of the form $S(\alpha, \beta)$,⁽⁸⁾ inelastic scattering to discrete levels, inelastic scattering to continuum, $(n, 2n)$, $(n, 3n)$, and $(n, \text{fission})$.

Two distinct classes of weighting spectra may be specified for the group-averaging of each mixture:

- (i) that used for the production of material-independent data; and
- (ii) that used for the production of material-dependent data, including the reciprocally averaged transport cross section, if required.

Each of these spectra may, in each group, be a linear combination of up to six basic spectra. The allowed basic spectra are:

- (1) E^{-x} , $x \geq 0$ (E:energy);
- (2) a Maxwellian distribution of specifiable mean energy;
- (3) tabular values, from which intermediate values are derived by assuming linearity on a log-log scale.
- (4) } The above three forms may be divided by the total cross
- (5) } section of the mixture in question.
- (6) }

Fission spectra are accommodated by applying standard forms of type (3) above.

Following the execution of the main section of GALAXY, there exists a magnetic tape containing, for each specified mixture, the processed data described above. These are the averaged data for each reaction and material separately, no combination of reactions or mixing of data for different materials having been effected. In particular, the group-transfer matrices have dimensions $G(G+2)$ to allow for transfer above and below the range of interest. This magnetic tape could be used as input to suitably prepared neutronics codes, either directly or after special processing. It was thought desirable, however, to provide general facilities for mixing, condensing, combining, and substituting. These are effected by the output scheme which operates on the above-mentioned magnetic tape.

The substitution facility, allowing a user to replace some GALAXY-produced quantities by specified alternatives, is not available at present. The remaining three options, which are operational, are the following:

- (1) mixing; corresponding averaged cross sections of the materials comprising a mixture may be added together in specifiable proportions;
- (2) condensing; the computed data may be condensed to fewer groups using a specified spectrum;
- (3) combining; certain combinations of group-averaged data may be formed. For instance, all parasitic absorption cross sections $[(n, \gamma), (n, p), (n, \alpha), \text{etc.}]$ may be added. Similarly, all nonfission group transfer cross sections may be combined.

The IBM-7090 version of the code, written in the FORTRAN II language, is working and in use. Part 2 of the code, the output scheme, also functions on the IBM-7030 (STRETCH) and accepts as input a BCD tape produced by Part 2 of the 7090 version. The code is now being prepared for the English Electric-Leo-Marconi KDF 9 computer.

A description of the capabilities of GALAXY and the preparation of input decks is given in Ref. 4.

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DPC, A TWO-DIMENSIONAL DATA PREPARATION CODE*

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INTRODUCTION

Accurate preparation of reactor engineering design data into a form suitable for neutronic code input is a time-consuming and tedious task. Such calculations, which involve, in the main, the performance of a large number of simple repetitive manipulations, are ideally suited for computer processing. However, a code for this application must be applicable to the great variety of materials configurations that appear in reactor designs, while, at the same time, it should retain a basic simplicity and ease of use in its application to the various problems.

The FORTRAN code DPC was developed primarily for preparing (r,z) input data for the two-dimensional codes DDK⁽¹⁾ and CRAM.⁽²⁾ The techniques developed through application of the code to several different reactor designs are illustrated in the succeeding description of the code.

INPUT DESCRIPTION

For a code such as DPC, input flexibility and readability are of paramount importance. Flexibility of format in the input numbers is achieved, first of all, by processing all input data through the Hassitt-Mitchell Input Routine, DECIN.^(3,4) This routine has been described as accepting any data that can be read by eye. In addition, mnemonic names are used in the input to identify the various data items. Thus the input is specified in a rather narrative style which promotes readability.

Since the storage of data is controlled by the identifying data names, the order of specification is immaterial. This allows multiple specification of data, with only the latest data being used. With this feature, specific corrections or modifications are achieved merely by appending the appropriate changes at the end of the problem deck. Likewise, in a series of related problems, only the required changes to the parent problem need be specified in subsequent problems. Since all data are printed out immediately on being read, a complete record of all such data modifications is maintained for future reference.

*Work performed under the auspices of the United States Atomic Energy Commission.

In the following description of the data types, upper case words are the key words used to identify the data types. The word "name" in every case stands for an alphabetic name supplied by the code user to identify the elements, mixtures, regions, etc., that are used in the problem specifications. Elements and mixtures are described by one word names; boundaries and regions may be assigned names including from zero to four words. Other lower case words, or letters, are used to represent numerical data items. In particular, i , j , k , ℓ , m , or n represent data identification numbers.

Standard Specifications. The specification of a standard cylindrical region may include such statements as given below:

$$\text{REGION } k \text{ name SIDES } i_1 i_2 j_1 j_2 \text{ MTL } m_k \text{ TEMP } t_k \quad (1)$$

$$\text{MTL } m \text{ name } w_1 n_1 w_2 n_2 \dots \text{DENSITY } d \text{ EXPN } x \quad (2)$$

$$\text{ELEMENT } n \text{ name atomic weight} \quad (3)$$

$$\text{RADIAL BOUNDARY } i \text{ name dimension } ,\ell_i \text{ MTL } m_i \text{ TEMP } t_i \quad (4)$$

$$\text{VERTICAL BOUNDARY } j \text{ name dimension } ,\ell_j \text{ MTL } m_j \text{ TEMP } t_j \quad (5)$$

In this example, it is assumed the cylindrical region contains a single material identified as MTL m_k in statement (1). The weight fractions w_i and identification numbers n_i of the constituent elements in the mixture are supplied in statement (2); one statement of type (3) must be supplied for each of the constituent elements. DPC computes the thermally expanded atomic densities based upon the region temperature specified in statement (1) as TEMP t_k . The reference material density in g/cc at 20°C and linear expansion coefficient needed for computing the expanded atomic densities are contained in statement (2) as DENSITY d EXPN x .

Boundaries of the region are stipulated in statement (1) as SIDES $i_1 i_2 j_1 j_2$. The four boundary identification numbers $i_1 i_2 j_1 j_2$ specify in order: inner, outer, bottom, and top boundaries of the given region. Boundary positions in the overall array of regions are defined in statements like (4) and (5). The dimension in these statements is the distance, positive or negative, from the given boundary to any previously defined reference boundary denoted by ℓ_i or ℓ_j . The material and temperature controlling the expansion of dimension are prescribed by MTL m_i or m_j and TEMP t_i or t_j .

The specification of a complete problem consists simply of describing all the regions in any order, using for each region the set of statements (1)

through (5). An arbitrarily selected vertical boundary for the entire system of regions defines $z = 0$, and is automatically assigned the identification number $j = 1$. Similarly, the radial reference boundary, $i = 1$, is taken at $r = 0$. Regions describing the component parts of the reactor may be defined more or less in the natural order in which the parts are assembled in the reactor.

The code computes the absolute expanded position of each boundary and reorders the boundaries accordingly. Consequently, the code can be used to check the net clearances between parts after expansion. The masses of all materials are also computed. This, in addition to providing an inventory of the fuel and/or blanket materials, provides a systematic check on the total weight that must be supported by the reactor structure.

A list of the region data, including the computed regional boundaries and atomic densities, is included in the output print. The code also constructs a picture plot of the regional identification numbers k , which identifies the relative positions of the regions in the array. In constructing the picture plot, tests for omission or overlap of regions are performed. Deliberate overlap of regions is permitted, however, if desired.

It is normally good practice at this stage in the development of the problem specifications to perform a preliminary run. The only additional specifications needed for this purpose are a title card at the front of the problem deck, and a STOP directive at the end of the data. STOP indicates the end of data and initiates processing without saving data for sequential cases. If it is desired to save the data for subsequent problems, the directive NEXT is used instead of STOP.

The ordered list of boundaries and the picture plot of the ordered array of regions obtained in a preliminary run are useful aids in choosing a mesh prescription for subsequent neutronic calculations. The mesh is prescribed by statements

$$\text{MESH} \left\{ \begin{array}{l} \text{RADIAL} \\ \text{VERTICAL} \end{array} \right\} m_1 \ell_1, m_2 \ell_2, \dots, m_n \ell_n, \quad (6)$$

where the pair of numbers $m_i \ell_i$ indicates that m_i mesh intervals are to be inserted between boundary ℓ_i and the immediately preceding boundary. The code will automatically establish one mesh interval between adjacent boundaries for which no mesh is prescribed.

In considering the final array, it is frequently found that some of the less significant and/or smaller regions may be combined with their neighbors. Such combinations or homogenizations may be accomplished through the specification

COLLAPSE $k_1 k_2 \dots k_n$ INTO k_i , (7)

where $k_1 \dots k_n$ are the identification numbers of the regions to be collapsed, and k_i is the region number assigned to the collapsed region. With the COLLAPSE facility available, the original region set may be defined in strict accordance with the actual design. Following this procedure, a formal and exact record of the assumptions of the model is retained, and hand calculations of any sort are avoided. Boundaries which are rendered superfluous by the region collapse are ignored in the establishment of the mesh unless they appear in the mesh specification of statement (6).

Noncylindrical Regions. In the previous discussion, only a standard cylindrical region was considered. In any practical reactor design, many of the component parts do not fit this simple cylindrical scheme or, in fact, any of the geometrical options available in the neutronic codes. Some procedure must therefore be used to simplify the geometry of the reactor calculational model.

In handling noncylindrical configurations in DPC, a parent cylindrical region is first selected and specified by a type (1) statement. This parent region is described as being composed of a number of subregions (≤ 20) each of which is specified by a statement like

SUBREGION ℓ type number d_1 BY $d_2 \dots$ BY d_n MTL m_ℓ . (8)

The subregions are then mixed by the code to form a homogenized mixture for the parent region. The various available types of subregions are listed in Table I, and are illustrated in Figs. 1 and 2. It is found in practice

Table I
SPECIFICATIONS OF SUBREGION DIMENSIONS

Type	Name	$d_1(1)$	$d_2(1)$	$d_3(2)$	$d_4(1)$	$d_5(1)$
Solid-of-revolution						
Curved Boundary	DISH	R	a	H		
Solid-of-revolution						
Straight-line Boundary	CONE	R_1	R_2	H		
Cylindrical Shell	CYL	outside R	inside $R^{(3)}$			
Cylindrical Annulus Cut						
by Cylindrical Surfaces	LOAF	R_1	R_2	H	R_3	R_4
Cylindrical Annulus Cut						
by Planes	TROUGH	X_1	X_2	H	R_1	R_2
Cylindrical Slice	FLAT	thickness	radius	H		
Spherical Shell	SHELL	outside R	inside $R^{(3)}$			
Hexagonal Shell	HEX	outside pitch	inside pitch ⁽³⁾	H		
Triangular Prism	TRI	base	altitude	H		
Parallelepiped	RECT	base	altitude	H		

(1) If zero or not needed, no value need be supplied, and the list of dimensions may be shortened by one

(2) H is height. If not specified, H is taken as the parent region height

(3) For shell regions (CYL, SHELL, and HEX) the pitches or radii may be given in either order and the positive volume will be selected

CASE A

CASE B

DISH

SOLID OF REVOLUTION WITH ARC BOUNDARY

LOAF

TROUGH

CYLINDRICAL ANNULUS
CUT BY A CYLINDERCYLINDRICAL ANNULUS
CUT BY A PLANE

CONE

SOLID OF REVOLUTION WITH
STRAIGHT LINE BOUNDARY

CYL

CYLINDRICAL SHELL

HEX

HEX SHELL

TRI

TRIANGULAR PRISM

FLAT

HEMI-CYLINDER CUT BY A PLANE

SHELL

SPHERICAL SHELL

RECT

PARALLELEPIPED

Fig. 1

Fig. 2

Subregion Types

that essentially all configurations normally encountered in reactor designs may be specified by combining in various ways the basic volume types in Table I.

In statement (8) type refers to one of the subregion names DISH, CONE, CYL, etc., given in column 2 of Table I. Number is the multiplicity of the particular subregion within the parent region, i.e., it determines the number of times the subregion volume is to be used in computing the composition of the parent region. It should be noted that number is not integral in many applications, and may be positive or negative. The list d_1 BY d_2 BY d_n specifies the subregion dimensions in accordance with the last five columns of Table I.

An overlay scheme of subregion specifications may be adopted by replacing MTL m_ℓ in statement (8) by the statement

$$\text{MTL } m_\ell \text{ DISPLACES } m_i. \quad (9)$$

If the given subregion volume is V , this simply means that a volume V of material m_i is subtracted from the total volume of material, and a volume V of material m_j is added. If a material is specified in the type (1) statement describing the parent region, by MTL m_k , then the subregions should be specified as overlays on the parent region. Overlays of subregions upon regions or other subregions, and the multiplicity specification are the principal mechanisms whereby the basic volume types of Table I are combined to obtain a great variety of configurations.

If the word CELL or CELLS is included in the specification of a region, the region is treated as a repetitive array. In this case the composition of only one cell is required in the specifications of subregions. Thus the volume and normal composition specifications of the parent region are ignored in determining the composition of CELL regions.

Several of the subregion types are redundant. For example, HEX, CYL, and TRI can all be derived from FLAT. However, the former three types of subregions are defined for convenience because of their frequent appearance in reactor designs. As an illustration of the method, a hexagonal shell of inner pitch one inch, outer pitch 2 in., and height 3 in., can be specified simply by the statement

```
SUBREGION 1 HEX 1 2 BY 1 BY 3 MTL  $m_1$ .
```

Again by constructing the hexagon from six equilateral triangles, the hexagonal shell is specified by

```
SUBREGION 1 TRI 6 1.155 BY 1 BY 3 MTL  $m_1$ ;
```

```
SUBREGION 2 TRI 6 0.577 BY 0.5 BY 3 MTL  $m_1$ .
```

Finally, in terms of FLAT, the hexagonal shell is specified more deviously by

```
SUBREGION 1 FLAT 36 1.155 BY 1 BY 3 MTL  $m_1$ ;
```

```
SUBREGION 2 FLAT -24 1.155 BY 1.155 BY 3 MTL  $m_1$ ;
```

```
SUBREGION 3 FLAT -36 0.577 BY 0.5 BY 3 MTL  $m_1$ ;
```

```
SUBREGION 4 FLAT 24 0.577 BY 0.577 BY 3 MTL  $m_1$ .
```

To illustrate further the specification flexibility, the following sets of specifications are presented as equivalent descriptions of the hexagonal shell described above; it is assumed additionally in these cases that the material m_2 is enclosed by the shell of material m_1 :

```
SUBREGION 1 HEX 1 2 BY 1 BY 3 MTL  $m_1$ 
```

```
SUBREGION 2 HEX 1 1 BY 0 BY 3 MTL  $m_2$ 
```



```

SUBREG 1.0 HEX 0.01E+2 5.04 CM BY 1.0 IN BY 3 MTL m1
SUBREGION 2 HEX 1 1 BY 3 MTL m2

SUBREG 1 HEX 1 1 BY 2 BY 3 MTL m1
SUBREG 2 HEX 1 1 BY 3 MTL m2

SUBREG 1 HEX 1 2 BY 3 MTL m1
SUBREG 3 HEX -1 1 BY 3 MTL m2
SUBREG 2 HEX 1 1 BY 3 MTL m2

SUBREG 1 HEX 1 2 BY 3 MTL m1
SUBREG 2 HEX 1 1 BY 3 MTL m2 DISPLACES m1

SUBREG 1 HEX 1 2 BY 3 MTL m1
SUBREG 2 HEX -1 1 BY 3 MTL m1 DISPLACES m2

```

Special Facilities. A number of special facilities are included in DPC to shorten the work of problem specification. A fixed library of element and mixture data is provided which may be read in and modified as desired. Atomic densities may be read in directly to define mixtures. Facilities are available for handling materials with nonlinearities in their expansion coefficients.

Statement types are provided which enable the specification of all, or any portion of, the boundary or regional temperatures in a single statement. If a region has contents similar to those of a previously specified region, it may be introduced by the statement

```
REGION k1 name LIKE k2. (10)
```

This may be followed by modifying statements for region k₁ without disturbing the original contents of region k₂. Means for computing the effective radii of regions containing a collection of hexagonal cells are incorporated in DPC, and the expansion displacement of the top boundary of a liquid mixture contained in a tube may be taken into account.

OUTPUT

DPC currently supplies output in the form of punched cards for input to either the DDK S_n code or the CRAM diffusion code. The input supplied to either code is for the two-dimensional (r,z) geometry option. Although the DPC printed output can be used in setting up one-dimensional problems, this may be inefficient. With automated input available for two-dimensional

applications, it is frequently more advisable, even in survey work, to simplify the two-dimensional specifications to obtain quick results than to resort to synthesis of two-dimensional results from one-dimensional calculations.

The desired output is specified in the DPC input by either the PRINT or PUNCH directives, followed by the name or names of the codes, DDK and/or CRAM, for which output is desired. PRINT causes the output to be printed only, whereas PUNCH calls for both printed and punched output.

ERRORS

A major advantage gained by the use of automated input to the neutron codes results from the reduction of input errors. In the first place, errors caused by violations of rigid format specifications and misarrangements of data are eliminated in DPC. The elimination of many tedious hand calculations reduces error production. Finally, an extensive set of diagnostic checks are made in DPC which facilitate the identification and correction of errors.

It was mentioned previously that tests for omission or overlap of regions are included. In general, diagnostic comments are printed if reference is made to data that are not defined. This includes references to undefined elements, materials, boundaries, or subregion types. Overflow evaluations and comments are provided for dimensioned variables. Checks are provided in the Hassitt-Mitchell routine DECIN and in DPC, for incorrectly specified data and control words.

As might be surmised, the development of error checks is continuing. It is planned to add to DPC a test for the incorrect inclusion of void regions in CRAM diffusion problems. It has also been proposed that reasonableness tests be placed on all data. In such tests the code would provide comments whenever inordinately large or small values are encountered for such parameters as densities, temperatures, and dimensions.

MACHINE REQUIREMENTS AND LIMITATIONS OF PROBLEM SIZE

The present version of DPC is coded for an IBM-7094 with a 32-k core size, with two disks, each of 10,000 tracks, and with two drums, each of 400 tracks. Limitations of problem size are summarized in Table II.

APPLICATIONS

The initial version of DPC was developed in an application to post-operational calculations of critical mass of LAMPRE I.⁽⁵⁾ Fifty-nine

regions were required for the initial precise representation of this reactor; forty-two regions were used in the collapsed version for neutronic calculations. In the course of this study, the effects of varying calculational parameters, such as the number of energy groups, the mesh prescription, and the regional delineation, were evaluated. It was concluded from this study that eigenvalues for complex reactor designs may be obtained from two-dimensional calculations, which are just as accurate as those obtained for simple critical experiments, if sufficient attention is given to detail.

Table II
LIMITS OF PROBLEM SIZE

Type of Data	Maximum Number Allowed
Elements	100
Materials	100
Elements per Material	20
Densities and Expansion Coefficients for Nonlinear Case	6
Radial Boundaries	100
Vertical Boundaries	100
Regions	100
Subregions per Region	20
Regions in Collapse Set	20

In a subsequent set of calculations,⁽⁶⁾ the efficiency of DPC techniques was tested. In the two-week interval available for performing these calculations, two-dimensional eigenvalues, reaction rates, etc., were obtained for the four quite different designs, both with the sodium coolant included and omitted. In these calculations the CRAM diffusion code was used initially to obtain preliminary fluxes which were subsequently input to the DDK S_n code for final determinations. This procedure yields considerable economy in computing times in two-dimensional work where transport theory results are needed.

The design calculations for cores which will be operated in the Fast Reactor Core Test Facility⁽⁷⁾ have provided the first application of DPC throughout the entire development of a reactor design. This work began with a parameter study which has culminated in a preliminary core design proposal.

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SESSION IV

KINETICS STUDIES

Tuesday, May 18, 1965

CHAIRMAN: J. J. Syrett
Central Electricity Generating Board--United Kingdom

CO-CHAIRMAN: Clarence Lee
Los Alamos Scientific Laboratory

SCIENTIFIC SECRETARIES: Charles Cohn
Jerry Kaganove
Argonne National Laboratory

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A SYSTEM OF CHAINED COMPUTER CODES FOR REACTOR FUEL CYCLE ANALYSIS*

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(Paper presented by E. T. Merrill)

The comparative evaluation of reactor fuel cycles is a complex problem in analysis because, in addition to the sheer number of economic considerations, there are variations in fuel performance which are traceable to differences in cross sections, in neutron yield per fission, in heat liberation per fission, etc. Comparative evaluations based on a single performance factor such as the enrichment level required to achieve a given exposure, or the exposure resulting from a given enrichment level, can be reported only when lengthy explanations and qualifications are attached. Reconciling such comparisons is further complicated by the inaccuracies inherent in theoretical calculations of fuel exposures and fuel depletion rates. The influence of such inaccuracies can be great because a fuel which may not even appear to reach criticality in one design may be superior in another. The effects of these inequities can be reduced by comparing fuel cycles at appropriately selected optimum operating points. The amounts of data and the iterative procedures associated with such studies are so great that accurate and timely execution of the work is feasible only with fully automatic computers and data-processing systems.

In 1961, when reactor burnup codes were still few and far between, we set out to calculate plutonium values in thermal reactors. Calculations of this nature required burnup analyses of thermal reactor systems in which the fuel was either enriched uranium or a combination of uranium and plutonium. It also required an integrated economic analysis of these same systems so that the value could be determined by comparing the cost of a uranium-fueled system with the cost of a recycle plutonium system. The codes used are listed in Fig. 1.

MELEAGER	To Supply The Reactor Fuel Burn-Up Data ("Physics")
QUICK	To Supply The Cost Data By Operating on Meleager Results
MINIMIZER	To Determine The Minimum Fuel Cost
PUVE	To Establish The Plutonium Value Resulting From An Appropriate Recycle Sequence

Fig. 1

MELEAGER Chain
Computer Code

In order to complete a value calculation for each reactor type which was analyzed, about fifty burnup calculations were required for enrichments

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which yielded exposures averaging 20,000 MWd/ton. Another set of fifty calculations was required for each of several variations of economic situations, fuel management schemes, lattice spacings, and fuel claddings for each reactor type. A total of approximately 7,500 burnup calculations were performed during the course of this one study.

To be able to make 7,500 burnup calculations within a reasonable time, we were compelled to use a reactor burnup code that would be very rapid--one that would require less than about 30 sec of machine time per case. This meant that we had to consider a burnup code which had a small number of groups, yet would give reliable results. This led to the development of MELEAGER, a burnup code which utilized the Westcott two-group cross-section representation.

MELEAGER has since been modified to a four-group formalism. The calculation of the Westcott dilute g and s values in the SIGMA subroutine of MELEAGER is based on the neutron temperature from a preceding calculation. The effective s is computed by the single-level, narrow-resonance, infinite-mass absorber method using the concentration of the given isotope plus a fraction of the concentration of other isotopes with interfering resonances. Next, the portion of g in excess of 1.0 is reduced by the resonance integral correction factor just computed. The total thermal absorption cross section for the fuel is used to obtain the thermal-flux depression needed for calculation of the effective value of g . The effective neutron temperature is computed, and the entire cross-section calculation is repeated if necessary.

The spectral index is essentially the ratio of the effective thermal absorption cross section of the cell divided by the slowing-down power ($\xi\Sigma_s$) of the cell. However, the slowing-down power must be reduced by a fraction of the resonance absorption cross section, especially in a reactor with a large epithermal reaction rate. Slowing-down calculations in codes such as GAM have indicated that this fraction is about 0.8 in homogeneous systems, and we have found that still smaller values reproduce flux measurements and burnup data for heterogeneous systems. Reactivity, flux, and related data are then computed. The SIGMA subroutine of MELEAGER requires 50 to 100 msec per pass.

The actual burnup is conducted at constant flux and constant cross section by the Runge-Kutta technique, which amounts to a Simpson's rule for integration of the rates of change of concentration of each isotope. The cross sections and decay constants are presented in two-dimensional arrays, in which the diagonal is the removal rate and the nondiagonals are the production rates from Isotope I to Isotope J. The third stage of the Runge-Kutta calculation provides a predicted concentration which is corrected in the fourth stage. We use this correction as an indication of precision. If the fractional value of this correction exceeds an input limit for any isotope, the time step is halved and the calculation repeated. If all are less than a lower limit, the time step will be doubled for the next calculation. Thus, small

initial steps do not limit the speed later in the calculation. This subroutine requires 100 to 150 msec per time step. Flux is recalculated at each time step, but an input number determines the number of time steps between cross section calculations. Output data not otherwise needed in the burnup calculation are computed only when required for writing to tape, and this is usually done while the preceding line is being transmitted.

In order to avoid the delays caused by transferring data from the burnup analysis into a code to do economic analysis, the two primary codes, MELEAGER and QUICK (each requiring over two-thirds of the available 7090 memory space), were chained together. Since the start of the plutonium value studies, we have improved the system and added several more links to the chain. The system which has evolved from these efforts is shown in Fig. 2. The MELEAGER burnup code, which was zero-dimensional, has been expanded into a one-dimensional code; optimization and report-generating codes have been linked into the chain.

Fig. 2. Chained Fuel-cycle Analysis System

Although the main use of this system is for surveys in which we make preliminary evaluations of concepts and outline the area where more intense investigation should be followed, the system must be capable of performing more exact and more detailed burnup calculations. For this reason, we have designed it so that we can substitute other burnup codes into it. The only requirement that another burnup code must meet is that it must produce a burnup-data tape which is compatible with the rest of the system. The burnup tape contains the fuel concentrations, the heat produced, and a time reference at set intervals during the irradiation. Presently, at Battelle-Northwest, there are four burnup codes available which meet this requirement.

The ZODIAC system, one of the codes now being used at Battelle-Northwest, uses a revision of GAM for the epithermal spectrum and is connected with the TEMPEST code for the thermal spectrum. It has one-dimensional capabilities with the diffusion calculation (HFN) and a burnup section called "ALCHEMY." This system, although more accurate for certain cases than the MELEAGER code, requires approximately 30 minutes per burnup, whereas MELEAGER requires only 5 to 30 seconds per burnup. The ZODIAC coding system, although it requires more time, is used for detailed analyses; the results are used to calibrate the constants which are used by the rapid burnup system to correct the neutron spectrum and some of the resonance shielding parameters.

Recently, we have coupled the Battelle-Northwest basic cross-section library to all of the codes in this fuel-cycle analysis system which use cross sections. This library contains descriptions of the cross sections of four hundred isotopes. The descriptions consist of an arbitrary number of data sets which apply over specified energy ranges; each set takes one of four forms as a function of energy. These forms are linear, logarithmic, one-over-v, and Breit-Wigner. The GANDS code computes the 2200-meter cross sections and the coefficients of a fourth-order polynomial representation of g and s as functions of neutron temperature. It also computes the resonance and Doppler coefficients for shielding the dilute resonance integrals. Formulations of the GAM and TEMPEST libraries, as well as the g and s parameters of the Westcott notation used in MELEAGER directly from the Battelle-Northwest nuclear data library, is a feature which adds a very useful consistency to the entire analysis system.

To supplement the MELEAGER burnup code and to allow for rapid analysis, wholly external calculation of cell data is required. This is handled by the JASON code which, using the P-3 approximation to the transport equation, yields initial values of thermal utilization, fast effect, and the flux depression as functions of fuel blackness. This code also homogenizes the lattice and develops the required input parameters which are used to calculate the neutron spectrum and resonance shielding for a given cell in the MELEAGER code. The calculating time for this code is about 2 to 5 sec.

To make this system still more reliable and to reduce user time in developing input, a case-generating code has been developed which will define cases and produce the data required for economic analysis without requiring the user to make advance assumptions about the performance of a given fuel. In other words, the code called SUPERCASE GENERATOR does not require that you tell it what fuel enrichments you would like run in order to supply suitable burnup data on tape to the economic system. Instead, you simply tell it the geometry, and it will determine what enrichments should be run and define the cases for the burnup code, which then does the burnup calculations. If SUPERCASE finds that there are discontinuities in the data, it will automatically increase the density of the data around such discontinuities. If the user is interested in data over a particular range of, say, fuel exposures, fuel enrichments, or reactivities, he may increase the importance weighting, or data density, in this range. During operation, the burnup code is under the control of the SUPERCASE code, which defines two or three cases at a time. The burnup code then analyzes these cases. Then, based on these results, additional cases are defined by the SUPERCASE code to round out the burnup data as required to facilitate economic analysis.

Normally, the MELEAGER calculation is at constant local power, which is not truly representative of the behavior in a power reactor. In order to account for this, and to expand the applicability of this code, a code called PROTEUS analyzes and adjusts the burnup data to correct to flux conditions which are more realistic. A PROTEUS curve fits all of the data on the burnup-data tape against time, then adjusts the flux to an equivalent constant value, and rewrites the burnup-data tape. At the same time, because of the information this code has stored, it is also capable of performing a number of other services.

PROTEUS, although using zero-dimensional burnup data, can calculate the average control requirement for a multiregion fuel irradiation. This is done by examining the reactivity of the fuel at various stages in its lifetime, and through proper integration of these data, determining the average loss of neutrons which must have occurred through either leakage or control-system losses. Again, since curve-fitted data exist, it is easy to terminate the calculation at some limit other than reactivity. For example, PROTEUS can determine when heat transfer limits have been exceeded, and thus superimpose engineering limitations on the physics limitations pertinent to the burnup code. One may also find that the leakage of the reactor may have been different than that which was initially used in the MELEAGER run. The final k_{eff} at which burnup was terminated can be adjusted by PROTEUS when it makes the new burnup-data tape. In effect, a change in reactor size has been simulated without the necessity of rerunning the entire burnup. The PROTEUS code takes about one-third as long to generate any, or all, of these data as MELEAGER takes to do a complete burnup calculation.

In order to make valid comparative analyses of various reactor systems, it is necessary to make these comparisons between minimum cost-operating conditions for each reactor. QUICK, the economics code, contains a subroutine for minimization of fuel-cycle cost, usually as a function of fuel exposure. With data from the burnup tape for a number of cases--each case calculated to some reactivity, power distribution, or heat-transfer-limited exposure--the fuel cost for a given economic environment is calculated. QUICK requires 20 msec to complete calculation of the total fuel cost for a given set of economic parameters. However, 10- to 18-economic-parameter sets are often examined with the same burnup data. These data are curve-fitted as a function of fuel exposure so that the operating conditions yielding minimum fuel cost can be determined.

When the QUICK code was first linked to the burnup code, we had considerable difficulty in determining exactly which operating condition was optimum, using either polynomial fits or analytical functions. One reason was that there were step functions in the fuel-cycle cost: for example, how much fuel would one accumulate at a reactor site before sending it to a separations process--the cost of which is a function of the batch size. Also, we found that valid comparisons usually require accuracy in the fourth significant figure. While trying to eliminate these difficulties, we observed that if we arranged the components of fuel cost into appropriate terms, each could be a simple function when plotted against fuel exposure. These groupings, which are used by MINIMIZER, are shown in Fig. 3.

Fig. 3
Cost Components and Fuel
Exposure as a Function of
Fuel Enrichment

One such term is the net burnup cost plus the reprocessing costs. A second useful term is the fabrication cost plus any losses which occur

in this process. A third term is the interest charges which occur out-of-reactor, and a fourth term is the in-reactor working capital charges. Grouping the cost components into these terms yields smooth functions of exposure. The accuracy of curve fitting could be improved still more if linear functions could be found. Consequently, each of these cost-component terms has been transformed slightly and fitted as cost in dollars per cubic centimeter of fuel, instead of mils per kilowatt hour, as shown in Fig. 4. This transformation, together with the grouping of terms, produces the required accuracy. In determining the minimum fuel cost, we found that, although these fits are simple polynomials, adding them together and solving for the derivative leads to several local fuel-cost minima within the range of the data. To get around this, we use a simple "hunting" method in which we take rather large initial steps to avoid the local fuel-cost minimum points which occur on the curve. This allows us to proceed to the vicinity of the primary minimum--the one of interest. Each time a minimum is found, the hunting step size is reduced, and only the area immediately surrounding that of the indicated minimum is searched further. The curve-fitting and minimization take approximately 160 msec per set of economic parameters.

Fig. 4

Numerator of Cost Components
and Exposure as a Function of
Fuel Enrichment

We have found it necessary to add a second step to the optimization procedure, optimization of the lattice spacing or fuel density, as well as enrichment. As shown in Fig. 2, another chained code, OPTIMIZER, was added to the economic system so that we are able to optimize the fuel cost as a function of physical or geometrical parameters such as lattice spacing or fuel density. A curve-fitting system, similar to that previously described, was adopted for the OPTIMIZER. The minimum fuel cost for a data tape containing the results of several burnup calculations for each of several lattice spacings is made available by the MINIMIZER routine and

the Economics code to OPTIMIZER, which then curve fits these minima, and calculates the lattice spacing, the fuel enrichment, and the discharge exposures which produce the minimum total fuel cost, as shown in Fig. 5. If desired, this system will also perform burnup calculations for that specific case so that a more detailed burnup analysis of the optimum point can be made available. We are now capable of starting with a choice of several reactor lattice designs and then optimizing under a given economic environment on the lattice which should be chosen to find some minimum for a reactor of a given type. We can optimize on such things as the amount of D₂O or total uranium usage. However, most optimization is done against fuel-cycle cost. With the speed that is available with this system, an analysis similar to that described would take about 20 min of 7090 time.

Fig. 5. Total Fuel Costs as Affected by Moderator Index and Enrichment of Fuel for a Water-moderated Reactor with Stainless Steel-clad, U²³⁵-enriched Uranium Fuel

An alternative calculation to the cell optimization which may be based on a prior optimization involves the program PUVe, which determines plutonium value. In this method, the enrichment producing minimum cost

is transmitted to MELEAGER for a burnup calculation to obtain specific data for use in PUVÉ. The plutonium recycle amount and composition are transmitted to SUPERCASE GENERATOR to obtain a new series of burnup data for QUICK and MINIMIZER. In this way, several burnup calculations using recycled plutonium under optimum conditions are available for calculations of plutonium value.

Variations in plutonium value can be reflected by a logical (although complex) extension of the simple indifference plutonium value determination which defines plutonium value as the price yielding the same fuel cost whether the plutonium discharged is sold or recycled. Proper accounting must acknowledge that the plutonium being recycled within an operation is not "free," but is sold at a price from one cycle to the next. Thus, re-cycling plutonium within an operation can be treated as the sale or purchase of goods among several operations. As indicated in Fig. 6, a higher price for plutonium would lower the fuel cost for a U^{235} -enriched cycle and would raise costs for plutonium enrichment. If the selling price of plutonium is less than its value, it is likely that it would be recycled and not sold. Thus, plutonium value is a basic number which must be considered for each reactor discharge to assure consistent selection of lowest cost operations. Since this determination is limited to a single operation, the resulting values should not be confused with market prices which reflect the influence of many operations.

Fig. 6

Fuel Cost and Assigned Plutonium Price for a Hypothetical Nonbreeding Reactor

Generally, the productivities of plutonium of feed composition and of the resulting ash composition in the same thermal reactor are different. This can be reflected in value by use of a method, described as PUVÉ, which employs the premise that the value of a discharged plutonium batch is determined by use of that batch as feed for the next cycle. Recycle analysis by PUVÉ uses an equation for each cycle involving the unknown value of the plutonium feed, the unknown value of the plutonium ashes, and the fuel cost. The fuel costs for successive plutonium recycle can, as indicated in Fig. 7, be written as a set of equations. The value of a batch

leaving the reactor in cycle $j-1$ is conditionally determined by use of that batch as feed for the next cycle j . The recycle process is repeated until some logical constraint can be applied to obviate the necessity of further cycles. In some cases, final plutonium batch values can be set to an arbitrary figure representing some other use. If an equilibrium plutonium composition has been reached, the last two batch values can be set equal. If neither of the foregoing conditions can be applied, it is often possible to use an extrapolation technique based upon composition. Five to seven recycle steps will usually provide an adequate value for plutonium in 20 or 30 min of 7090 time.

$n-1$ = Number of Times Plutonium Produced in the Reactor is Recycled to the Reactor

F_n = Total Fuel Cost in mill/kwh_e on the nth Step

X_{n-1} = Value in \$/gram of Plutonium Supplied to the Reactor in the nth Step

X_n = Value in \$/gram of Plutonium Discharged from the Reactor in the nth Step

$A_n, B_n,$ and C_n are Coefficients Appropriate for Each Step

Fig. 7. Successive Plutonium-recycle Flow Sheet

Obviously, one of the main things we are going to produce is such a tremendous amount of output that it would take a considerable amount of effort to analyze.

To assist in this analysis, we have added another link to the chain shown in Fig. 2, the PLOTTER code, which prints out a three-page summary analysis for each burnup calculation. This summary includes

such information as the initial, final, and average cross sections of all materials used in the burnup; the mass balances of all materials involved in the burnup; the alpha values of the fissionable isotopes; the production of possible higher isotopes or fission products that might have economic value; the consumption of uranium; the heat output and the variation in heat transfer rates; the fluxes; initial and final fuel enrichment; and composition. The summary also includes complete neutron balances: initial, final, and averaged over the fuel cycle. To further assist in reporting this information, the printer has been utilized in preparing graphical output. More recently, peripheral digital plotters working from machine-prepared tapes are being used to graph various output-data combinations of interest. Our codes are set up in such a manner that by using normal input procedures, rather than by recompiling, we can plot any items of data that are either generated internally, or are printed out, against any other such item. These methods of output analysis have been developed to the point where the output is almost a complete report by itself. The output report is largely devoid of the esoteric notations and abbreviations which are common features of burnup and cell calculating codes.

Another analysis code is HESTIA, which evaluates the properties of uranium conservation in a reactor. This code calculates such quantities as the tons of natural uranium required per megawatt (electrical) installed and per megawatt-year (electrical) generated, the fissile plutonium discharged per total fissile material charged, and various indices of the uranium-conservation performance of a reactor.

With these tools, we have the capability of starting with a basic description of the lattice cell, and then by varying this description, find the lattice and enrichment that should be chosen to produce optimum fuel cost for a stated economic environment. These same data may be automatically plotted and reported in nearly complete form, all in a single 20-minute computer pass. In addition to attaining our original objective of developing a system with high calculational speed, we have case-generating codes and data-expanding codes, which make the system more efficient to use by reducing the requirement for basic information and input effort (and, incidentally, input errors) on the part of the user. A typical complete optimization such as we have discussed requires about 150 input cards, of which probably 100 are almost standardized for a given type of analysis.

To review, the uses which have been made of this system include such diverse studies as: (1) definition of optimum cell geometry for a given cycle in a reactor type, (2) identification of the economic incentive for defining reactor physics parameters with greater accuracy, (3) estimation of the impact of changing economic environments, (4) evaluations of the cost impact of transplutonium isotope production, (5) evaluation of the type of reactor to be developed for a given fuel resource availability situation, (6) calculations of plutonium values, and (7) operation of reactors

with bred-fuel recycle. The system possesses the iterative capability of using the information from one optimization as input to generate additional cases--a technique used in automatic recycle of plutonium for plutonium value analysis.

As an example of the application of these chained computer codes to a typical survey problem, I would like to discuss the manner in which these codes are used to evaluate the uranium-conservation characteristics of a reactor. The problem is to determine the amount of uranium which will be used over a long period of time by an expanding nuclear power economy. The uranium resources which are available to us are limited. We wish to make the best use of these natural resources and obtain the maximum amount of energy from them. Let us assume we also have available an estimate of the future growth of the nuclear power industry over the next several decades. The problem is one of determining which reactors, or which reactor types, can be introduced into our economy to fulfill the nuclear-power demand which is represented by this growth projection without exhausting the fissile content of our natural resources.

There are several courses of action available. We can build thermal reactors which consume more fissile material than they produce. Obviously, after a long period of time, we will exhaust the supply of available fissile materials, and we will not have replaced the supply with sufficient fissile material to continue to provide the growth which was hypothesized. We can also build breeder reactors which do replace their fissile inventories. However, breeders will only be introduced as they become economical and are able to produce nuclear power at a cost equal to, or possibly slightly greater than, the cost of production by thermal reactors.

Let us assume that breeder reactors will be built only as rapidly as plutonium is available to fuel them. If we wait too long to introduce breeder reactors, all of the fissile material available to us will have been used without our reserves having been replenished. If we introduce breeder reactors before a sufficient plutonium inventory has been established, we will be limited by the rate at which plutonium is produced for inventories.

Let us suppose that the nuclear generating capacity which is to be installed in the near future to fill the demands of this growth curve will be predominantly thermal reactors, probably similar to a PWR or BWR. Later growth demands will be met by construction of fast reactors. Let us suppose that the fast reactor will be fueled with plutonium and will use depleted uranium in its blanket. Suppose that when fast reactors become available we will install them as rapidly as plutonium is available for fueling them. Suppose, further, that the amount of plutonium available to fuel fast reactors will not be sufficient to allow us to build as many as we would wish. The deficit in new capacity will have to be met by the construction of additional thermal reactors.

Prior to the introduction of economic breeders, that is, for the next several years, thermal reactors will be constructed exclusively. These reactors will be recycling all the plutonium that they produce. However, by the time the plutonium which a reactor produces has gone through the separations and refabrication processes and then has been recycled to the point of being charged back into the reactor, a certain amount of time will have gone by. During this time, we will have constructed more reactors, presumably of the same type. So we wish to take the plutonium that was produced earlier by a smaller number of reactors and recycle it in a larger number of reactors. This is equivalent to recycling in a reactor only part of the plutonium which it produces. The rate of growth of the nuclear-power industry can be expressed by the ratio of the total generating capacity installed as of some time and the total capacity installed one fuel-cycle length earlier. This ratio can be considered a partial recycle rate and can also be used as a parameter to express the method of operation. Plutonium will only be recycled when we are not building fast reactors, or when there is an excess of plutonium above the amount required to fuel fast reactors.

As we look at the future growth of the economy, there will be four distinct periods to consider. First, thermal reactors alone will be constructed. These reactors will recycle the plutonium which they produce. Second, fast reactors fueled with plutonium will be introduced into the economy as rapidly as we have plutonium available to supply their inventories. During this period of time, the thermal reactors will operate on uranium only and will not recycle their own plutonium. During the third period of time, we will have sufficient plutonium available to fuel enough breeder reactors to satisfy the growth of the economy, and still have some plutonium for partial recycle in the thermal reactors that have already been constructed. However, during this period there will not be enough plutonium for complete recycle in the thermal reactors. During the fourth period, there will be an excess of plutonium, even though we will recycle as much as is economical in thermal reactors.

How are these chained computer codes applied to this problem of uranium conservation? For each reactor that will be constructed in the expanding economy hypothesized, we wish to optimize the actual reactor operation within each of the economic environments anticipated. First, for one uranium price and for one rate of growth, which is expressed as a recycle fraction, we go through a complete optimization using these codes. We know that the price of uranium will vary continuously over the future, but we will approximate this by the use of six discrete prices. The installation rate of the reactors will vary with the growth rate of the overall economy and with the rate of introduction of other types of reactors. So we will express a range of installation rates by six discrete rates of plutonium recycle, or recycle fractions, and then use the optimized results for these points to curve fit and find the optimum operation for any growth rate that will be encountered at some time in the future.

The steps that will be required in the optimization for one recycle fraction and for one uranium price are shown in Fig. 8. First, we use SUPERCASE and MELEAGER to calculate burnups using seven or eight uranium enrichments. Then, the results of these burnups go to QUICK and to MINIMIZER to find the enrichment which gives the net minimum fuel cost for this one uranium ore price. Now, with this enrichment, we return to MELEAGER to calculate the burnup at this optimum enrichment. The next step is to recycle a fraction of the plutonium which has been produced at this optimum enrichment, a fraction which corresponds to some given power-reactor growth rate, with each of seven or eight uranium enrichments. These enrichments are generated by the SUPERCASE program, and then the MELEAGER code calculates the burnups. Finally, we return to QUICK and to MINIMIZER to find the enrichment which gives the minimum fuel cost for this fraction recycle and for this uranium ore cost. We return to MELEAGER to compute burnup for the optimum enrichment with this fractional recycle. These optimum enrichments depend upon the value of plutonium to see whether or not we started with a reasonable estimate. If we did not, then the optimization should be repeated with an improved estimate of plutonium value. The next step is to use the PLOTTER program to generate curves of the results and to produce neutron- and material-balance reports on the characteristics of this reactor for optimum plutonium recycle at this given uranium price. From PLOTTER we go to the HESTIA program, which calculates the uranium-usage parameters which will be used as input data to the VESTA program. HESTIA

1. Use SUPERCASE to Generate Cases for Fueling with Uranium Only
2. Use MELEAGER for Burnup Calculations
3. Use QUICK for Economics Calculations
4. Use MINIMIZER for Fuel Cost Optimization
5. Use MELEAGER for Burnup Calculations at Optimum Enrichment
6. Use SUPERCASE to Generate Cases for Fueling with Uranium and Recycle Plutonium from Optimum
7. Use MELEAGER for Burnup Calculations
8. Use QUICK for Economics Calculations
9. Use MINIMIZER for Fuel Cost Optimization
10. Use MELEAGER for Burnup Calculations at Optimum Enrichment
11. Use PUVe to Check Plutonium Value Estimates
12. Use PLOTTER to Generate Output Report Curves
13. Use HESTIA to Calculate Uranium Usage Parameters
14. Use VESTA (not on chain) to Evaluate Uranium Usage for a Hypothesized Economy

Fig. 8. Chain Calculations for the Problem of Uranium Conservation

calculates such quantities as the number of tons of natural uranium which will be required per megawatt of installed electrical capacity, the amount of natural uranium which will be required per megawatt-year of electrical energy generated, the initial and final enrichments of uranium and plutonium, and the amount of fissile plutonium produced per unit of fissile material that is charged to the reactor. Data such as these will be generated for each of six ore prices and five recycle rates. This requires thirty complete optimizations, thirty complete passes through this series of programs. Each pass through this series starting with SUPERCASE and MELEAGER and ending with PUVe and HESTIA, requires approximately 7 min. The thirty optimizations require a total time of about $3\frac{1}{2}$ hr. The results of these machine calculations are sufficient to describe the characteristics of one reactor which will then be used by the VESTA program in making calculations on the hypothesized economy.

Figure 9 shows some of the output from VESTA. First, the total installed capacity for each type of reactor that we assume will be introduced in the future is shown. Figure 10 shows the amount of uranium which will

Fig. 9. MW(e) Installed Capacity if 20-year Doubler Introduced after 1980 and 7-year Doubler Introduced after 1990

Fig. 10. Uranium Utilization of 20-year Doubler Introduced after 1980 and 7-year Doubler Introduced after 1990

be used as a function of time over the same period for the same economy. The discontinuities in the curves of Fig. 9 represent a change in ore price. When the price changes, we rework the cascade tails material before buying additional uranium at the higher price. In Fig. 11, we see the amount of uranium that will be required for one hypothesized economy, as well as a comparison between this amount of uranium and the results of similar calculations for other hypothesized economies. From this, we are able to make evaluations of the importance of the construction rates and of the types of breeder reactors which may be introduced. In this work, so far, there is no attempt to optimize the relative numbers of the different types of reactors which might be built. Each reactor is optimized without considering the impact it may have on other reactors and also without considering the impact that other reactors may have on it.

Fig. 11

Relative Uranium Usage
for Various Breeder
Introduction Dates

The next extensions to the system of chained codes which are planned include the use of the optimum operating parameters calculated for several types of reactors, together with forecasts of the expanding economy, to produce a linear-programming formulation of the conservation problem. Then we can determine the minimum amount of uranium to be used over a future period and the associated costs. So the next link in our chain will be a matrix-maker program to take the output from the MELEAGER, QUICK, and VESTA codes, and combine them in linear-programming descriptions of several reactors. Finally, the output from this link on the chain will be used as input to a linear-programming code which will then proceed to solve for the overall optimum and determine the optimum amount of plutonium recycle for each reactor in order to minimize such quantities as the amount of fissile material, the amount of uranium, or the total energy cost over a short- or long-period of time.

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Discussion of Paper
Presented by Mr. Merrill

MR. CHURCH (DuPont Savannah River Laboratory): Mr. Merrill, would you comment as to the utility of the Runge-Kutta technique in place of an explicit solution to the burnup equation?

MR. MERRILL: This choice was originally made by John Triplett and Gary Busselman, and I have continued with that selection because it appears to be rapid and permits an expansion of the time step. We can start with any small number, such as a time step of a day or so, and expand the time step as the error limits permit. This permits the variation of cross sections of all isotopes independently throughout the irradiation. The calculation of cross sections is carried out at some set interval of time. For instance, the plutonium-240 cross section is quite sensitive to the amount of that isotope present in a sample. If you start with a uranium-235 situation, you can create a very large discrepancy if you make some prior assumption about what that cross section is going to be, rather than to calculate it based on the growth of the plutonium.

MR. CHURCH: But in each case you could change the cross sections as a function of time step.

MR. MERRILL: Yes, the cross sections are recomputed.

MR. CHURCH: You could do this for the explicit solution also. I wondered if it was more flexible in coding.

MR. MERRILL: That, probably, is the prime reason that we had.

MR. GRIGGS (Windscale): Is it possible to deduce from your work any figures of merit for plutonium vis a vis uranium-235 as an enriching material for these reactors?

MR. NEEF: This is primarily the result of the calculations with the PUVÉ program. The value of plutonium which results from this is based on the assumption of a uranium ore price and other charges. A whole price schedule for uranium is used to calculate the fuel cost of a reactor operating on uranium, and then the value of plutonium is calculated to give the same fuel costs. This value of plutonium is based then on a direct substitution or indifference to operation with either plutonium or with uranium.

MR. GRIGGS: I was wondering whether there would be an atom to atom equivalent in any sense. Do you have any calculations where one atom of plutonium would have been as good as one atom of uranium-235 to give a lifetime or something like that?

MR. MERRILL: Generally, no.

MR. ROBBINS (Nuclear Utility Services): Is so much optimization really justified in view of the uncertainties in the uranium-235 price? Secondly, are you doing anything to get some better predictions as to what the uranium-235 price might do in the future?

MR. NEEF: We are just as much in the dark as anyone as to what will happen in the future. We know that the price of uranium will possibly go down a little bit in the near future, but will certainly go up a large amount as we exhaust the available ores. We try to characterize our reactors by looking at several uranium prices which we think cover the range that we will encounter over the future.

MR. ROBBINS: The problem seems to be that the optimization will be dependent upon what the uranium-235 price really is, and I wonder if so much optimization is justified since the uncertainties in the price are caused by the uncertainties in the reserves which are quite large.

MR. MERRILL: In order to make anything comparative, the only valid comparisons occur at minima; if you want to make a study of case A versus case B, you have to be far more precise than the actual accuracy of the data in either case A or case B in order to see if one circumstance versus another is beneficial or not.

MR. RAVETS (Westinghouse Astronuclear): Is there any trouble involved in doing zero-dimensional burnup calculations and forcing yourself into a wrong position, that is, a wrong saddle point, in the multidimensional phase space you have in these surveys, or are things going so smoothly in this system that you don't get into such trouble?

MR. MERRILL: We normally check the situations that are crucial with the one-dimensional code on an occasional basis, rather than routinely, to confirm that the minimum actually is a minimum.

MR. RAVETS: A number of years ago there was a lot of motion towards the direction of experimental design or statistical analysis to pick your design point, rather than going through a zero-dimensional study, after a multidimensional study, selective points were picked to make an experimental design. This was then fit by means of a regression technique so that only a few detailed calculations need be made. Has this thought ever come up in this sort of program?

MR. NEEF: No. We are more interested in survey work where not all the parameters are known. A whole range is covered so we need to do many calculations rapidly. We could substitute other, slower burnup codes into our system if we wanted to look at one particular system in detail around some values of the parameters.

A NEW APPROACH TO WATER REACTOR LIFETIME WITH SPATIAL VARIATION STUDIES*

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(Paper presented by M. Console)

I. Introduction

This paper presents a new approach to the solution of the burnup problem coupled with the few-group diffusion in one and two dimensions, for pressurized water reactors.

A family of monodimensional digital computer programs: MELE-1, MELE-2, and MELE-3 (Modal Expansion Lifetime Evaluation) is now running on the IBM 7090.

A bidimensional program, CONDOR, is now being tested. Our approach assumes, as a starting point, the series expansion of the spatial flux and the variational technique for the solution of the diffusion equations.

The application of the spatial modal expansion to solve neutron-diffusion problems is not a new one, but was first developed by Foderaro and Garabedian,^(1,2) and Federighi and Kaplan.⁽³⁾ With the present work, the authors have intended to exploit the potential rapidity implicit in the modal expansion to generate fast computer programs for lifetime evaluation.

Before the establishment of the final mathematical model employed in the programs mentioned above, several routes were tried, and many possibilities and alternatives investigated, which fall in four main subjects:

- i) search of the best suitable basis of functions for the series expansion of the fluxes;
- ii) determination of the reactor critical conditions by means of a uniformly distributed poison without passing through parametric searches;

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- iii) study of the feasibility and convenience also of expanding in series the isotopic densities in the reactor;
- iv) coupling of flux series expansion with finite differences, in order to improve the local flux representation, especially in the thermal group.

II. Basic Equations

The one-dimensional few-group diffusion equations are

$$\left. \begin{aligned} -\text{div} [D^{i,t}(x) \text{grad } \phi^{i,t}(x)] + \left[\Sigma^{i,t}(x) + t^i \Sigma_p(x) \right] \phi^{i,t}(x) = \\ \frac{\chi_i}{\lambda} \sum_{j=1}^{n_g} \nu \Sigma_f^{j,t}(x) \phi^{j,t}(x) + \Sigma_R^{i-1,t} \phi^{i-1,t} \quad (i = 1, 2, \dots, n_g) \end{aligned} \right\} \cdot (\text{II-1})$$

The meaning of the symbols is as follows:

$$\Sigma^{i,t} = \Sigma_a^{i,t} + \Sigma_R^{i,t} + B^{2,i} D^{i,t}$$

$$D^{i,t} = \text{diffusion coefficient}$$

$$\Sigma_a^{i,t} = \text{macroscopic absorption cross section}$$

$$B^{2,i} = \text{transverse buckling}$$

$$\Sigma_R^{i,t} = \text{macroscopic removal cross section}$$

$$\Sigma_p = \text{macroscopic cross section of the poison}$$

$$t^i = \text{poison fraction in group } i$$

$$\chi^i = \text{fission spectrum in group } i$$

$$\nu \Sigma_f^{i,t} = \text{macroscopic fission cross section times } \nu$$

$$\phi^{i,t} = \text{neutron flux.}$$

The superscript i refers to the group i , and the superscript t refers to the fact that the stationary equations (II-1) are solved at the particular time t of the reactor lifetime. Indeed, Eqs. (II-1) are the time-dependent diffusion equations, already discretized with respect to time.

A number of time steps of pre-fixed magnitude is given. At the beginning of each time step, Eqs. (II-1) are solved and, keeping the fluxes stationary throughout the time step, new isotopic number densities and a new set of diffusion constants are calculated by solving the burnup equations (II-2) below.

The new number densities will be used for the diffusion calculations in the next time step.

The burnup equations have the general form

$$\left. \begin{aligned} \frac{dN_m(x,t)}{dt} = & -\lambda_m N_m(x,t) - N_m(x,t) \left[\sum_i \sigma_{a,m}^i \phi^{i,t}(x) \right] \\ & + \lambda_{m'} N_{m'} + N_{m-1}(x,t) \left[\sum_i \sigma_{a,m-1}^i \phi^{i,t}(x) \right] \end{aligned} \right\} \quad (\text{II-2})$$

Here N_m , N_{m-1} , and $N_{m'}$, are the isotopic densities of different isotopes, λ_m is a decay constant of isotope m , and $\sigma_a = \sigma_c + \sigma_f$ is the microscopic absorption cross section.

A thermal self-shielding factor is also included, but not explicitly indicated, in Eqs. (II-2) for the sake of simplicity.

III. Search for the Basis of Functions

In order to solve Eqs. (II-1) the group fluxes are expanded in series of eigenfunctions:

$$\phi^{i,t}(x) = \sum_{h=1}^N \alpha^{i,t} W_h(x), \quad (\text{III-1})$$

The coefficients $\alpha^{i,t}$ are determined in such a way that the group functionals (III-2) are stationary (Ref. 3):

$$\left. \begin{aligned} F^i [\phi^{i,t}(x)] = & \int_{\text{REACTOR}} \left\{ -\frac{D^{i,t}}{2} \left[\frac{d\phi^{i,t}}{dx} \right]^2 - [\Sigma^{i,t} + t^i \Sigma_p] [\phi^{i,t}]^2 \right. \\ & \left. + \left[\frac{\chi_i}{\lambda} \sum_{j=1}^{ng} \nu \Sigma_f^{j,t} \phi^{j,t} \right] \phi^{i,t} \right\} dx. \end{aligned} \right\} \quad (\text{III-2})$$

After substitution of (III-1) into (III-2) the following few-group matrix equations are obtained:

$$\left. \begin{aligned} A^{i,t} \alpha^{i,t} + t^i P^t \alpha^{i,t} &= \frac{\chi_i}{\lambda} \beta^t + R^{i-1,t} \alpha^{i-1,t}; \\ \beta^t &= \sum_{j=1}^{n_g} S^{j,t} \alpha^{j,t} \end{aligned} \right\}, \quad (\text{III-3})$$

where:

$$\left. \begin{aligned} |A^{i,t}|_{h,k} &= \int_{\text{REACTOR}} \Sigma^{i,t}(x) W_h(x) W_k(x) dx \\ &+ \int_{\text{REACTOR}} D^{i,t} B_k^2 \dot{W}_h(x) \dot{W}_k(x) dx \\ |P^t|_{h,k} &= \int_{\text{REACTOR}} \Sigma_p^t(x) W_h(x) W_k(x) dx \\ |S^{i,t}|_{h,k} &= \int_{\text{REACTOR}} \nu \Sigma_f^{i,t}(x) W_h(x) W_k(x) dx \\ |R^{i,t}|_{h,k} &= \int_{\text{REACTOR}} \Sigma_R^{i,t}(x) W_h(x) W_k(x) dx \end{aligned} \right\} \quad (\text{III-4})$$

is the absorption + leakage matrix,

is the poison matrix,

is the fission matrix, and

is the removal matrix.

The first step is to determine which kind of eigenfunctions $W_h(x)$ are best suitable for rendering stationary the functionals (III-2).

Lunelli and Maggioni, working under the same contract as the authors, have investigated the matter with an IBM-7090 code, TEST, whose purpose is that of solving the one-group diffusion with several choices for the basis functions W_h . The functions tried were:

- 1) $\sin h\pi x/L$;
- 2) $\cos (2h - 1)\pi x/2L$;
- 3) $J_0\left(x_h \frac{x}{L}\right)$
- 4) $\cos \frac{h\pi(x/L - 1)}{x/L}$;
- 5) $[1 - (x/L)]x/L^h$;
- 6) $\frac{x}{L} \prod_{k=1}^h \left(\frac{k}{h} - \frac{x}{L}\right)$;
- 7) $J_1\left(\beta_h \frac{x}{L}\right)$;
- 8) functions W_h which are the solutions of a problem

$$W_h + [\lambda_h g(x) - f(x)]W_h = 0$$

with continuity conditions at the interfaces and vanishing at external boundaries.

Types 1), 2), and 3) are the usual eigenfunctions of Refs. 1, 2, and 3 for the three geometries: asymmetric slab, symmetric slab, and cylinder. Types 4), 5), 6), and 7) have been proved unsatisfactory, whereas type 8) has shown some improvement, especially for the representation of the flux near the interfaces, with respect to types 1), 2), and 3). Inasmuch as the complexity of computation of eigenfunctions 8) overshadows the small gains in the precision of the results, this has been dropped. It has been concluded that the best suitable functions were the trigonometric functions. The cosines are used for cylindrical geometry instead of the Bessel functions J_0 because of the existence of the simple addition formulae for the trigonometric functions.

These addition formulae were thought to be essential for the code MELE-1, in which the isotopic number densities are also expanded in series. The use of the cosines for cylindrical geometry has been retained in MELE-2, MELE-3, and in CONDOR.

IV. Solution of the Depletion Equations

The depletion equations considered are the 13 space- and time-dependent equations of the type (II-2) for the 13 isotopes (U^{235} , U^{236} , U^{238} , Pu^{239} , Pu^{240} , Pu^{241} , I^{135} , Xe^{135} , Pr^{139} , Sm^{139} , Lumped Fission Product, and two burnable poisons). The treatment of the space variable has given rise to two distinct approaches and to two different computer programs: MELE-1 and MELE-2.

The first approach is based on the series expansion of the isotopic densities $N_m(x,t)$ in the same basis $W_h(x)$ in which the fluxes are expanded. This is the more radical and, in a sense, more elegant approach, for the entire lifetime calculations remain in the same functional space (the Fourier space) without transition to Cartesian space, as happens in the second approach. In the latter the depletion equations are solved in any of the small regions into which the reactor is divided.

As an illustration of the first approach, consider the U^{235} depletion equation, which is the simplest:

$$\frac{dN(x,t)}{dt} = - \sum_{i=1}^{n_g} N(x,t) \sigma_a^i \phi^i(x,t). \quad (IV-1)$$

In symmetric slab geometry, it is

$$\phi^i(x,t) = \sum_{h=1}^N \alpha_h^{i,t} \sqrt{\frac{2}{L}} \cos \frac{(2h-1)\pi x}{2L}. \quad (IV-2)$$

Substituting (IV-2) in (IV-1), multiplying (IV-1) by $\cos (k-1)\pi x/L$ and by $\cos \left(k - \frac{1}{2}\right) \pi x/L$, and integrating between 0 and L (= reactor length), one obtains the following set of differential equations:

$$\begin{aligned} \dot{N}_k &= \frac{1}{2} \sum_{i=1}^{n_g} \sum_{h=1}^N A_h^i \left[M_{(h+k-1)} + M_{|h-k+(1/2)|+(1/2)} \right]; \\ \dot{M}_k &= \frac{1}{2} \sum_{i=1}^{n_g} \sum_{h=1}^N A_h^i \left[N_{(h+k)} + N_{|h-k|+1} \right], \end{aligned} \quad (IV-3)$$

with

$$\begin{aligned} A_h^i &= \sigma_a^i \alpha_h^i; \\ N_k &= \int_0^L N(x,t) \cos \frac{(k-1)\pi x}{2L} dx; \\ M_k &= \int_0^L N(x,t) \cos \left(k - \frac{1}{2}\right) \frac{\pi x}{L} dx. \end{aligned} \quad (IV-4)$$

It is sufficient to solve as many systems (IV-3) as there are time-variable isotopes. Then, knowing N_k for each isotope, calculation of the matrix elements (III-4) is straightforward. For instance,

$$|R^{i,t}|_{h,k} = \frac{1}{2} \sum_{j=1}^{\text{ALL ISOTOPES}} \sigma_{R,j}^i \left[N_{h+k}^{j,t} + N_{|h-k|+1}^{j,t} \right].$$

This first approach, programmed in MELE-1, did not give good results for practical calculations for two reasons:

- a) Too many terms in the expansion of atomic densities are needed to ensure a practical convergence.
- b) Serious difficulties have been encountered in solving the depletion equations of the Xe^{135} and Sm^{139} , for the modified Euler method does not converge unless the time-step length be of the order of few hours.* This, of course, is too small compared with the order of magnitude of the reactor lifetime. Thus, the program MELE-1 works only in the cases in which the average reactor flux is very low, so that the above conditions are fulfilled.

In order to get rid of these difficulties, two alternatives have been explored. In the first, the depletion equations are solved for a set of pre-fixed mesh points; the Fourier coefficients for each isotopic density are then calculated by numeric integration. In the second, the core is divided into a number of subregions in which average fluxes and average number densities are calculated. The second alternative has proved to be more accurate and has been programmed in MELE-2, Ref. 4.

V. Criticality Searches

The criticality searches are performed by determining the value of the control parameter (poison boundary or poison cross section) such as $\lambda = 1$ in Eqs. (V-1):

$$\left. \begin{aligned} A^i \alpha^i + t^i P \alpha^i &= \frac{\chi^i}{\lambda} \beta + R^{i-1} \alpha^{i-1}; \\ \beta &= \sum_{j=1}^{n_g} S^j \alpha^j. \end{aligned} \right\} \quad (\text{V-1})$$

*The convergence condition for this method is

$$\sigma_a^i \alpha_h^i \Delta t \ll 1.$$

The meaning of the symbols is given in Sect. III, except that here the time superscript t has been dropped. Only the poison matrix P is a function of the control parameter.

In order to solve the problem of the criticality searches as stated above, several methods have been examined. First of all, it is not convenient to determine the criticality conditions by means of the parametric searches employed by the finite-difference programs known to us. For in these latter the calculation of the eigenvalue λ , in the outer iterations successive to the first, is much accelerated by using, as an initial guess, the converged flux of the preceding iteration. This policy is not suitable to our approach, in which the matrices at the left hand of Eqs. (V-1) are directly inverted at each outer iteration. Therefore alternative methods have been sought:

1) An attempt has been made to determine the poison cross section directly from the eigenvalue Eqs. (V-2):

$$\mu t^i P \alpha^i = \chi^i \sum_{j=1}^{n_g} S_j \alpha^j + R^{i-1} \alpha^{i-1}. \quad (V-2)$$

Equations (V-2) can be put in the form

$$\left. \begin{aligned} \mu T \alpha &= Z \alpha; \\ \mu \alpha &= T^{-1} Z \alpha; \\ \mu \alpha &= \Omega \alpha, \end{aligned} \right\} \quad (V-3)$$

where

$$\left. \begin{aligned} T &= \begin{pmatrix} t^1 P & 0 & 0 & \dots & 0 \\ 0 & t^2 P & 0 & \dots & 0 \\ \vdots & & & & \\ 0 & 0 & 0 & \dots & t^{n_g} P \end{pmatrix} \\ Z &= \begin{pmatrix} \chi^1 S^1 & \chi^1 S^2 & \dots & \chi^1 S^{n_g} \\ \chi^2 S^1 & \chi^2 S^2 & \dots & \chi^2 S^{n_g} \\ \vdots & & & \\ \chi^{n_g} S^1 & \chi^{n_g} S^2 & \dots & \chi^{n_g} S^{n_g} \end{pmatrix} \\ \Omega &= T^{-1} Z. \end{aligned} \right\} \quad (V-4)$$

This method requires only the inversion of the matrix P . We realized that the physically significant eigenvalue is the largest algebraically, which in

this case does not coincide with the one of maximal modulus. Nevertheless, a standard method for finding the algebraically largest eigenvalue was applied, by shifting the eigenvalue spectrum. Unfortunately, the ratio of the eigenvalue of maximal modulus and the largest algebraically turned out to be of an order of magnitude unpredictable a priori, at least on the basis of preliminary considerations made for a bare homogeneous reactor. Consequently, the procedure of shifting the spectrum of eigenvalues is not applicable, due to evident numerical criticalities.

2) The determination of the eigenvalue defined as follows:

$$\frac{1}{\mu} t^i P \alpha^i = \chi^i \beta + R^{i-1} \alpha^{i-1}, \quad (V-5)$$

does not present the inconveniences found in method 1), but requires the inversion of the matrices (V-4), which is not profitable from the standpoint of computational time.

3) Let us consider an eigenvalue defined as follows:

$$\mu A^i \alpha^i = \chi^i \beta + t^i P \alpha^i + R^{i-1} \alpha^{i-1}, \quad (V-6)$$

where the poison matrix P is a function of the control parameter. The eigenvalue problem is readily set up in the form

$$\mu B \alpha = C \alpha,$$

where

$$\left. \begin{aligned} B &= \begin{pmatrix} A^1 & 0 & 0 & 0 \\ 0 & A^2 & 0 & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & A^{ng} \end{pmatrix}; \quad \alpha = \begin{pmatrix} \alpha^1 \\ \alpha^2 \\ \vdots \\ \alpha^{ng} \end{pmatrix}; \\ C &= \begin{pmatrix} \chi^1 S^1 + t^1 P & \chi^1 S^2 & \dots & \chi^1 S^{ng} \\ \chi^2 S^1 + R^1 & \chi^2 S^2 + t^2 P & \dots & \chi^2 S^{ng} \\ \dots & \dots & \dots & \dots \\ \chi^{ng} S^1 & \chi^{ng} S^2 & \dots & \chi^{ng} S^{ng} + t^{ng} P \end{pmatrix}. \end{aligned} \right\} \quad (V-7)$$

To perform a criticality search by varying the control parameter until $\mu = 1$, it is sufficient to invert the matrices A^i only one time, and this is very favorable from the standpoint of computational time. Also, in this case the physically acceptable eigenvalue is the largest algebraically, but fortunately

the two eigenvalues are of the same order of magnitude, and it is possible to evaluate, by means of a simple formula, an upper bound of the spectrum, so that the spectrum is easily shiftable and the eigenvalue largest algebraically readily found by means of the classical power method.

4) The following method is a variant of the preceding one. The eigenvalue equations are

$$\left(A^i + t^i P_{\max}\right) \alpha^i = \frac{1}{\mu} \chi^i \sum_{j=1}^{n_g} \left(\beta^j + \delta_{i,j} t^i \delta P\right) \alpha^j + R^{i-1} \alpha^{i-1}. \quad (V-8)$$

Here $P_{\max}$ is the matrix corresponding to an upper bound of the control parameter and

$$\delta P = P_{\max} - P.$$

For any value taken by the control parameter, the diffusion differential operator and the corresponding matrix operator (formed by discretizing it with finite differences) have an eigenvalue of maximal modulus and a corresponding eigenfunction everywhere nonnegative, Ref. 4. It is natural to suppose this property holds also for Eqs. (V-8); this has been rigorously proved for one group, but all the calculations performed have confirmed the validity for more general cases. The critical searches then can be made by changing the critical parameter until $\mu = 1$. As before, this procedure requires only the inversion of the matrices $(A^i + t^i P_{\max})$.

This method has been employed in MELE-2 and MELE-3, and in the two-dimensional program CONDOR.

VI. Numerical Results and Comparison between MELE-2 and Finite Difference Programs.

The results obtained with MELE-2 have been compared with those obtained with CANDLE and FEVER.

The comparison with CANDLE has been made for a cylindrical reactor consisting of a core, a steel baffle, and a water reflector. The calculations have been made with four groups, with the critical parameter Σ_p (macroscopic poison cross section) taken to be uniformly distributed in the core.

Table I shows the values of Σ_p at the various time steps, the linearly extrapolated value of the reactor life, and its deviation from the value obtained with CANDLE. Also computing times are shown. The agreement between CANDLE and MELE-2 with 15 harmonics is good as regards Σ_p ,

the fluxes, and the isotopic density distributions (see Figs. 1 and 2). MELE-2 with 10 harmonics shows an increasing deviation of the Σ_p , with a maximum deviation of 10% at the last time steps. Anyway, the lifetime estimate is wrong only by 2%.

Table I
COMPARISON OF THE VALUES OF THE CRITICAL PARAMETER, Σ_p ,
OBTAINED FOR EACH TIME STEP

Time Step	Hours	Σ_p CANDLE (150 meshpoints)	Σ_p MELE (15 harmonics)	Σ_p MELE (10 harmonics)
1	0	0 0254	0 0254	0 0255
2	100	0 0205	0 0206	0 0207
3	2000	0 0165	0 0166	0 0167
4	4000	0 0122	0 0123	0 0125
5	6000	0 00758	0 00767	0 00789
6	8000	0 00294	0 00306	0 00331
Lifetime T		9268 hr	9331 hr	9447 hr
ΔT		0 hr	63 hr	179 hr
Computation Time on IBM-7090		4 min 20 sec (IBM-7094)	4 min 03 sec (IBM-7090)	1 min 03 sec (IBM-7090)

Fig. 1. Comparison between MELE and CANDLE

Fig. 2. Isotopic Densities
t = 8000 hr

The comparison between MELE-2 and FEVER has been conducted for a cylindrical reactor made of a three-zone core and a water reflector. Table II shows the results of 4-group calculations. The agreement is good enough with regard to the critical parameter Σ_p , but the thermal flux distribution is very poor, as shown in Fig. 3, presenting many oscillations around the true curve.

Table II
COMPARISON OF THE VALUES OF THE CRITICAL PARAMETER Σ_p ,
OBTAINED FOR EACH TIME STEP

Time Step	Hours	Σ_p FEVER (140 meshpoints)	Σ_p MELE-2 (20 harmonics)	Σ_p MELE-2 (15 harmonics)	Σ_p MELE-2 (10 harmonics)
1	0	0 02305	0 02312	0 02342	0 02397
2	2,000	0 02378	0 02380	0 02405	0 02455
3	4,000	0 02262	0 02263	0 02286	0 02339
4	6,000	0 02038	0 02039	0 02064	0 02129
5	8,000	0 01754	0 01756	0 01781	0 01853
6	10,000	0 01432	0 01439	0 01466	0 01536
Computation Times on IBM-7090		7 min	6 min 40 sec	4 min 20 sec	3 min

Fig. 3. FEVER vs MELE-2

VII. Improving the Flux Distribution by Coupling the Series Expansion with Finite Difference: MELE-3

The results obtained with MELE-2 have shown that the method of series expansion is able to determine with good accuracy the criticality

factor (k_{eff}) or the critical parameter (poison cross section or poison boundary) with a reasonable number of harmonics (≤ 20). The thermal-flux distribution, on the contrary, is not adequate in cases more complex than the simple core-reflector systems, especially when a high peak occurs. In order to improve the thermal-flux distribution, the following mechanism has been chosen:

- i) to determine the control parameter and the group fluxes by means of the series expansion;
- ii) to recalculate the thermal flux with a one-iteration finite-difference scheme, using the eigenvalue and the fast fluxes already determined as the source term for the thermal flux. The normalization factor and the thermal flux averaged over the subregions, necessary for the depletion calculations, are obtained by numerical integration of the point flux by Simpson rule.

Following these ideas, a new one-dimensional program, MELE-3, has been set up. The criticality searches may be effected either with the harmonics method or with finite differences. Also it is possible to perform the criticality searches with the harmonics method, and then to continue the calculations with finite differences, using the previous results as a starting approximation.

The continuation may be performed in two modes:

- a) With the iterative search of the control parameter and the group fluxes, calculations going on until the convergence criterion is met.
- b) With one iteration, calculating one or more group fluxes with finite differences. This is a refinement only of the previously determined fluxes.

Moreover, to reduce further the computation times, MELE-3 includes the following features:

- i) the number of harmonics is group-dependent. Indeed, the nonthermal fluxes, being more regular, need not have the same number of harmonics as the thermal flux. As the computation time is greatly dependent on the number of harmonics used, a good saving is obtained, especially in four-group calculations.
- ii) another method of matrix inversion is employed, suitable for large symmetric matrices, which needs half the number of operations as the method employed in MELE-2.

To check the new features of MELE-3, six 2-group calculations have been run and compared with the FEVER results. The reference reactor was highly heterogeneous, with a very strong thermal peak in the reflector. It is again a three-zone core and a water reflector.

The six calculations are the following:

- 1) MELE-2: 20 harmonics in both groups, no finite differences.
- 2) MELE-3: 10 harmonics in both groups, no finite differences.
- 3) MELE-3: 10 harmonics in fast group, 20 in thermal group, no finite differences.
- 4) MELE-3: 10 harmonics in fast group, 20 harmonics in thermal group, finite differences in thermal group.
- 5) MELE-3: 20 harmonics in both groups, finite differences in thermal group, one iteration.
- 6) MELE-3: 20 harmonics in both groups, finite differences in both groups, more than one iteration.

Table III shows the critical parameter Σ_p obtained from the six runs of MELE-3 and from FEVER, together with the computation times.

Table III
COMPARISON OF THE VALUES OF THE CRITICAL PARAMETER, Σ_p ,
OBTAINED FOR EACH TIME STEP

Time Step	Hours	Σ_p FEVER (86 points)	Σ_p MELE-2 (1)	Σ_p MELE-3 (2)	Σ_p MELE-3 (3)	Σ_p MELE-3 (4)	Σ_p MELE-3 (5)	Σ_p MELE-3 (6)
1	0	0.02856	0.02864	0.02968	0.02883	0.02883	0.02864	0.02864
2	2000	0.02322	0.02318	0.02394	0.02331	0.02333	0.02319	0.02318
3	4000	0.02238	0.0224	0.02309	0.02253	0.02256	0.02242	0.02241
4	6000	0.02077	0.02077	0.02147	0.0209	0.0209	0.02080	0.02078
5	8000		0.0187	0.01943	0.01884	0.01891	0.01875	0.01871
Computation Times on IBM-7090		4 min 10 sec	3 min 08 sec	1 min 22 sec	1 min 40 sec	2 min	2 min 30 sec	2 min 56 sec

As regards the critical parameters, run 6 is very good, run 5 is also very good, runs 4 and 3 are fairly good, run 2 is poor, and run 1 is very good.

The thermal-flux representation is now interesting to look at. Figure 4 shows the thermal flux at the beginning of life. FEVER and run 6 coincide (the maximum deviation is 0.1%, not detectable in the figure). The flux of run 5 is also very good. Figure 5 shows the thermal flux at beginning of life, from FEVER and run 4. The agreement is fairly good. Figure 6 shows the thermal flux at beginning of life, from FEVER and run 1. The agreement is very poor. Figure 7 shows the fast flux at beginning of life, from FEVER, from run 3, and run 1. This plot shows that the fast flux is very well represented by 20 harmonics. Hence, it is

Fig. 4. Thermal Flux at Beginning of Life

Fig. 5. Thermal Flux at Beginning of Life

Fig. 6. Thermal Flux at Beginning of Life

Fig. 7. Fast Flux at Beginning of Life

Discussion of Paper
Presented by Mr. Console

MR. NESTOR (Oak Ridge National Laboratory): We wrote a similar harmonics code some years back for spherical two-region reactors and found that, when we came to solve for the expansion coefficients, we had one more equation. When you come to solve for the expansion coefficients you have one more equation than you have coefficients because it is a homogeneous problem.

MR. CONSOLE: Yes.

MR. NESTOR: One method for a 10-harmonics problem would be to set one of the coefficients to unity and solve for the other nine. We found, however, that this procedure often produced a wildly oscillating flux distribution, sometimes even negative fluxes, but we could get rid of this if we took the 10 x 9 set and solved it as a least-squares problem. This might account for some of the disagreement in your thermal-flux calculation.

MR. CONSOLE: I see, thank you.

MR. EMON (Texas A&M): One of the problems you have when solving finite-difference codes is the guess as to initial source. I would imagine if one looked back to the mathematics that the rate of convergence is directly dependent on the initial guess. Could you use some low-order approximation, such as P-10 or -15, for an initial source? Then, since the running time is reasonably low as you indicated, could you use this for a guess in a finite-difference approximation?

MR. CONSOLE: Yes, we made similar calculations using few harmonics, ranging from five to twenty harmonics, hoping that a lower approximation could give a good initial guess, but we obtained a bad eigenvalue. Accordingly, we have iterated the finite difference to improve the eigenvalue. With a good eigenvalue as a start, only one iteration will give the thermal flux. We also tried several combinations using different numbers of harmonics in the different groups, say, 10 harmonics in the fast group and 20 in the thermal one.

BISTRO, AN INTEGRATED COMPUTATIONAL SYSTEM FOR PREDICTION OF THE HISTORY OF BOILING WATER REACTORS

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1. INTRODUCTION

The problem of calculating burnup (i.e., the energy released from a certain amount of nuclear fuel) in a given nuclear power reactor has been the subject for a number of methods of solutions, and a family of computer programmes of various degrees of sophistication exists for this purpose. Together with the problem of burnup determination, numerous problems associated with long-term reactor behaviour, such as control rod programming and power distributions, are attempted to be solved within the same calculational system. The complexity of the problems presented here implies that it is next to impossible to find their solutions by one computer programme of sufficient generality to treat most types of power reactors.

The BISTRO system is designed in order to facilitate reactor history calculations for light-water boiling reactors. The notation "BISTRO system" refers to a system of computer programmes and routines, some of which were already available at the time of development of the system. The BISTRO programme denotes the actual programme performing the necessary data transmission and various auxiliary calculations associated with the various codes used in the BISTRO system. BISTRO is developed for the one-bank version of the CDC 3600 and is written as an overlay programme in FORTRAN 63.

This paper describes briefly the various aspects of the system. Section II deals with its scope, Section III describes briefly the configuration of parameters used, and Section IV is devoted to a description of the physical models used in connection with particular problems. Section V deals with the data-transmission system, and in Section VI is given a brief discussion of various features of the system.

2. SCOPE AND GENERAL LAYOUT

The BISTRO system was developed in order to facilitate lifetime calculations for light-water boiling reactors. One of the main objectives was that of automatic data processing combined with simple operating characteristics and a fairly high degree of flexibility. For the sake of simplicity, several already existing codes were used, thus putting the emphasis on data transmission and editing in the BISTRO programme itself.

The reactor lifetime is divided into a number of time steps within which the flux and power distributions are assumed constant. Between each time step, one or several BISTRO runs may be performed in order to evaluate the reactor characteristics at that particular time, and in order to provide parameters to be used in the subsequent run. The uncontrolled core of the reactor is at any time assumed to be completely characterized by a burnup distribution, a power distribution, and a void distribution. It is further assumed that all relevant core parameters are functions of burnup and void fraction, which are treated as independent variables. In other words, for a core parameter Σ ,

$$d\Sigma = \frac{\partial \Sigma}{\partial \alpha} d\alpha + \frac{\partial \Sigma}{\partial E} dE \quad (1)$$

is assumed to be a true exact differential. Here, α and E denote void fraction and burnup, respectively. These assumptions imply that the core parameters may be precalculated and tabulated as functions of E and α , and their desired values may at any stage be retrieved by interpolation. For the purpose of calculating core parameters $\Sigma = \Sigma(E, \alpha)$ the point burnup model contained in the METHUSELAH programme⁽¹⁾ was chosen. Thereby is assumed a constant power level during reactor life.

The flux and power distributions are desired in two dimensions, necessitating the use of a diffusion-theory code working in R-Z geometry. The programme TWENTY GRAND⁽²⁾ was found useful for this purpose. Evaluation of 2-dimensional void distributions is a rather complicated problem, and it was decided to solve this problem by synthesis of a number of one-dimensional calculations with the VOIFLO code,⁽³⁾ according to a principle described in Section IV. A simplified block diagram showing the layout of the main parts of the system is given in Fig. 1. The notations "JOB" and "CASE" refer here to the reactor-lifetime problem and a unit run, respectively.

Fig. 1. Flow Diagram for BISTRO

Further, because of the general method of approach, a criticality search procedure was not found desirable. Instead, information pertaining to a subsequent point on the time scale regarding the effects obtained by various movements of control elements was found to be of great value. In practice this is achieved by prescribing a number of black control-element configurations, for which approximate criticality factors are obtained in a manner sketched in Section IV.

3. PROBLEM CONFIGURATIONS

The METHUSELAH programme works in a 4-group scheme of neutron energy, and this representation of the core parameters is retained in BISTRO. Since the computation time for multigroup diffusion calculations is approximately proportional to the number of energy groups used, the option of applying 2-group representation for an arbitrary case is included. This is achieved by simply including the unnormalized epithermal group fluxes in the set of core parameters, and condensing the epithermal group parameters in the usual fashion.

The geometrical representation of the reactor is that used by TWENTY GRAND, i.e., characterized by the usual division into mesh regions. Because of requirements imposed by the use of VOIFLO (see Section IV), it is, however, necessary that the region boundaries within the core form straight lines penetrating the entire core in an R-Z plane, thereby dividing the core radially in a number of annuli. Each region is assumed to have a uniform physical composition at any time.

The model applied for the control of the reactor allows for both thermally black and grey (burnable) control elements. The latter are assumed to have permanent positions within the reactor core.

The representation of the absorption properties of the control elements is consistent with the 4-group model. Each control element is assumed to be of cruciform shape and need not be partially inserted in any region.

As is evident from Fig. 1, the first step is essentially initialization of the problem. Any other case may, by definition, be either SEQUENTIAL, meaning that a time step has been taken since the previous case, or REPEATED, meaning that no time of the reactor life has elapsed since the previous case. The option represented by the latter type of case is particularly important in connection with updating of void distributions, and of power distributions when control rod movements have just occurred.

4. PHYSICAL AND MATHEMATICAL MODELS

4.1 Calculation of void distributions

As mentioned above, the evaluation of void distributions is performed one-dimensionally by utilization of the steady-state, loop-boiling model contained in VOIFLO. The use of this program within the BISTRO system is a two-step operation.⁽⁴⁾ First, a hydraulic loop problem is defined by the core, riser, and downcomer, and a VOIFLO calculation is performed in order to find the pressure drop ΔP over the core and the temperature T_i of water at the core inlet.

One-dimensional calculations are then performed for each annulus (omitting riser and downcomer) with ΔP and T_i as boundary conditions. In this fashion, an axial void distribution is obtained for each annulus. These are in turn integrated into regionwise averages, as the geometrical representation assumed in VOIFLO does not correspond to the axial mesh-region division used in TWENTY GRAND.

4.2 Updating of burnup, interpolation of core parameters, and correction of xenon cross section

The updating of the burnup matrix is in most cases self-evident, and the generation of core parameters, denoted by X , performed at a point i on the time scale is twofold, namely,

$$X_{i+1} = X_{i+1}(B_{i+1}, V_i) \quad (2)$$

for the sequential case, and

$$X_i = X_i(B_i, V_i) \quad (3)$$

for the repeated case. Here, B and V denote burnup and void matrices, respectively. Since a set X_i always is available, this set is used if no new information is obtained from the case under processing, i.e., if

a) the reactor is nonboiling

or

b) a sequential case is being processed.

While processing a repeated case, the matrix B_i is updated according to

$$B_i = (B_i^1 + B_{i-1} + \Delta \cdot P_i) \cdot 0.5, \quad (4)$$

where Δ and P_i denote time step and power matrix, respectively, and the burnup matrix B_i^1 is the one available from the last run for point $i - 1$.

The generation of x (which is an element of X) as indicated in (2) and (3) is performed as a two-dimensional interpolation. Initially, any parameter x is given for a series of discrete burnup (E) and void values (α). During initialization, x is expanded as a polynomial:

$$x = \sum_{\ell=1}^M a_{\ell} \alpha^{\ell-1} \quad (5)$$

for all given values of E , where M is the total number of discrete values of α used in the representation. The coefficients a_{ℓ} are included in the so called job information. For elements E_m and α_m of the B and V matrices, four values E_k belonging to the original discrete set of arguments are found, preferably ordered as

$$E_1 < E_2 < E_m < E_3 < E_4. \quad (6)$$

For each E_k , an $x_{k,m}$ is found from (5), and finally $x_{m,m}$ is found by third-degree interpolation between these values.

The thermal absorption cross section Σ_{A4} obtained in the manner just described does not contain the contribution Σ_{Xe} from xenon.

By assuming that xenon is in equilibrium within each region, and that the production of xenon is proportional to the power density, the following formula is obtained for the absorption cross section for xenon in an arbitrary region:

$$\Sigma_{Xe} = \Sigma'_{Xe} \frac{P}{P'} \frac{\lambda_{Xe} + \sigma_{Xe} \Phi_4'}{\lambda_{Xe} + \sigma_{Xe} \Phi_4}, \quad (7)$$

in the usual notation. Here P is the power density and the primed quantities refer to tabulated values.

4.3 Calculation of equivalent poison cross sections

The evaluation of the equivalent poison cross section for the black control elements follows quite closely a well-known method due to Henry.⁽⁵⁾ For grey absorbers, the same principles are utilized. A thermal $1/v$ -absorber is assumed in the present version of the system, and self-shielding is taken into account only for the thermal-energy group.

In the calculation of the depletion, the effects of construction material in which the grey absorber is embedded are neglected.

The original time step or burnup interval Δ is divided into a number of substeps, and the effective cross sections are re-evaluated between each

substep. The depletion of the grey absorber during each substep is found by the use of a self-evident, exponential depletion formula.

4.4 Calculation of approximate multiplication factors

The information desired in order to facilitate control element positioning is, in BISTRO, given in the form of approximate multiplication factors for the subsequent sequential case, each pertaining to a specified configuration of control elements. From the case under process, which represents point i in the time scale, the following relation is trivial:

$$k_{\text{eff } i} = \frac{P_i}{A_i + L_i}, \quad (8)$$

where P , A , and L denote production, absorption, and leakage, respectively. By assuming that

$$\Phi_{k,m,i+1} = \Phi_{k,m,i},$$

where k and m denote group and region, one gets

$$k_{\text{eff } i+1} = \frac{P_{i+1}}{A_{i+1} + \frac{P_i}{k_{\text{eff } i}} - A_i}. \quad (9)$$

This formula, together with Eq. (10) of Section VI, is used for each trial control configuration. In spite of its crudeness, (9) has been found quite useful. The absolute value of $k_{\text{eff } i+1}$ is, of course, somewhat in error, but the relative effects from different control configurations are very well described.

5. INFORMATION FLOW

A simplified diagram showing the information flow within the system is given in Fig. 2. This diagram is relevant to a noninitial case. Most output routines, as well as job-information reference, have been omitted for simplicity. Routines performing editing and/or calculations are symbolized by circles; the associated letters give in alphabetic order the chronology of programme flow. Reference to Section IV is made for some of the routines. The various information groups given as buffers contain the following information:

Buffer 1: 4-group, regionwise poison cross sections for black and grey control elements and burnable poison isotopic concentration.

Buffer 2: Group constants in 4 groups (i.e., D , Σ_R , Σ_A , $\nu\Sigma_F$, and in conventional notation, for all regions; Σ_A is here uncontrolled).

Buffer 3: Regionwise burnup distributions.

Buffer 4: Groupwise energy release (i.e., watt/unit neutron flux) for all regions.

A. Editing	G. Interpolation and correction of group parameters (4.2)
B. TWENTY GRAND	
C. Integration	H. Calculation of grey poison cross section (4.3)
D. Integration	I. Calculation of black poison cross section (4.3)
E. Void calculation (4.1)	J. Calculation of k_{eff} test values (4.4)
F. Updating of burnup (4.2)	

Fig. 2. Simplified Flow Diagram for BISTRO

Since the input data for any new case (introduced at A) may prescribe either a repeated or a sequential case, all information given in these buffers has to be in two sets. The selection of these sets is a part of the editing performed at A. On the other hand all calculations are necessary in order to produce these data twice, once for each set.

All information referred to as buffered is actually contained on one magnetic tape, by which information is transferred from the completion of one case to the start of the following. Another tape is used in connection with the TWENTY GRAND programme.

The input to an initial case consists (apart from the METHUSELAH data tape) mainly of data specifying the TWENTY GRAND and VOIFLO geometries, thermohydraulic data for VOIFLO, control-material specifications, as well as reflector data and other time-independent parameters.

If no adjustments are made in group number, time step, or TWENTY GRAND iteration parameters, the case input consists only of data specifying black control-element configuration. If the complete control rod program for the reactor is known, the entire reactor lifetime, represented by an arbitrary number of sequential and repeated cases, may be obtained in one computer run. Specifically, a void-power control-element iteration may be performed automatically with a minimum of input data by running one sequential and a number of repeated cases continuously.

The output for each case is essentially made up of regionwise edits of neutron flux, power, and void fraction, together with the criticality and power peaking factors. In addition, the test values for k_{eff} are given for the prescribed control-element configurations. An option is a regionwise edit of the concentrations of the most relevant part of the isotopic library contained in METHUSELAH. This feature is included in order to facilitate detailed studies of any of the core regions by separate, more sophisticated programmes.

6. DISCUSSION

As is well known, very limited experimental information exists that is suitable for testing of macroscopic burnup calculations. The best documented reactor history seems to be that for the first core of YANKEE.^(6, 7)

The YANKEE history has been simulated by BISTRO with quantitatively good results.⁽⁸⁾ As expected from previously published works on the METHUSELAH physics model,⁽⁹⁾ the average end-of-life burnup value shows a small discrepancy, approximately 6%. Moreover, the general agreement regarding controlled criticality indicates that the model for black control rod effectiveness applied in BISTRO is correct within 10-20% (in equivalent cross sections). The theoretical regionwise burnup values are well within 10% of the reported ones.

The situation is probably less satisfactory when boiling water reactors are treated, mainly because of the approximation made in the tabular two-dimensional representation of the core parameters. However, this approximation would not introduce any error if the void distribution, for a particular reactor, was independent of time. This is, of course, unrealistic, but there are two tendencies which will reduce the total effect of the approximation, namely,

- a) the regionwise void content undergoes relatively small variations during the reactor lifetime;
- b) the average void content is almost constant during life.

These features, which have been found true for the boiling water reactors investigated, tend to reduce the errors in the integral parameters, such as multiplication factor and average burnup. The region characteristics will, of course, still be somewhat influenced.

In particular, the effects of this approximation are emphasized when regionwise and total void-reactivity coefficients are to be evaluated. This is done in a separate programme which is associated with, but at present not included in, the BISTRO system. The method used here is that of two-group perturbation theory, and group-constant increments associated with a void increment are then needed. The increments obtained by usual interpolation are then written as

$$d\Sigma = \frac{\partial \Sigma}{\partial \alpha} d\alpha + \sum_i \frac{\partial \Sigma}{\partial N_i} dN_i, \quad (10)$$

where N_i refers to the concentration of the isotopes used in the METHUSELAH model. The desired increment is here the first term on the right-hand side of (10), and the necessary corrections are introduced by simply writing

$$\frac{\partial \Sigma}{\partial N_i} = \sigma_i, \quad (11)$$

where σ_i is the effective microscopic cross section for isotope i , and approximate values for these quantities are then given as additional information.

Another point on which there exists considerable room for improvement is that of evaluation of control rod worth. In particular, this approximation may, when used in connection with burnable poison calculations, lead to accumulating errors as the life calculation proceeds. No comparisons have, however, been made with more detailed methods, and it is therefore very difficult to assess this effect quantitatively in terms of, say, residual poison.

It is believed, however, that a cell-diffusion-theory method should be included instead of the present scheme.

The computing time is, of course, mainly dependent on the two-dimensional diffusion-theory problem. In addition to the execution time for TWENTY GRAND, some 3 to 4 minutes are needed per case. As the present version of TWENTY GRAND is comparatively slow, a significant reduction in computing time is believed possible by speeding up this part of the system, or by replacing it with a faster group-diffusion code.

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A REACTOR SYSTEM DYNAMICS CODE: AIROS*

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I. INTRODUCTION

In order to achieve economic nuclear power without compromising the need for safety, it is vitally important to be aware of potential problems in the design and operation of future reactor systems as well as to improve the understanding of present reactors. There is need for a tool capable of investigating the general area of reactor dynamics in order to develop a fundamental understanding and seek out potential problems concerning the safety of reactor systems. With such a tool, theories can be formulated, tested, and verified by new experiments or by application of previous measurements.

It is important to have such a tool, with realistic models of the dynamic behavior of reactor systems, in order to understand their basic safety. The intent of this work was to develop a flexible digital-computer program as a tool which can lead to an understanding of the dynamic behavior of reactors; and to be able to use this tool for parametric safety studies, design studies, and hazard analysis.

The specifications for this tool fall into three areas: (1) a fast scheme of numerical integration with automatic switching, (2) adequate representation of physical phenomena with flexibility for changing models, and (3) special programming features.

The numerical integration scheme chosen was that developed by Cohen⁽¹⁾ with an interval switching routine developed by the authors. The integration scheme was used in the earlier AIREK codes^(2,3) with considerable success and is coded separately for three classes of differential equations: (1) prompt-neutron equation, (2) delayed-neutron-precursor equations, and (3) generalized feedback equations.

Physical phenomena represented are heat transfer by conduction and convection, decay of coolant flow for simulation of pump failure or line rupture, representation of decay-heat production, rod withdrawal, simulation of programmed control or scram rod insertion, fuel melting, coolant

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vaporization and boiling, simulation of instrument response to scram signals and others. No specific geometry model is built in, but the user divides the heat transfer geometry into channels, each having as many axial and radial nodes as is desired; e.g., 3 channels each having 5 axial and 3 radial nodes. In this manner flexibility of coding and physical models was achieved.

Prime requirements for a production code are ease of data input and availability of special features. Every attempt has been made to provide these features in AIROS. Examples are the treatment of startup, extensive graphical display, the multiple-case feature with built-in initialization of much of the input, and the modularity and accessibility of the physical models (see Figs. 1, 2, and 3).

Fig. 1. AIROS-startup from Cold Shutdown, Rod Withdrawal

Fig. 2. Rod Withdrawal Protected by Sequenced Rod Drop

Fig. 3. Rod Withdrawal Protected by Sequenced Rod Drop

II. PHYSICAL MODELS

Let us now briefly describe the physical models.

AIROS⁽⁴⁾ solves the space-independent reactor kinetics equations and provides for the determination of reactivity by solving, in addition, the discretized equations which represent the spatial heat and mass transfer model for several fuel channels. Also, variation of the film coefficient with flow is accounted for, along with the provisions for flow decay and afterglow heating. Scrams can be initiated by delayed signals from instruments which sense any quantity calculated, e.g., power, inverse period, or temperature.

A. Neutron Behavior

The space-independent prompt and delayed-precursor neutron equations as used in AIROS are

$$\dot{N}(t) = \left[\frac{\rho(t) - \beta}{\ell} \right] N(t) + \sum_i \lambda_i C_i(t) + S_0 \quad (1)$$

$$\dot{C}_i(t) = \frac{\beta f_i}{\ell} N(t) - \lambda_i C_i(t), \quad (2)$$

where the symbols are defined in Appendix A, and the reactivity $\rho(t)$ is a known function of time, power level, and the feedback variables.

It is assumed in these equations that the effective prompt lifetime ℓ , the precursor fractions f_i , and β are constant. In general, these parameters are affected by changes in temperature, spectrum, control rod position, and other variables of the system. Fortunately, for most applications the consequences of postulated accidents are not changed by accounting for these variations. Often the uncertainty in the parameters is greater than their variation during a transient.

These equations are well known and widely discussed elsewhere. They are solved numerically by a technique whose details are found in Ref. 4. Fifteen delayed neutron-precursor equations are provided to allow for photoneutron production in addition to the usual 6-group model.

B. Feedback Equations

Generalized feedback equations are used to provide flexibility in the models that represent multichannel heat transfer including conduction and convection, energy, pressure, and other phenomena. Both differential and algebraic equations are provided, and are of the form

$$\begin{Bmatrix} \dot{F}_j(t) \\ F_j(t) \end{Bmatrix} = P_j Q(t) + U_j N(0) + Y_j F_j(t) + \sum_i \alpha_{ij}(t) F_{k_{ij}}(t), \quad (3)$$

with

$$Q(t) = q(t) + [1 - q(0)] N(t);$$

$$\alpha_{ij}(t) = \begin{cases} C_{k_{ij},j}; & k_{ij} > 0 \\ \omega C_{k_{ij},j}; & k_{ij} < 0, \end{cases}$$

and k_{ij} is the number of the i th feedback "connected to" the j th ($i = 1, 8$), representing a transformation from a sparse indexing set, $\ell, \ell = 1, NF$; $j, j = 1, NF$ to the condensed indexing set, $i, i = 1, 8$; $j, j = 1, NF$.

Thus, if, for some j , $k_{1j} = 5$, $k_{2j} = 10$, $k_{3j} = 17$, then feedback variables 5, 10, and 17 are the first, second, and third variables, respectively, "connected to" Node j . The transformation is used to save storage space in the computer, but limits the number of variables which can be "connected" to any other to eight.

The coefficients $\alpha_{ij}(t)$ are conduction and convection of the form $(UA)/(\rho C_p V)$ and $(\dot{\omega} C_p)/(\rho C_p V)$, respectively, for a nodal heat transfer calculation. Thus the form of α_{ij} permits flow-dependent conduction coefficients, e.g., the film coefficient and convection terms.

Since $N(t)$ and $q(t)$ [consequently $Q(t)$] are usually expressed as fractions of full power, the coefficients U_j and P_j have units of $^{\circ}\text{F}/\text{sec}$, whereas Y_j and α_{ij} are relaxation times with units sec^{-1} .

1. Simple Feedback Equations

Many kinds of feedback variables can be represented by Eq. (3). By setting $U_j = Y_j = \alpha_{ij} = q = 0$ for some j , Eq. (3) becomes

$$\dot{F}_j(t) = P_j N(t). \quad (4)$$

If P_j represents the initial reactor power in megawatts, the $F_j(t)$ is the energy produced to time t .

2. Heat Transfer

Multichannel discretized heat transfer equations can be represented by Eq. (3). One hundred feedback equations are sufficient to follow several channels representing the hot fuel element, the average fuel element and one or more special test elements each having five radial and three axial nodes.

3. Instrumentation Response

In a real reactor system, abnormal behavior such as high temperature, power, or inverse period is sensed by a fission plate, thermocouple, or period meter, and in general by some instrument having its own response to the signal. This signal is finally relayed to a servomechanism which, in turn, initiates the scram.

It is convenient, then, to use an additional feedback equation to represent the response from each instrument which may initiate the scram signal. Let $F_k(t)$ represent the response of some instrument. Then, from Eq. (3), we see that by setting

$$Y_k = -\frac{1}{\tau}; \quad \alpha_{ik} = \frac{1}{\tau}; \quad P_k = U_k = 0,$$

we have

$$\dot{F}_k(t) = \frac{1}{\tau} [F_j(t) - F_k(t)], \quad (5)$$

which is the desired equation for the instrument response to one of the F_j 's. Response to the power can be found by setting $P_k = 1/\tau$, $Y_k = -1/\tau$, $\alpha_{ik} = U_k = 0$; $i = 1, 8$, viz.,

$$\dot{F}_k(t) = \frac{1}{\tau} [Q(t) - F_k(t)], \quad (6)$$

where τ is the instrument response time. Similarly, other instrument response functions can be simulated.

C. Reactivity

The reactivity subroutine is quite flexible, in that any equation can be programmed and many special equations have been coded for special application. Examples are the simulation of the reactivity worth of the control drums for SNAP and bubble (void) models for AIREK-KEWB.^(3,5) The form chosen for the production version of AIROS is as follows,

1. Normal Reactivity

$$r(t) = r(0) + \text{MIN}[\gamma_1 t, \gamma_4] + \sum_j (\delta \rho)_j; \quad t \leq (t_s + \tau_{D1}), \quad (7)$$

where

$r(0)$ = the initial reactivity given in the input or determined by the solution of the inhour equation for constant inverse period in dollars.

γ_1 = linear reactivity insertion rate (dollars/sec).

γ_4 = maximum reactivity insertion (dollars).

$$(\delta\rho)_j = \int_{F_j(0)}^{F_j(t)} \left(\frac{\delta\rho}{\delta F_j} \right) dF_j$$

$$\left(\frac{\delta\rho}{\delta F_j} \right) = \text{reactivity coefficient for the } j^{\text{th}} \text{ feedback.}$$

t_s = time at which the scram signal is sensed as discussed below.

τ_{D_1} = delay between the time the signal is sensed and the first rod motion starts and is found from j_s

where

j_s = the number of the feedback causing the scram (see Eq. (8)).

Equation (7) represents reactivity from (1) step insertion at $t = 0$, (2) linear reactivity insertion, which is assumed to terminate after a scram occurs or at a maximum insertion, and (3) reactivity feedback due to the deviation of the feedback variables from their initial conditions.

It is assumed that the reactivity feedback coefficient $(\delta\rho/\delta F_j)$ can be represented as follows:

$$F_j^{\theta_j} \left(\frac{\delta\rho}{\delta F_j} \right) = A_j, \text{ a constant.}$$

with θ_j usually taken to be 0, 1/2, or 1. Thus the reactivity contribution of the j^{th} feedback variable up to time t , namely, $(\delta\rho)_j$, is

$$(\delta\rho)_j = \begin{cases} \frac{A_j}{1 - \theta_j} [F_j^{1 - \theta_j}(t) - F_j^{1 - \theta_j}(0)]; & \theta_j \neq 1 \\ A_j \ln[F_j(t)/F_j(0)]; & \theta_j = 1. \end{cases}$$

The time at which the scram occurs, t_s , is determined by comparing each of the feedback variables which can initiate a scram against a scram level FM_j specified in the input. Thus t_s is the earliest time at which the condition

$$F_j(t) \geq |FM_j|; \quad j = j_s \tag{8}$$

is satisfied. The absolute value of FM_j is taken because the program determines those feedbacks, j , which can initiate a scram by the condition

$$FM_j < 0. \quad (9)$$

2. Reactivity after a Scram

Reactivity after scram is assumed to be due to up to 4 scram rods dropping from the full-out position, downward through the core under the influence of gravity, each with its own delay time. It is further assumed that the axial flux distribution is a sine function; so that the importance (relative worth) is given by a sine-squared function. Thus the reactivity after scram is given by

$$r(t) = r(0) + \gamma_1(t_s + \tau_{D1}) + \sum_j (\delta\rho)_j + \sum_{k=1}^4 \xi_k \sin^2\left(\frac{\pi}{2} \frac{X_k}{L_k}\right), \quad (10)$$

where

$$t \geq t_s + \tau_{D1}$$

ξ_k = maximum rod worth (dollars) of the k^{th} rod.

L_k = distance through which rod k falls.

$X_k(t)$ = distance from top of core at time t , viz.,

$$X_k(t) = \begin{cases} 0; & t \leq t_s + \tau_{Dk} \\ \frac{1}{2} a_k [t - (t_s + \tau_{Dk})]^{N_k}; & 0 \leq X_k(t) \leq L_k; \quad t > t_s + \tau_{D1} \\ L_k; & t_s + \tau_{D1} < t \rightarrow \infty \end{cases} \quad (11)$$

where

$N_k = 2$, $k = 1, 3$, i.e., free fall under gravity, and $N_4 = 1$.

The constant a_k is the acceleration of gravity (ft/sec²) as modified possibly by a friction factor.

D. Flow Equations

At the present time, provisions for two flow conditions are available, allowing for constant flow, flow decay from full power, and after a scram. This subroutine is quite flexible and subject to frequent change. The current form is as follows.

1. Flow Decay from Full Power

It is assumed that the reactor is operating at some level at $t = 0$, and that an accident such as pump failure or pipe rupture occurs which causes the flow to decay from its normal value according to the following relation:

$$\dot{\omega}(t) = A \exp(Bt) + C + \text{MAX}[0, E(F - t)]; \quad t \geq 0. \quad (12)$$

This option can also be used to simulate pump startup for increasing power levels, although no provision (other than end of problem) is made to terminate the increase.

2. Flow Decay after Scram

In this case, the reactor operates according to Eqs. (1), (2), (3), and (10), and at constant flow up to the time of a scram, i.e.,

$$\dot{\omega}(t) = D; \quad t \geq (t_s + \tau_{\dot{\omega}}^o), \quad (13)$$

where $\tau_{\dot{\omega}}^o$ is a delay time and according to

$$\begin{aligned} \dot{\omega}(t) = & A \exp\{B[t - (t_s + \tau_{\dot{\omega}}^o)]\} + C \\ & + \text{MAX}\{0, E[F - (t_s - t - \tau_{\dot{\omega}}^o)]\}; \quad t > (t_s + \tau_{\dot{\omega}}^o) \end{aligned} \quad (14)$$

thereafter.

E. Afterglow Heating

The formulation for afterglow heating is a 2-term exponential based on Ref. 6:

$$q(t) = \begin{cases} q(0); & t \leq t_s \\ \delta_1 \exp[\delta_3(t - t_s)] + \delta_2 \exp[\delta_4(t - t_s)]; & t > t_s. \end{cases} \quad (15)$$

One can simulate the afterglow heating for a startup after a previous scram [$q(0) \neq 0$], afterglow after a scram [$q(0) = 0$; $\delta_1, \delta_2 \neq 0$], or combinations. Improved formulations can be coded as data become available.

F. Fuel Melting and Coolant Boiling

Several models have been used to describe fuel melting and coolant boiling. One such model is described in Ref. 7, but was crude and will not be reported herein. Another is a simplification of the TRANS-FUGUE⁽⁸⁾ code, incorporating two-phase flow. Currently, fuel-capsule melting experiments are under way at TREAT. It is anticipated that a realistic model for

fuel melting will be developed and will be incorporated into AIROS, along with the two-phase flow model.

III. SPECIAL FEATURES

AIROS has several special programming features which can be used to great advantage. These features either reduce running time or make the program easier to use, i.e., require less input data.

A. Initial Conditions on Neutron Levels

Since the program solves a system of first-order differential equations, it is necessary to provide the initial conditions for the prompt- and delayed-precursor neutron levels, reactivity, flow, etc. To make input easy, the user can set certain of the initial conditions by a combination of three methods.

1. At the beginning of the first run of a set of cases, the initial neutron- and delayed-precursor levels are set equal to one; i.e.,

$$N(0) = W_i(0) = 1; \quad i = 1, 15. \quad (16)$$

These values are used as the initial conditions for all cases until changed by one of the two methods which follow. Note that the initial reactivity $r(0)$, flow $\dot{V}(0)$, and feedback levels $F_j(0)$ are not initialized by the program.

2. Initial conditions can be input.
3. Initial conditions can be obtained from a solution to the inhour equation.

B. Preset Data

As a convenience, portions of the data are preset prior to the first case and are used in subsequent cases unless changed by input data. In addition to setting the neutron levels equal to one, the following values are preset.

1. Delayed-neutron-precursor Decay Constants and Fractions

The delayed-neutron-precursor data⁽⁹⁾ are for thermal fissions in U^{235} , and are built in or can be changed.

2. Maximum Values of Feedbacks

In order to preclude problem termination because of exceeding the maximum value of some feedback which is not used in the problem, all

feedback maxima are set equal to 10^{35} . Those feedbacks which are used to terminate the problem or to initiate a scram must have maximum values provided in the input data.

C. Interval Switching

The interval size h is automatically adjusted by AIROS so that a given accuracy results. Since it is extremely difficult to perform an exact analysis of the truncation error or of the propagation of error, an approximate method was developed which has proven to be satisfactory. This method is discussed in Ref. 4 and will not be repeated here.

D. Startup Problems

One of the classic accidents investigated in every hazards report is the startup accident. In this accident, a shim rod is withdrawn to achieve full power, and because of some malfunction continues to withdraw, causing the reactor to go highly supercritical. The initial power level (that of the source) is sufficiently small--1 watt, say--so that negligible heat is generated during a large part of the transient. Consequently, no useful information is gained in solving Eq. (3) for the temperatures, as they are constant; however, a large amount of computer time is wasted, since we are solving many feedback equations.

Provision is made in AIROS to solve only Eqs. (1), (2), and (7) for the prompt-neutron level, delayed-neutron-precursor levels, and reactivity, respectively, until such time that $N(t) \geq N_{\min}$, where $N_{\min}$ is provided as input data; thereafter Eq. (3) is also solved. The user can bypass this option if desired by setting $N_{\min} = 0$, in which case the feedback equations will be solved at all time-points. Normally, however, $N_{\min}$ should be such that the feedback equations are solved when the prompt power exceeds 0.1% of full power. This feature reduces the running time by 75% in typical cases.

E. Problem Termination

Normal termination of a problem occurs when one of the following three conditions is met:

1. $t \geq \text{TIMEM}$, the maximum problem time specified in the input;
2. $N(t) \geq N_{\max}$, the maximum neutron level specified in the input;
3. $F_j(t) \geq FM_j$, the maximum value of one of the feedbacks.

F. Restart from Previous Case

A feature is provided in AIROS which permits restarting a case from cards punched by a previous case. These cards contain the information required to continue the problem, the last computed values being used for the

initial conditions. Punching of restart cards is automatic if difficulty is encountered in completing a case, but optional otherwise (see the previous remarks regarding problem termination).

G. Printing and Graphical Display Options

Several options provide control over output:

1. Frequency of output--the user can specify that every n^{th} point is output.
2. Delayed-neutron-precursor levels are optional.
3. Time scale--the time scale for printed and graphical output can be divided into two parts for startup problems:

$$0 \leq t \leq t_0 \text{ AND } t_0 \leq t \leq t_{\text{MAX}},$$

where t_0 represents the time at which 0.1%, say, power occurred.

Options provide for display of power, reactivity, inverse period, and delayed neutrons in each of several ways on separate frames:

- a) $0 \leq t \leq t_{\text{MAX}}$
- b) $0 \leq t \leq t_0 \text{ AND } t_0 \leq t \leq t_{\text{MAX}}$
- c) $0 \leq t \leq t_0 \text{ AND } 0 \leq t \leq t_{\text{MAX}}$
- d) $t_0 \leq t \leq t_{\text{MAX}}$

4. Choice of Feedback Variable Output

The user of AIROS can indicate which feedback variables are to be printed and which are to be displayed. Furthermore, any feedback variables can be grouped on a given frame. The feature allows, for example, grouping of all fuel nodes.

H. Multiple Cases

Input data are divided into six groups as follows:

1. title card;
2. floating-point data, such as error bounds, initial conditions, and control rod worths;
3. integer data describing output options for the feedback variables;
4. floating-point data containing the heat transfer coefficients;

5. integer data indicating how the nodes are connected;
6. restart data (may not be present).

Since addressable data are used, multiple cases can be run with only changes in data specified; all other data remain from previous cases.

APPENDIX A

Main Symbols

<u>Quantity</u>	<u>Definition</u>
t	Time(sec)
$N(t)$	Prompt-neutron level at time t
$\rho(t)$	Total reactivity, $(\delta k/k) = \delta k/k \beta$
β	Effective fraction of delayed neutrons
ℓ	Neutron lifetime (sec)
f_i	Fraction of delayed neutrons in group i
λ_i	Decay constant for delayed-neutron-precursor group i
$C_i(t)$	Delayed-neutron-precursor group i concentration at time t
S_0	Source term
F_j	Feedback variables
P_j, U_j, Y_j	Proportionality constants
$r(t)$	Total reactivity, dollars
$W_i(t)$	Normalized concentration of delayed-neutron-precursor group i
S	Normalized source term
A_j	Feedback coefficients in the reactivity equation
γ_1	Time coefficient in the reactivity equation
$\omega(t)$	Inverse reactor period
k_{eff}	Effective multiplication constant
$\alpha_{ij}(t)$	Heat transfer coefficient between feedbacks i and j
$Q(t)$	Sum of neutron level and afterglow-heating level (normalized)
ND	Number of delayed-neutron-precursor groups
NF	Number of feedback equations
$q(t)$	Afterglow heat

$\dot{\omega}(t)$	Mass flow rate
t_s	Time at which a scram occurs
τ_{D_1}	Scram delay time

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Discussion of Paper Presented by Mr. Blaine

MR. SHAFTMAN (Argonne National Laboratory): What geometry did you use? Also, do you have an automatic way of readjusting your time interval when you get into numerical instability, if you do get into it?

MR. BLAINE: The geometry is quite arbitrary; no specific geometry is built into the code. It is strictly a nodal representation of the heat transfer. As for the second question, the integration scheme is the same as used in the earlier AIREK codes. The time interval is automatically

adjusted by doubling or halving according to a prescribed error bound--a thoroughly typical method. We use a new and more satisfactory definition of the error from that used in the AIREK codes. The most frequent kind of instability we ran into, of course, was hydrodynamic instability, but by appropriate choice of the error bound, this vanished.

MR. VAUGHAN (Central Electricity Generating Board): On the question of geometry, in practice do you mostly use axially-averaged quantities so that the representation is virtually pointwise, or do you take account of axial variation? Also, in representing fuel pin temperatures, you divide your pins into a number of annular regions; for investigations of start-up accidents about how many regions do you use?

MR. BLAINE: In terms of the number of nodes that are normally used, Atomix International reactors to date have been sodium-graphite reactors which use 7 to 19 rods in a cluster. This was the geometry used in HALLAM and in SRE. We have not designed a reactor with pin geometry; however, there are people doing studies with pin geometry. I don't know how fine a division they are using. We, normally, use three to five radial nodes, and three to five axial nodes per channel.

FREAK--A FAST REACTOR MULTIGROUP KINETICS PROGRAM

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1. Introduction

The treatment of reactor kinetics normally adopted⁽¹⁾ is to use a one-point reactor model and to assume monoenergetic neutrons. These assumptions neglect any changes in spatial neutron distribution and energy spectrum during transients. Hence the results obtained from such a treatment are likely to be accurate only for any integral type of disturbance. The objects of writing a program to deal with multienergetic neutrons with two-dimensional spatial distribution were, firstly, to check the normal treatment of kinetics of fast neutron reactors for integral disturbances (e.g., step and ramp changes in reactivity) and, secondly, to investigate those types of local disturbance (e.g., movement of some of the fuel elements and partial flow blockage) for which the point model is clearly unacceptable. Since the program was intended to deal specifically with fast power reactors it was considered necessary to treat multienergetic neutrons and also to be able to follow in some detail the movements of fuel elements, since this can be a major source of reactivity feed-back in such systems.

The general basis of the program is described in Section II, which outlines the steady-state calculations. Treatment of time-dependent behavior is given in Section III. The Doppler effect is treated in Section IV, reactor control and scram in Section V, and editing routines associated with the main program in Section VI. In Section VII some comparisons are made between results obtained from the program and those from a point reactor treatment.

2. Steady-state Calculations

Before describing the time-dependent section of the program it is convenient to outline the general basis of the treatment with reference to a steady-state calculation. The neutron behavior is treated by standard multigroup diffusion theory. The basis of the program is a multigroup diffusion-theory program⁽²⁾ called CRAM, which has been in extensive use for over 3 yr. In general, CRAM can handle up to 100 energy groups and allows scatter from any one group to any other group. Cross sections may be put in directly or they may be obtained from one of several multigroup libraries in the program. At present the libraries available are (1) ANL 11-group,⁽³⁾ (2) Roach 16-group,⁽⁴⁾ (3) Yiftah 16-group,⁽⁵⁾ (4) 33-group.⁽⁶⁾ It is easy to add any other libraries as required, and a group-condensation routine is provided. The kinetics program uses the version in RZ geometry which computes $k_{\text{effective}}$, but with a modification to include delayed neutrons.

Up to 10 groups of delayed neutrons are allowed. Fissile isotopes have to be specified separately, with the delayed fractions β_i as extra input data. Also required are the delayed-neutron energy spectra ξ_{ig} for each delayed group i and energy group g . It is assumed that the delayed spectra are the same for all isotopes.

The fission source term in group g is thus of the form

$$\frac{1}{k} \sum_{i,g',n} [\chi_g(1 - \beta_n) + \xi_{ig}\beta_{in}] (\nu\Sigma_f)_{g'n} \phi_{g'},$$

where n denotes isotope. The full time-dependent diffusion equation used is given as Eq. (1) in Appendix 1.

The program computes k and obtains the flux distribution (see Ref. 2 and Appendix 2). From this the specific power distribution (in Watts per cc), given by Eq. (3) in Appendix 1 is calculated corresponding to a specified total reactor power given by Eq. (4) in Appendix 1. (The normalization constant is retained throughout subsequent kinetics calculations.) The power distribution is used to determine the temperature distribution in each reactor material by means of Eqs. (5)-(10) in Appendix 1. The materials considered are fuel, canning, structure, flowing coolant, and static coolant. Variation of temperature across a fuel pin is treated by considering the pin as divided into two zones and introducing a center fuel temperature associated with the inner zone and a surface fuel temperature associated with the outer zone. If required, two types of fuel and two types of canning can be handled. The mean outlet temperature of the coolant is obtained from Eq. (11) in Appendix 1, allowing for the mass of coolant in the outlet plenum chamber. In the coolant equations the variation of heat transfer coefficient with mass flow is allowed for through an index h . The mass flow may be varied radially to allow for gagged elements. The density and specific heat of each material are allowed to be temperature dependent.

A further temperature equation allows a simple simulation of the effect of disturbances travelling around the external coolant circuit.

The next section of the program deals with the effect of temperature gradients on the position of fuel elements. The displacement of each mesh point with respect to its original position at some uniform reference temperature T_0 is calculated. The displacement in the z direction is obtained from Eq. (13) of Appendix 1, which allows expansion to be governed by canning or fuel temperature. Boundary conditions are used which assume that the reactor is divided into a number of axial zones, within each of which the can or fuel is fixed to the structure. The structure [see Eq. (14) of Appendix 1] is assumed to be fixed at a hold-down plate at the inlet ($z = 0$) end of the reactor. Displacement in the r direction [see Eq. (15) in Appendix 1] allows for bowing of elements to be governed by structure

temperature and bowing of pins to be governed by can or fuel temperature, and also takes into account the temperature gradient between successive radial mesh points. Boundary conditions put the radial displacements at $z = 0$ equal to the expansion of the hold-down plate. The derivation of Eq. (15) of Appendix 1 assumes that the axial power distribution is independent of radius. A program correction is planned in which the term proportional to power gradient is replaced by two terms, one proportional to power gradient and one proportional to the gradient of the power integrated in the z direction.

If the radial displacements due to thermal effects are sufficient to take up the initial clearances between the elements, elastic displacements are caused. These are calculated by Eqs. (16)-(18) of Appendix 1, in which elastic deflection of successive elements is allowed for. The elastic displacements (if any) are then added to the thermal displacements in the r direction. The general result of the displacement section of the program is to obtain a new r - z mesh corresponding to the calculated temperature distribution, allowing for all displacements relative to the reference frame for the temperature T_0 . A further effect of the temperature distribution is the expansion of each material, resulting in a reduction in density and hence macroscopic cross section. The new density is given by

$$\rho'_m = \rho_m \left[1 + \ell_m (T_m - T_0) + \frac{\alpha_m}{2} (T_m - T_0)^2 \right]^{-1}.$$

A further change due to temperature has also to be allowed for, namely, the change in volume fractions f_m due to expansion of and displacement of materials in the reactor, by means of Eqs. (19)-(21) in Appendix 1. The resultant new macroscopic cross sections are given by

$$\Sigma'_m = \frac{f'_m}{f_m} \frac{\rho'_m}{\rho_m} \Sigma_m.$$

The next stage of the program is to go back to the diffusion equations with the new macroscopic cross sections and solve them again, using the new mesh. The new flux distribution produced is then the start of the next cycle of calculations. An iterative procedure is thus commenced within each cycle of which the flux distribution, temperature distribution, and displacements are converged to a specified accuracy. The overall convergence criterion is that there must be only one iteration each of flux, temperature, and displacement in any one cycle (see Appendix 2). At each stage of the calculation an estimated value of $k_{\text{effective}}$ is produced, the first one being that corresponding to the uniform reference temperature T_0 and the last that corresponding to the reactor power specified. Calculation can be done at zero power and will then produce a $k_{\text{effective}}$ corresponding to a uniform reactor temperature equal to the specified coolant inlet temperature. In this way direct calculation of total temperature and power

coefficients can be made. These may be compared with perturbation-theory calculations (see Section VI).

At the end of the steady-state calculation the final fluxes, temperatures, displacements, and delayed-neutron distributions are written onto a history tape.

It is possible to start any new steady-state calculation, or re-start one which has not been fully converged, by use of a flux guess from a tape previously produced. For this purpose one can use either a CRAM dump tape or a FREAK history tape. If a FREAK history tape is used, then the temperature distribution and displacements contained on it can also be used as starting estimates for new cases.

3. Time-dependent Calculations

The effect of any physical disturbance to the system can be obtained by changing the appropriate item of input data, e.g., zone composition, coolant flow rate, and inlet temperature. It is also possible to simulate the usual integral type of disturbance used in point-model kinetics, e.g., a reactivity step, by making temporary changes to the cross-section library. Input data for a kinetics run also include the number and size of time steps for the ensuing calculation. The program picks up the steady-state ($t = 0$) fluxes, etc., from the history tape and new data from the input cards, and commences a kinetics run. The diffusion equation [(1) of Appendix 1] and delayed-neutron precursor equation [(2) in Appendix 1] are solved simultaneously, by the usual source-iteration technique, using the first-order difference approximation for the time differential. The flux distribution obtained is used to produce a power distribution (using the same normalization factor as calculated in the steady state) and the time-dependent temperature equations [(5)-(10) of Appendix 1] are then solved by means of the first-order difference approximation. The displacements are then determined, and the same iterative procedure is followed for convergence of flux, temperature, and displacements as was adopted for the steady state.

During the running of the program the output is restricted to flux iteration details, total power, outlet temperature, and maximum fuel and coolant temperatures. However, at specified time intervals the program dumps on to the history tape full fluxes, temperatures, displacements, and delayed-neutron distributions. Any part of this information may then be printed out as required later.

It is always possible to start a kinetics run at any time reached in a previous run by using the history tape. Hence a transient does not have to be followed in full in any one run. The history tape produced in any re-started run contains all the information from the original history tape as well as any new information produced during the new run.

4. Doppler Effect

As has been described in Sections II and III, the effects of thermal expansions and displacements of reactor materials are allowed for in the diffusion equation by the program. These effects produce the reactivity feedback effect due to direct changes in reactor composition.

Another very important reactivity effect due to temperature changes is the Doppler effect. Doppler-broadened effective capture and fission cross sections can be calculated in any specified energy-group structure by the program ERIC.⁽⁷⁾ In order to incorporate this effect in FREAK, a subsidiary program, FRTD, was written. This program takes the capture and fission cross sections for a set of temperatures, as produced by ERIC, and combines these with FREAK input data to produce macroscopic cross sections Σ_T and $\nu\Sigma_f$ for each fuel material (group condensed if necessary) as required in the diffusion equation.

A modified library is thus produced for fuel material consisting of tables of cross sections at a specified set of temperatures. The FREAK program now finds by linear interpolation in these tables the value of the cross section corresponding to the average fuel temperature:

$$T_e = xT_{es} + (1 - x) T_{ec},$$

at each mesh point.

Thus, in a kinetics run the reactivity feedback due to the Doppler effect is allowed for by the changes in macroscopic fuel cross section with temperature.

It is possible to use FREAK both with and without Doppler-broadened cross sections. Hence, the reactivity change due to the Doppler effect can be found in the steady state, for both uniform and nonuniform temperature distributions. These direct calculations can be compared with those from perturbation theory (see Section VI).

5. Reactor Control and Scram

Also available in the time-dependent part of FREAK is a facility for control rod movement. Control rods are assumed to move vertically in channels and to be interchangeable with coolant when moved. The initial data required consist of the radial location of the rod, depth of insertion, composition of the rod, and volume fraction of coolant displaced on movement of the rod. The movement is governed by the difference ΔQ between the demanded value and the actual calculated value of some control quantity Q . Control quantities available are coolant temperature, power from any channel, and central fuel temperature. (It is an easy matter to allow any other desired control quantity.) From the difference ΔQ is obtained an

error signal ϵ [see Eqs. (18)-(20) in Appendix 1] which allows for time delay, for each region, and overall. A composite region signal is then found by weighting. An action signal equation [see Eq. (22) of Appendix 1] allows for phase advance of the signal. Finally, the control rod movement, given by Eq. (23) in Appendix 1, is calculated, there being assumed a dead bandwidth for the signal below which there is no movement and a value for the signal above which there is no further movement.

Scram rods may either be treated in the same way as control rods (i.e., automatically) or may be treated as subject to manual control. With automatic control the action signal is obtained in the same way as for the control rods, but the movement of the scram rod is assumed to start at a fixed value of the action signal and to proceed with a uniform acceleration. With manual control the scram rod is simply assumed to move with uniform acceleration starting at a fixed time.

It is intended to employ the control section of the program in two ways. Firstly, for small disturbances the effectiveness of various control rod arrangements and the dependence of the stability of the control system on circuit constants can be investigated. Secondly, for large disturbances the effectiveness of the scram rods and the dependence of satisfactory curtailment of the incident on delay time and rate of scram can be investigated.

6. Editing Routines Associated with FREAK

In the usual one-point reactor kinetics treatment certain quantities are used which are neither input nor output explicitly in FREAK. These are the effective delayed fraction (β_{eff}), the prompt-neutron lifetime (ℓ^*), and temperature or power coefficients of reactivity. For the purposes of comparison of FREAK results with one-point-model results, it is desirable to use consistent values of these quantities. This section describes editing routines which have been written to obtain β_{eff} , ℓ^* , and the reactivity coefficients. These routines are all based on the use of multigroup perturbation theory.⁽²⁾ The first requirement for their use is to have both a regular flux and an adjoint flux available on tapes from CRAM calculations. It is a simple matter to do CRAM calculations using the same input data (as regards mesh, reactor composition, and cross-section library) as in FREAK to produce these regular and adjoint flux tapes.

The β_{eff} routine requires as input data the delayed-neutron fractions in each delayed group for all fissile isotopes in the problem, the prompt-neutron fission spectrum, and the delayed-neutron spectrum for each delayed group. By means of the standard multigroup perturbation expression,⁽⁸⁾ the routine produces the total effective delayed fraction plus the contributions from each delayed group and from each isotope.

The ℓ^* routine requires as input data the inverse neutron velocities for each energy group. By use of the standard multigroup perturbation expression,⁽⁸⁾ the routine produces the prompt-neutron lifetime for each zone and for the whole system.

The reactivity coefficient routine requires, besides regular and adjoint flux tapes, a FREAK history tape. The routine uses multigroup perturbation theory to obtain the reactivity change from zero power to the FREAK power due to changes in reactor composition. The effects allowed for are density changes due to axial expansion of each material, volume expansion of coolant, change in coolant volume fraction due to radial expansion of can and structure, change in fuel length, and radial displacement of elements. The routine also computes the reactivity change due to change in fuel cross sections (through the Doppler effect).

The routine produces temperature coefficients per unit expansion coefficient and reactivity changes from zero power to FREAK power for expansion of each material in each zone and sums over zones, reactivity change due to Doppler effect, and reactivity change due to radial displacements.

7. Comparison of FREAK Results

The steady-state part of the FREAK program has been working satisfactorily for some time. It has been used to determine reactivity changes from zero to full power. These have been compared with results of perturbation-theory calculations by means of the routine discussed in Section VI. The calculated total reactivity changes obtained from summing contributions from the different effects (fuel movement, Doppler effect, etc.) from the perturbation routine are in good agreement with those obtained directly from FREAK.

Time-dependent calculations with FREAK have up to now been restricted to reactivity steps. Calculations have been made for a power reactor using a model having 16 axial and 16 radial mesh points. Six delayed groups and five energy groups were used. Calculations were also made with one energy group only. None of these calculations has yet been carried very far in time because of the machine time involved. Efforts are at present being made to reduce the running time per time step and to find some acceptable method of automatically increasing the time step within the program. For the limited range over which comparison is possible there appears to be little difference between the FREAK results and those obtained with a point model, as was anticipated for the integral type of disturbance considered (a step change of 0.25% in ν).

Calculations have also been made for a somewhat simpler model having 8 axial and 10 radial mesh points covering a reactor core only.

Only one delayed group and one energy group were used. The results obtained for a step of 0.03% in ν at low power are in reasonable agreement with those obtained from a one-point-model treatment.

Acknowledgments

The programming of FREAK was performed by A. Hassitt and A. Fielden. The derivation of the equations of the temperature and displacement sections was made by P. E. Simmons and G. McAreavey. The edit routines were written by R. M. Lord and J. K. Fletcher.

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APPENDIX 1

Equations

Diffusion equations:

$$\frac{1}{v_g} \frac{\partial \phi_g}{\partial t} = D_g \nabla^2 \phi_g - \Sigma_{rg} \phi_g + \sum_{g'} \Sigma_{g'g} \phi_{g'} + \sum_{g',n} \chi_g (1 - \beta_n) (\nu \Sigma_f)_{g'n} \phi_{g'} + \sum_i \xi_{ig} \lambda_i C_i, \quad (1)$$

where

$$\Sigma_{rg} = \Sigma_{cg} + \Sigma_{fg} + \sum_{g'} \Sigma_{gg'}; \quad \beta_n = \sum_i \beta_{in}; \quad Dg = \frac{1}{3\Sigma_{trg}}.$$

Precursor equations:

$$\frac{\partial C_i}{\partial t} = \sum_{g,n} (\nu \Sigma_f)_{gn} \beta_{in} \phi_g - \lambda_i C_i. \quad (2)$$

Specific power (for material m):

$$P_m = \sum_{g,n} \left\{ e_{fn} \Sigma_{fgn} + e_{cn} \Sigma_{cgn} \right\} \phi_g \times 1.6 \times 10^{-13} \text{ W/cc.} \quad (3)$$

Normalization--total power:

$$P = \int_V \sum_m P_m dV \times 10^{-6} \text{ MW.} \quad (4)$$

Temperature equations:

(a) Flowing coolant ($T_d = T_{in}$ at $s = 0$)

$$M_d \left\{ \rho_d f_d \frac{\partial T_d}{\partial t} + w \frac{\partial T_d}{\partial s} \right\} = p_d + H_b w^h (T_b - T_d) + H_s w^h (T_s - T_d). \quad (5)$$

(b) Static coolant

$$M_{d0} \rho_{d0} f_{d0} \frac{\partial T_{d0}}{\partial t} = p_{d0} - H_{b0} (T_{d0} - T_b) + H_r \left\{ \frac{\partial^2 T_{d0}}{\partial r^2} - \frac{T_{d0} - T_{in}}{\phi} \frac{\partial^2 \phi}{\partial r^2} \right\}. \quad (6)$$

(c) Structure

$$M_b \rho_b f_b \frac{\partial T_b}{\partial t} = p_b - H_b w^h (T_b - T_d) + H_{b0} (T_{d0} - T_b). \quad (7)$$

(d) Canning

$$M_s \rho_s f_s \frac{\partial T_s}{\partial t} = p_s + H_{es} (T_{es} - T_s) - H_s w^h (T_s - T_d). \quad (8)$$

(e) Fuel surface

$$xM_e\rho_{efe}\frac{\partial T_{es}}{\partial t} = xp_e + H_{ec}(T_{ec} - T_{es}) - H_{es}(T_{es} - T_s). \quad (9)$$

(f) Fuel center

$$(1-x)M_e\rho_{efe}\frac{\partial T_{ec}}{\partial t} = (1-x)p_e - H_{ec}(T_{ec} - T_{es}). \quad (10)$$

(g) Outlet

$$WT_{out} + m\frac{\partial T_{out}}{\partial t} = 2\pi \int_0^R T_d(outlet) wrdr. \quad (11)$$

(h) External circuit

$$T'_{in} + \frac{K}{W} \frac{\partial T'_{in}}{\partial t} = F(T_{out}); \quad T_{in}(t) = T'_{in}(t - t_a). \quad (12)$$

Displacements:

z mesh:

$$\begin{aligned} \frac{\partial y_z}{\partial z} = & B_s \left\{ \ell_s(T_s - T_0) + \frac{\alpha_s}{2} (T_s - T_0)^2 \right\} + B_{es} \left\{ \ell_e(T_{es} - T_0) + \frac{\alpha_e}{2} (T_{es} - T_0)^2 \right\} \\ & + B_{ec} \left\{ \ell_e(T_{ec} - T_0) + \frac{\alpha_e}{2} (T_{ec} - T_0)^2 \right\} \end{aligned} \quad (13)$$

Structure:

$$\frac{\partial y_b}{\partial z} = \ell_b(T_b - T_0) + \frac{\alpha_b}{2} (T_b - T_0)^2. \quad (14)$$

Boundary conditions: $y_z = y_b$ at fixed points and $y_b = 0$ at $z = 0$.

r mesh:

$$\begin{aligned} \frac{\partial^2 y_r}{\partial z^2} = & -\frac{1}{p} \frac{\partial p}{\partial r} \left\{ A_b[\ell_b + \alpha_b(T_b - T_0)](T_b - T_{in}) + A_s[\ell_s + \alpha_s(T_s - T_0)](T_s - T_{in}) \right. \\ & + A_e[\ell_e + \alpha_e(T_{es} - T_0)](T_{es} - T_{in}) \\ & \left. - A_b \left[\frac{g_{J-1,J} + g_{J,J+1}}{2 \left(1 + \frac{H_b}{H_{b0}} wh \right)} \{ \ell_b + \alpha_b(T_b - T_0) \} \right] \right\} \end{aligned} \quad (15)$$

where g is the structure temperature gradient from one radial mesh point to the next.

Boundary conditions at the tube-plate $z = 0$: $\frac{\partial y_r}{\partial z} = 0$ and

$$y_r = (1+a) \frac{1}{r} \int_0^r \left\{ \ell_b (T_b - T_0) + \frac{\alpha_b}{2} (T_b - T_0)^2 \right\} r dr \\ + (1-a) \frac{r}{R^2} \int_0^R \left\{ \ell_b (T_b - T_0) + \frac{\alpha_b}{2} (T_b - T_0)^2 \right\} r dr.$$

Elastic: Let $Y(j)$ denote the maximum value for the j^{th} radial mesh point of y_r . Denote by z' the axial mesh point where the maximum $Y(j)$ of $y(r)$ occurs. Residual clearance between elements is

$$C_j = \frac{C_0}{b} (r_j - r_{j-1}) + Y(j) - Y(j-1). \quad (16)$$

If $C_j < 0$ for $j = p$ to q , then

$$Y_{\ell}(j-1) = Y_{\ell}(j) + C_j \text{ for } j = p \text{ to } q \text{ and } \sum_{j=p-1}^q r_j Y_{\ell}(j) = 0; \quad (17)$$

$$y_{\ell}(z, k) = \frac{1}{2} Y_{\ell}(j) \left(\frac{z}{z'} \right)^2 \left(3 - \frac{z}{z'} \right). \quad (18)$$

Volume fractions:

$$f'_{d0} = 1 - \frac{(1 - f_{d0})}{\left(1 + \frac{\partial y_r}{\partial r}\right)} \left[1 + 2\ell_b (T_b - T_0) + \alpha_b (T_b - T_0)^2 \right]; \quad (19)$$

$$\left. \begin{aligned} f'_d &= \frac{1}{\left(1 + \frac{\partial y_r}{\partial r}\right)} \left[f_d + (f_s + f_e + f_d) \{ 2\ell_b (T_b - T_0) + \alpha_b (T_b - T_0)^2 \} \right. \\ &\quad - f_s \{ 2\ell_s (T_s - T_0) + \alpha_s (T_s - T_0)^2 \} \\ &\quad \left. - f_e \{ 2\ell_e (T_e - T_0) + \alpha_e (T_e - T_0)^2 \} \right] \end{aligned} \right\}; \quad (20)$$

$$f'_m = \frac{f_m}{\left(1 + \frac{\partial y_r}{\partial r}\right)} \quad \text{for } m = b, s, e. \quad (21)$$

Control rods:

Difference between demanded and actual value of control quantity

$$\Delta Q_J = Q_J - Q_{aJ} \quad \text{for region } J. \quad (22)$$

Error signal

$$\tau \frac{d\epsilon_J}{dt} + \epsilon_J = \Delta Q_J \quad \text{for region } J; \quad (23)$$

$$\tau \frac{d\epsilon_M}{dt} + \epsilon_M = \Delta Q_M \quad \text{for overall average.} \quad (24)$$

Composite signal

$$\gamma_J = (1 - d_J) \epsilon_J + d_J \epsilon_M. \quad (25)$$

Action signal

$$\eta_J = N_J \left\{ \mu \frac{d\gamma_J}{dt} + \gamma_J \right\}. \quad (26)$$

Control rod movement

$$\begin{aligned} \frac{dz_C}{dt} &= G_J f(\eta_J) \text{ where } f(\eta) = 0 \text{ for } |\eta| \leq \delta \\ &= |\eta| - \delta \text{ for } \delta < |\eta| < \Delta \\ &= \Delta - \delta \text{ for } |\eta| \geq \Delta. \end{aligned} \quad (27)$$

Scram rods:

(a) Action signal η_I obtained as for control rods

Scram rod movement

$$\left. \begin{aligned} z_s &= 0 & \text{for } |\eta_I| < E_I \\ \frac{dz_s}{dt} &= St & \text{for } |\eta_I| \geq E_I \end{aligned} \right\}. \quad (28)$$

(b) Manual

$$\left. \begin{aligned} z_s &= 0 & \text{for } t < t_s \\ \frac{dz_s}{dt} &= St & \text{for } t \geq t_s \end{aligned} \right\}. \quad (29)$$

APPENDIX 2

Outline of program flow

The FREAK program is written in FORTRAN for the IBM-7090 computer. It is conveniently divided into several distinct sections. Of these the flux, acceleration, and library sections are identical with those of CRAM.(2). The print and restart sections are similar to those of CRAM but modified to allow treatment of temperature distributions and displacements. Those peculiar to FREAK are the time-dependent flux, delayed neutron, temperature, displacement, and control sections.

As in CRAM the flux section computes the quantity Λ given by

$$\Lambda^n = \left(\frac{I^n}{I^{n-1}} \right)^{1/2}, \quad (30)$$

where

$$I^n = \sum_{j, k, g} \left\{ \phi^n(j, k, g) \right\}^2$$

and $\phi^n(j, k, g)$ is the flux at point (j, k) in group g in iteration n . At every iteration the program prints Λ^n , and at some iterations it also prints an estimate of k , $F_{\max}$, and $F_{\min}$, where

$$F_{\max} = \text{Max}_{j, k, g} \left\{ \frac{\phi^n(j, k, g)}{\phi^{n-1}(j, k, g)} \right\}, \quad (31)$$

and similarly for $F_{\min}$.

The flux calculation finishes if all the following conditions are satisfied:

$$\left. \begin{aligned} F_{\max} - F_{\min} &< 0.00005 \\ |F_{\max} - 1| &< 0.001 \\ |F_{\min} - 1| &< 0.00005 \end{aligned} \right\}. \quad (32)$$

A steady-state calculation is commenced by the word ENTER and does a flux calculation with tests given by Eq. (32). When these are satisfied the final value of k is printed out and temperature calculation begins. A restarted calculation is commenced by the word RESTART, does a flux calculation (no tests are applied in this case), and goes straight to the temperature calculation. A kinetics calculation is commenced by the word KINETICS and goes straight into the temperature calculation (starting with flux, etc., from the history tape). The number of iterations taken in the calculation of a converged temperature distribution is counted. The convergence criterion is

$$\left| \frac{T^n - T^{n-1}}{T^n} \right| < 0.0001 \quad (33)$$

for every material at every mesh point. When this is satisfied, the program proceeds to the calculation of displacements. The number of iterations taken is counted until the following convergence criterion is satisfied:

$$\left| y_r^n - y_r^{n-1} \right| < 0.001 \quad (34)$$

at every mesh point. The programme then computes a new mesh and new macroscopic cross sections allowing for changes in material densities and volume fractions. A flux calculation is commenced with these new data by means of the convergence tests (32). The number of iterations taken is counted.

The next step is to compare the new value of Λ obtained with that at the beginning of the temperature calculation. If the change in Λ is greater than 0.0001, the programme goes back to the beginning of the temperature calculation for another cycle. The next stage is to inspect the number of iterations on each of flux, temperature, and displacements taken by the program in the last cycle. The calculation finishes when each count is unity. In a steady-state calculation the program then prints k , fluxes, etc. In a kinetics calculation the program either prints or proceeds to the next time step.

An outline of the program flow is given in the following flow diagram:

LIST OF SYMBOLS USEDMain Symbols

A	Factors defining relative importance of bowing	l	Coefficient of expansion
B	Factors defining relative importance of axial expansion	m	Mass of coolant in outlet plenum chamber
C	Concentration of delayed-neutron precursors	p	Specific power (heat rating)
D	Diffusion coefficient	r	Radial distance
E	Value of action signal for scram	s	Distance along distorted channel
G	Control rod gain	t	Time
H	Heat transfer coefficient	v	Neutron velocity
K	Constant in external circuit equation	w	Relative coolant mass velocity.
M	Specific heat	x	Fraction of fuel associated with surface of fuel pin
N	Control rod indicator	y	Displacement
P	Total reactor power	z	Axial distance
Q	Value of control quantity	α	Temperature coefficient of expansion coefficient
R	Outer radius of reactor	β	Delayed-neutron fraction
S	Scram rod acceleration	γ	Composite signal
T	Temperature	δ	Dead band semiwidth for control rods
V	Volume	ϵ	Error signal
W	Total coolant mass flow	η	Action signal
Y	Maximum displacement	λ	Precursor decay constant
a	Poisson's ratio for hold-down plate	μ	Phase-advance constant
b	Effective width of fuel element	ν	Number of neutrons per fission
c	Distance between adjacent fuel elements	ξ	Spectrum of delayed neutrons
d	Weighting factor for composite signal	ρ	Density
e	Energy per reaction	τ	Delay time (for error signal)
f	Volume fraction	ϕ	Neutron flux
g	Structure temperature gradient	χ	Spectrum of prompt fission neutrons
h	Index of mass velocity	Δ	Maximum value of action signal
k	Multiplication factor	Σ	Macroscopic cross section

Subscripts (or argument)

a	As calculated (for control quantity)	k	Axial mesh point
b	Structure	ℓ	Elastic
c	Capture	m	Material
do	Static coolant	n	Isotope
d	Flowing coolant	o	Reference level
ec	Center of fuel	out	Outlet
es	Surface of fuel	r	Radial direction
e	Mean fuel	s	Canning
f	Fission	z	Axial direction
g	Neutron-energy group	C	Control
i	Delayed-neutron group	I	Scram rod region
in	Inlet	J	Control rod region
j	Radial mesh point	S	Scram

Discussion of Paper
Presented by Mr. Perks

MR. VAUGHAN (Central Electricity Generating Board): In this work to what extent do you take cognizance of the external circuit? There is always this difficulty with kinetic models: what is assumed about variation in inlet conditions? What prospect is there of linking this code to some simplified description of what's going on in the external circuit?

MR. PERKS: We do have a possibility of linking it to a description of the external circuit. This has been left open, but at the moment we only have a simple differential equation which just allows for delay of transients in traveling around the circuit and simply relates the inlet temperature to the outlet temperature.

MR. UNDERHILL (UKAEA, AERE): Could you discuss why you choose to solve the kinetic problem with a time-dependent diffusion equation? Is the time-dependent term really important or, in the kind of situation you are solving, could the solution be carried out equally well with a series of time-independent diffusion solutions?

MR. PERKS: No, I don't think it could for the range of conditions which we are trying to cover, that is, very rapid transients arising from the block changes in composition and also very slow transients from minor changes in flow rate.

MR. SEGAL (Atomic Power Development Associates, Inc.): It seems to me that you have chosen to calculate reactivity changes by the direct method. To this end you have sacrificed the spatial description to a very coarse-mesh one. Would it be possible to stick to a perturbation-theory formulation for the space-reactivity effects? This would allow the use of large numbers of groups and points, and enable one to obtain a very detailed spatial description.

MR. PERKS: The object of the program was to allow for spatial dependence with time. We do have a digital program to do what you suggest, that is, to calculate reactivity coefficients from perturbation theory by use of as fine a representation as you like, spatially, and to use up to 100 nodal points for the heat transfer representation. We hope that the two programs will be complementary. The one I have just referred to is still being developed and will be used mostly in a survey fashion, whereas FREAK would only be used for a relatively few spot checks.

MR. OKRENT (Argonne National Laboratory): Do you believe that for the types of accidents or transient conditions you would be looking at that it would be insufficient to compute the steady-state flux distribution corresponding to the actual temperature and spatial conditions at that time? In other words, do you have to carry along the derivative of the flux with respect to time?

MR. PERKS: The flux distribution can certainly be calculated at any given power level at any given time, but I think the delay times, particularly for fuel and coolant, would get you into trouble.

MR. OKRENT: These are delays in the heat transfer. I am referring only to whether or not you need a time-dependent flux calculation.

MR. PERKS: This is something we are testing with this program. It was only developed in a way to check these very points which you are bringing up.

A TIME-DEPENDENT MULTIGROUP DIFFUSION CODE WITH AUTOMATIC RESONANCE SELF-SHIELDING OF CROSS SECTIONS

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(Paper presented by A. Brickstock)

1. Introduction

The SWANTIME code was originally written to assist in the interpretation of pulsed experiments carried out with the VERA reactor at Aldermaston. These experiments are important for checking cross-section data and methods of computing Doppler coefficients. The objectives require the determination of neutron-energy spectra by time of flight, prompt-neutron lifetimes, delayed-neutron fractions, and effective reactivities.

The VERA cores used in these experiments have appreciable heterogeneity, being composed of fuel boxes filled with plates of fuel, moderator, etc., typical fuel-plate thickness being $1/8$ in. The systems can be broadly classified as "fast to intermediate."

It is essential to take into account, inter alia;

- (a) resonance absorption;
- (b) self-shielding of resonances;
- (c) the effect of heterogeneity on resonance self-shielding;
- (d) the effect of heterogeneity in heavily absorbing low-energy groups in which moderator flux peaking and fuel-plate flux-depression effects become important.

The energy region over which (c) is important is generally characterized by fairly low nonresonant cross sections, so that the "off-resonance" flux does not vary significantly across a fuel/moderator cell.

For U^{235} fuelled systems, effects (c) and (d) can be reasonably well-separated. In the energy range in which U^{235} has high nonresonant cross sections (that is, at energies below a few eV), there are no strongly absorbing resonances. This being so, the correction to resonance absorption due to "fine structure" in off-resonance flux is not important. The error in ignoring this correction should be small. However, in the case of heterogeneous Pu^{239} -fuelled systems this division is not possible since Pu^{239} has a very large resonance at about 0.3 eV, the nonresonant cross section being several hundred barns. This is sufficient to give strong fine structure for very thin plates. The methods used in the present version of the code are therefore not adequate for heterogeneous plutonium systems. It will be shown later that even when low-energy neutrons have little effect in the steady state, they can have an important effect on the time dependence following a neutron pulse.

It is well-known that the use of diffusion theory can lead to appreciable errors in steady-state calculations and cannot be expected to be very accurate for time-dependent problems. It is therefore pertinent to ask why diffusion theory should be used. The only other relevant programme in current use at Aldermaston is a Monte Carlo code. This was very expensive to run; even after 2-3 hours on the IBM-7030, it gave only limited information owing to poor statistics. Further, it did not take into account points (b) to (d) mentioned above.

Also, we had available a multigroup steady-state diffusion code SWAN,⁽¹⁾ which takes these points into account to the extent of calculating effective homogeneous cross sections in the input sections.

In view of the relative ease of programming the equations, the availability of SWAN input routines and data libraries, and the comparatively small computer time required, it seemed worthwhile to write a one-dimensional diffusion code, accepting its inherent inaccuracies.

Much of the input for SWANTIME is derived from that of SWAN.⁽¹⁾ More details of the equations solved by SWANTIME are given by Smith.⁽²⁾

Any number of compositions and regions are allowed, each composition being separately "self-shielded." The outer boundary condition is normally a logarithmic one, although zero flux is also allowed.

A full downscatter matrix is included, although in practice this can be truncated after relatively few groups in many cases.

2. Data-library Tapes: Resonant Cross Sections

Data input to the code is from one of several library tapes containing resonant and nonresonant microscopic group cross sections for most of the common isotopes. Currently available data sets include the Roach 16-group set,⁽³⁾ the GA-33 group set (an extension of the Yiftah, Okrent, Moldauer set⁽⁴⁾), and a set denoted by GAR-35 (GA-33 plus the bottom two groups of the Roach set).

Resonance self-shielding is taken into account by expressing the effective resonant group cross section of any isotope as a function of the total nonresonant cross section of the mixture in which the isotope occurs. Curves giving such a dependence have been given, for example, by Roach.⁽³⁾ Resonant cross sections are given in analytic forms by parameters derived from least-squares fits to these curves. Similar methods have been used for other data sets. These parameters are included with the resonant cross sections on tape.

3. Effect of Heterogeneity on Resonance Reactions

For a homogeneous medium consisting of a mixture of fuel (F) and moderator (M) with partial volumes V_M and V_F , the macroscopic non-resonant total cross section can be expressed in the form

$$\Sigma_T = V_F \Sigma_F + V_M \Sigma_M$$

in obvious notation.

We are interested in heterogeneous systems which can be approximated by a regular array of homogeneous fuel plates in a homogeneous moderator. In the method given by Bell,⁽⁵⁾ the moderator cross section Σ_M is replaced by an effective cross section $V_F \tau / V_M$, where

$$\tau = S_F \Sigma_M / (S_M + \Sigma_M),$$

and S_F and S_M are surface area/(4xvolume) for fuel and moderator, respectively.

If $V_M \Sigma_M$ is replaced by τV_F and use made of the relation $S_F / S_M = V_M / V_F$, this may be written in the form

$$\Sigma_M V_M / (1 + \mu \Sigma_M V_M),$$

where

$$\mu = 1 / V_F S_F.$$

The resonant cross sections may now be evaluated for total non-resonant cross sections modified in this way. Thus the effect of heterogeneity on the resonant cross sections may be approximated by means of the input parameter μ (one value for each composition).

4. "Disadvantage Factors" in Low-energy Groups

In the low-energy groups the "disadvantage factors" (mean moderator flux/mean fuel flux) are calculated by a method given by Cohen,⁽⁶⁾ which uses diffusion theory in the moderator and a consistent P_1 approximation in the fuel.

We assume a uniform source in the moderator and zero source in the fuel. The former is not unreasonable since for any group the source should be much flatter than the group flux. The disadvantage factor for any group can then be written as

$$\phi_M / \phi_F = abG + F(2a)$$

where $2a$ and $2b$ are fuel and moderator thicknesses per unit cell (in mean free paths),

$$G = (Kb \coth Kb - 1)/DK^2b^2,$$

$$F(x) = x[1 + 3E_4(x)]/[1 - 2E_3(x)],$$

and K and D are inverse diffusion length and diffusion coefficient in the moderator. All quantities are measured in terms of mean free paths in the appropriate medium. $E_3(x)$ and $E_4(x)$ are the usual exponential integrals.

K is calculated from the transport approximation, which may be written in the form

$$\ln\left(\frac{1+K}{1-K}\right) = 2KW,$$

where

$$W = \Sigma_T/\Sigma_S.$$

A subroutine XKAPPA expresses K in terms of W by means of simple analytic forms over various ranges. The fraction $F(x)$ is approximated by another subroutine, EXINT. The calculation of mean cross sections for all groups below a given group makes allowance for the flux ratios calculated in this way.

5. Solution of the Time-dependent Equations

The time-dependent multigroup diffusion equations derived from the P_1 approximations take the form

$$\frac{3D}{V^2} \frac{\partial^2 \phi}{\partial t^2} + \frac{1 + 3D\Sigma_a}{V} \frac{\partial \phi}{\partial t} = D\nabla^2 \phi - \Sigma_a \phi + \chi S + C + \frac{3D}{V} \frac{\partial}{\partial t} (\chi S + C),$$

where Σ_a denotes the total removal cross section from the group (absorption plus removal by moderation), S is the total fission source, χ the fraction of neutrons born into the group, and C the total source produced by scattering into the group.

Group subscripts have been omitted for simplicity. In the present code the second-order term has been omitted because:

(i) Its effect on the solution should have died out in a small fraction of a microsecond. This time region is not of much interest. Subsequently the term is small compared with the first order term.

(ii) It seriously complicates stability of the solution. Neglect of this term means in effect an infinite wave propagation velocity: any disturbance is seen instantaneously at all points in the medium.

(iii) It simplifies the equations from hyperbolic to parabolic form.

At the rates of change occurring in the present calculations, with the possible exception of the most subcritical case, the term containing the source derivative should not be important. Since it is difficult to include it in the present method of solution, which considers only an instantaneous pulse at time zero, this term also has been omitted.

It is uncertain precisely how much the neglect of these terms will affect the solution but we believe the effect to be small. The equations finally solved take the form

$$\frac{1 + 3D\Sigma_a}{V} \frac{\partial \phi}{\partial t} = D\nabla^2 \phi - \Sigma_a \phi + \chi S + C.$$

The method used to solve the resulting set of first-order coupled differential equations is that of Crank and Nicolson,⁽⁷⁾ with the addition of a standard source iteration technique. Space derivatives are approximated by

$$\frac{\partial \phi_m}{\partial r} = \frac{\phi_{m+1} - \phi_{m-1}}{2\delta r};$$

$$\frac{\partial^2 \phi_m}{\partial r^2} = \frac{\phi_{m+1} - 2\phi_m + \phi_{m-1}}{\delta r^2},$$

so that we can express the time derivatives in the symbolic form $\partial \phi / \partial t = F(\phi)$. We make the approximations

$$\left(\frac{\partial \phi}{\partial t} \right)_{t+\frac{1}{2}h} \sim \frac{\phi(t+h) - \phi(t)}{h} \sim 1/2 \left[F(\phi)_t + F(\phi)_{t+h} \right].$$

For any given configuration and boundary conditions it is possible to write the resulting equations for the fluxes at time-step n in the matrix form

$$\underline{A_n} \underline{\phi_n} = \underline{F_{n-1}},$$

where $\underline{F_{n-1}}$ depends only on quantities at time-step $(n-1)$ and

$$\underline{A_n} = \underline{A_0} - \frac{\gamma}{\delta t_n} \underline{I},$$

$\underline{A}_0$ being a constant matrix, γ being a constant for any group, and δt_n in general varying from step to step. $\underline{A}_n$ is a band matrix of width 3 (or "tri-diagonal" matrix) and is readily decomposed into the form

$$\underline{A}_n = \underline{L}_n \underline{U}_n,$$

where $\underline{L}_n$ and $\underline{U}_n$ have nonzero diagonal terms plus a nonzero term below or above (respectively) each diagonal term. Hence

$$\underline{L}_n \underline{U}_n \phi_n = \underline{F}_{n-1},$$

which can be solved directly for $\underline{U}_n \phi_n$, this in turn leading directly to ϕ_n .

Since the time interval in general varies from step to step, $\underline{A}_n$ also varies; thus $\underline{L}_n$ and $\underline{U}_n$ must be calculated at each time step (except when the interval is unchanged). However, this decomposition takes a small fraction of the total computing time.

The initial flux guess at each point for any time step (after the first) is made by the following extrapolation formula, corresponding to exponential extrapolation:

$$\phi_{n+2} \sim \phi_{n+1} (\phi_{n+1}/\phi_n)^x,$$

where

$$x = \delta t_{n+2}/\delta t_{n+1}.$$

This extrapolation technique effects a marked reduction in the number of iterations needed. The fluxes so calculated are used to compute the initial source guess, a standard source iteration technique then being used.

6. Neutron Pulse

Only an instantaneous pulse at time zero is allowed. However, since the problem is linear, the response to a pulse of finite duration may be obtained by superposition. A routine is provided for editing the output tape and integrating the fluxes and source over a finite pulse of arbitrary profile.

The instantaneous pulse is specified by the total number of neutrons in the pulse (PULSE) and a set of values PUXI(J) giving the fraction of these neutrons in each group J. The pulse is added uniformly over the volume bounded by any two mesh points (NWPV 1 and NWPV 2).

7. Time Intervals and Running Time

Owing to the short lifetimes in the higher energy groups, very small time intervals must be taken initially, while the high-energy pulse is decaying

rapidly. A process is provided for progressively increasing the interval subject to certain restrictions.

The time interval at successive steps is increased by a given constant ratio (FCTR) unless during the last time step either:

- (i) The fluxes changed by more than a specified ratio (RATST), or
- (ii) A given number of iterations (NSIT) was exceeded.

An efficient solution is normally obtained with an initial interval of 10^{-12} sec, FCTR ~ 1.25 , and NSIT = 6.

The criterion for convergence is that the sources at all mesh points should change by less than a given fraction (TOL) per iteration. Usually TOL = 10^{-4} .

RATST may be as high as 1.75, although the maximum number of iterations per step will normally override this test.

A provision for using Aitken's δ^2 process to speed the iterations is available, although this has not been found beneficial and is never used in practice.

We are normally interested in following the response to pulses 3 or 4 μ sec wide to times of order 50 μ sec. Such a run requires between 100 and 200 time steps. For a two-region spherical problem with 35 mesh points and 16 energy groups, the running time on the IBM-7030 is about 10-15 min.

8. Machine Storage

Variable dimensions are used throughout so that the only restriction is on total problem size. For the above example the total storage required (excluding programme) is about 14000 (decimal). The programme requires an additional 10000 stores (decimal). Modification to run on a 32-k machine would be quite easy.

9. Results

A number of runs with the 16-group Roach set have been carried out for a VERA system designated 5A. The composition of this system is given in the appendix.

Initially SWAN is used to give the core radii required for various reactivities. The desired reactivity in a SWANTIME run is then obtained by appropriate adjustment of the core radius.

In the past, agreement between measured and calculated values of α (decay constants) has been poor. Despite this there has been little attempt to investigate theoretically the time and energy dependence of neutron flux following a pulse.

It is often assumed that a few microseconds after a pulse the source decays as a pure exponential with a constant α -value given by the one-group expression $\alpha = (1 - k)/L$, where L is the prompt-neutron lifetime. Since $L = \ell_0 k$, where ℓ_0 is constant, this gives $\alpha = \rho/\ell_0$, the reactivity ρ being defined as $(1 - k)/k$. We shall show that this assumption is not tenable.

Figure 1 shows the variation, as calculated by SWAN, of "steady-state" lifetime with fuel-plate thickness. The effective delayed-neutron fraction is approximately 0.80% varying very slightly with plate thickness.

Figure 2 is typical of the decay of the total fission source following an instantaneous pulse at the core-reflector boundary, for a system 6.7% below delayed critical (7.5% below prompt critical). Curves are given for a homogeneous system and for one with 1/8-in.-thick fuel plates, the compositions being otherwise identical. Heterogeneity has a pronounced effect on the decay rate at later times.

For the first few microseconds the source in the heterogeneous run falls faster than in the homogeneous one. This is because

- (a) the effective fission cross sections in the low-energy groups are much lower in the heterogeneous case; thus we have to wait for the low-energy flux to build up much more before its contribution to the source is seen.
- (b) The low-energy steady-state source contribution is rather larger in the heterogeneous case. Thus, before the low-energy

flux has built up, the heterogeneous system is effectively slightly more subcritical than the homogeneous system.

Eventually the low-energy flux builds up and gives a larger source contribution in the heterogeneous system, and the source falls considerably more slowly.

Figure 3 shows the corresponding α -values for these runs (all values of α are in units of 10^4 sec^{-1}). It should be noted that the value

10. Comparisons with Experiment

Pulsed measurements have been made at a number of different reactivities.⁽⁸⁾ The neutron pulse was injected on the core-reflector boundary and was nominally 3 μsec wide. The actual pulse profile is shown in Fig. 5: response to this showed little difference from that for a uniform source 3 μsec wide.

The variation of flux with time was measured at the core center by a U^{235} -coated fission chamber (and other detectors). It should be noted that this does not measure the actual time variation of U^{235} fission rate in the reactor. This is because the effective cross sections of the fission chamber in the resonance and low-energy regions are much higher than the heavily-shielded effective cross sections in the reactor core. The fission chamber is thus biased to low-energy neutrons. Once the low-energy flux has built up, an appreciable fraction of the total fissions arises from low-energy neutrons, slowing down the rate at which the total count falls. This will, of course, lead to measured values of α lower than those deduced from the decay of total fission source.

Figure 6 compares the calculated time variations of U^{235} fission-chamber response and the total fission source at the core center for $k = 0.882$. These two curves differ significantly at times well after the pulse.

Figure 7 compares calculated and measured decay curves for a number of reactivities. In all cases the calculated curves are rather too steep, particularly soon after the pulse. At times in excess of 20 μsec all the curves have very nearly the correct gradient.

11. Discussion of Results

There are undoubtedly errors arising from

- (a) use of diffusion theory;
- (b) neglect of the second-order term;
- (c) approximations in treating resonance absorption;
- (d) approximations in treating heterogeneity.

However, it seems unlikely that the qualitative trends illustrated are seriously in error. This being so, the results presented indicate that in the interpretation of pulsed experiments it is important to take heterogeneity and spectral time dependence into explicit account. It is suggested that the frequently postulated attainment of a constant α a few microseconds after a pulse is not tenable; neither is a linear dependence of α on reactivity, except perhaps very shortly after an instantaneous pulse. The nonlinearity of α with ρ is due to the buildup of low-energy neutrons to a considerably greater proportion of the total flux than their steady-state contribution.

In addition to the above errors arising from theoretical inadequacies, when comparing with experiment there are further errors arising from

- (e) inadequate data;
- (f) incorrect geometry (the actual system is not spherical);
- (g) incorrect energy for the injected neutrons: the actual source energy was 14 MeV. In the calculations the neutrons were injected in the top energy group, extending from 3 to 10 MeV.

The effect of the first two is uncertain. Error (g) should have little effect, but this is easily checked in principle.

APPENDIX

Composition of VERA 5A

Isotope	Core density	Reflector density
	(atoms per 10^{-24} cm ³)	
U ²³⁵	0.006605	0.000250
U ²³⁸	0.000504	0.034400
H	0.006551	-
C	0.054610	-
Fe	0.006283	0.006464
Ni	0.000689	0.000708
Cr	0.001635	0.001682

The fuel in the core consisted of 1/8-in -thick plates of 93% enriched uranium. With a 40-cm-thick reflector, the calculated critical core radius was 18.13 cm. There were 14 mesh intervals in the core and 20 in the reflector.

Acknowledgment

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Discussion of Paper Presented by Mr. Brickstock

MR. SEMLER (National Aeronautics Space Agency): Did you get a chance to compare some of these answers directly with the Monte Carlo answers you talked of? How close were they?

MR. BRICKSTOCK: The Monte Carlo runs didn't really go sufficiently far to give any meaningful comparison. I think the furthest we took one of the Monte Carlos was about 8 μ sec after the pulse. The statistics were not good enough to get any very good comparison. They did seem to follow each other, roughly, but we couldn't get any real comparison.

MR. UNDERHILL (UKAEA, AERE): In the summary you mention an initial time step of 10^{-12} sec. Firstly, is that a practical time step, and if so, how do you explain it? It seems extraordinarily small compared with the prompt lifetimes you are dealing with. Is this just, perhaps, a function of diffusion theory used in a situation where transport theory is truly appropriate?

MR. BRICKSTOCK: I think the use of 10^{-12} sec was, perhaps, stretching things a little; the actual running time of the program is not very dependent upon the initial time step taken. The running time is not affected very much, perhaps, 5%, if 10^{-9} sec is used. We have used time steps as short as this to start up initially; it is convenient to put in a very short time step and not have to worry very much about what actual value you take.

PINETO--A FORTRAN CODE DESIGNED FOR THE SOLUTION OF NONLINEAR DIFFERENTIAL EQUATIONS IN NEUTRON DYNAMICS

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General Description

From a mathematical point of view, the dynamic behavior of a reactor can be described by a system of partial differential equations in the variables time and space (having supposed a group model for the energy variable). In fact, with the diffusion of fast computing facilities, an increasing effort is nowadays directed toward the numerical solution of systems of partial differential equations arising in particular space-dependent dynamic problems.

However, it still appears that, when rapid solutions are wanted, it is often worth-while to renounce to the spatial-time picture of the transient. In such a case, by integrating the partial differential equations with respect to space, a system of ordinary differential equations is obtained, describing the time variations of mean spatial values of the variables.

In such framework it appears that very often the system to be solved is made up of nonlinear equations having the following general form:

$$dV_i(t)/dt = r_i(t)V_i(t) + N_i(t),$$

where $r_i(t)$ and $N_i(t)$ are completely arbitrary functions depending on time directly or through any combination of the system variables t and $V_i(t)$. In fact, the differential equations describing one or multigroup, one or multiregion kinetics can be reduced to this type, and the same is true for the equations describing thermodynamic behavior of the reactor, and for other feedback equations taking into account control system, external loops, and poison.

PINETO integrates essentially up to 100 equations of the type introduced above. However, due to the fact that very often a one-group, one-region kinetic equation is used, the actual system solved by PINETO has been written in a form suitable to this kind of problem, namely, PINETO solves a system made up of the following equations:

- a) the one-group, one-region kinetic equation;
- b) up to 11 delayed-neutron equations;
- c) up to 98 equations of the general type introduced above.

When non-nuclear problems are treated, or when a one-group, one-region model is not employed, equations of type a) and b) are eliminated, and the problem to be studied is described entirely by equations of type c).

In order to achieve the maximum generality it is necessary that reactivity, appearing in an equation of type a), and the terms r_i and N_i appearing in equations of type c), may be any function of the system variables or any of their combinations. As for the way of introducing such functions, two choices are available to the user: the first, which requires knowledge of FORTRAN language, is to rewrite by means of some simple rules the subroutines by which these functions are specified. The second, requiring no knowledge of FORTRAN, is to use the standard form of PINETO, in which such functions are introduced in tabular and/or analytical form, this last being the sum of polynomials and transcendental functions (sine, cosine, log, exp), having as arguments any combination of the system variables. We would like to underline that the user of standard PINETO needs have no knowledge of programming, since the type of functions and arguments are introduced through the input data alone. Besides, in our experience the majority of the problems which can be encountered in coupling multigroup kinetic with thermodynamic theory, can be dealt with by the standard PINETO, which has proven to be a very efficient and flexible tool.

Another original feature of PINETO is the possibility of handling problems automatically in which some of the system equations change their form during transients. In fact, a great number of problems can be encountered in which during a transient there occur changes in physical status, such as fusion of fuel, boiling of coolant, and variation of type of flow. Correspondingly, the equations describing fuel temperature, coolant temperature, and flow change their form. The procedure generally followed until now was a very cumbersome one, that is, to stop the computation and to restart with a new set of equations having as initial conditions the final values of the preceding run. Note that this stop-restart procedure had to be repeated every time even one equation changed its form. In PINETO these changes may be accomplished automatically. In fact, it tests at every time step if some one of the conditions has been verified. If such is the case, the form of the corresponding equation is automatically changed, and the initial value of the new equation is set to be the last value obtained for the pertinent variable with the old equation. One has just to indicate which of the system equations can undergo a

change, what is the new form, and under what conditions the change occurs. Here again two choices are available to the user for the introduction of the change conditions. The first is to rewrite, following some simple rules, the subroutine by means of which such conditions are described; the second is to use the standard form of PINETO, in which for each equation which can undergo a change during transient, the pertinent condition is the changing of sign of any combination, also nonlinear, of the system variables. The type of combination is introduced through the input data, thus permitting the users to have no knowledge of programming. In all the cases we have considered, the standard form has shown to be sufficient.

The input of the code consists essentially of the description of the system to be solved, that is, the number of equations, initial conditions, constant terms appearing in the right-hand side of the equations, specification of the driving functions, reactivity, specification of r_i and N_i , if it is the case, of the conditions under which some of the system equations have to be changed. The output of the code consists of tables and also plots of results. The quantities to be tabulated or plotted may be chosen by the user through input data. The type of plot desired (linear or logarithmic) and the scaling may be chosen by the user or may be left under code control.

A restart option has been introduced in PINETO, in order to stop a transient whenever desired, and to start it again later on. This makes possible a better organization of the machine time required, and a solution by steps of problems that would otherwise require too much time.

PINETO, written in FORTRAN for the 7090, follows very closely the organization of the AIREK II code,⁽¹⁾ which appears very flexible since, for any logical set of operations required, a pertinent subroutine is present. The numerical method in PINETO is the one suggested by Cohen and Flatt⁽²⁾ in the case of quasi-linear differential equations, and which has proven effective in many applications. The time step can be kept constant in specified intervals or may be controlled by the code, depending on the behavior of equations of type a). In all the cases considered we have found that the integration method leads to very accurate answers, with a running time between 5 and 10 min on the IBM-7090 computer for the cases which are described below.

Applications

Three different examples are here reported in which PINETO, in its standard form, has been used, namely: the determination in three-group theory of the behavior of a fast pulsed reactor during one pulse of reactivity; the study of a startup accident in a fast reactor; the solution of differential equations of the Bessel type. The last example has been included in order to underline how PINETO can be used for problems not

connected with reactor theory and in order to point out the precision of the results in this particular case.

1. In the SORA fast pulsed reactor, the system of equations to be solved, for $0 \leq t \leq T_f$, in the study of the pulsed stationary state is the following:⁽³⁾

$$\begin{aligned}\dot{\eta}_1 &= \frac{\nu_c}{\Lambda_1} \left[(1 - \beta) - \frac{1}{\nu_c k_1(t)} \right] \eta_1 + \frac{\nu_c}{\Lambda_1} (1 - \beta) [\eta_2 + \eta_3] + \frac{\nu_c}{\Lambda_1} \beta, \quad [\dot{\eta}_1(0) = 0]; \\ \dot{\eta}_2 &= -\frac{\eta_2}{\ell_2(t)} + \frac{\Lambda_1}{\Lambda_2} \frac{\eta_1}{\ell_{12}(t)}, \quad [\dot{\eta}_2(0) = 0]; \\ \dot{\eta}_3 &= -\frac{\eta_3}{\ell_3(t)} + \frac{\Lambda_2}{\Lambda_3} \frac{\eta_2}{\ell_{23}(t)}, \quad [\dot{\eta}_3(0) = 0],\end{aligned}\tag{1}$$

where η_i are relative powers in the three-group approximation, Λ_i are generation times, β is total delayed-neutron yield, ℓ_{ij} are slowing-down times, ℓ_i are lifetimes, and k_1 is the multiplication factor for the fast group.

The variable terms of the right-hand side of the equations are expressed as follows:

$$\begin{aligned}1/k_1(t) &= x_1 + \delta x_1 f(t); \\ 1/\ell_2(t) &= \tau_2 + \delta \tau_2 f(t); \\ 1/\ell_3(t) &= \tau_3 + \delta \tau_3 f(t); \\ 1/\ell_{12}(t) &= \alpha_{12} + \delta \alpha_{12} f(t); \\ 1/\ell_{23}(t) &= \alpha_{23} + \delta \alpha_{23} f(t),\end{aligned}$$

where

$$f(t) = 1 - \frac{4}{T_f^2} \left(t - \frac{T_f}{2} \right)^2.$$

As for ν_c , it is to be considered as the eigenvalue of the problem and has the significance as the factor by which the value of ν must be multiplied in order to keep the pulsed reactor stationary. The condition which ν_c must satisfy in order that the reactor is periodically pulsed critical has the form

$$\int_0^{T_f} \sum_{g=1}^3 \eta_g(t, \nu_c) dt = B(\text{assigned value}).\tag{2}$$

For the solution of the problem described by means of PINETO, a fourth equation has been added to the system (1), that is

$$\frac{dQ}{dt} = \eta_1 + \eta_2 + \eta_3, \quad [Q(0) = 0],$$

in such a way that $Q(T_f)$ represents the integral appearing in (2). Only equations of type c) were used for the description of the problem. Many runs of PINETO have been carried on until condition (2) was fulfilled. The behavior of η_1 , η_2 , and η_3 , corresponding to stationary ν_c , is shown in Fig. 1 as directly obtained in the output plot. It is to be noted that the possibility offered by PINETO to treat the three-group model is shown to be very important, since the one-group treatment was proven to be quite insufficient to describe the kinetic behavior of a pulsed reactor like SORA.

2. An application of the possibility of handling equations that change their forms during transients is clearly shown in the case of the TAPIRO⁽⁴⁾ fast reactor.

As is well-known, the power transient in startup accidents in fast reactors depends strongly on the fuel temperature. The precision required in the results forced us to divide the core into four regions (or cells), each characterized by one temperature. The set of equations to be solved at the beginning of the transient is the following:

$$\dot{N} = \frac{\beta}{1} \left[\left\{ r_1(t) - 1 \right\} N + \sum_{J=2}^7 f_J X_J \right], \quad N(0) = 1;$$

$$\dot{X}_i = Y_i X_i + P_i N, \quad X_i(0) = 1 (i = 2, 3 \dots 7);$$

$$\dot{T}_1 = A_1 N + B_1 (T_1 - T_2), \quad T_1(0) = 0;$$

$$\dot{T}_2 = A_2 N + B_2 (T_1 - T_2) + C_2 (T_2 - T_3), \quad T_2(0) = 0;$$

$$\dot{T}_3 = A_3 N + B_3 (T_2 - T_3) + C_3 (T_3 - T_4), \quad T_3(0) = 0;$$

$$\dot{T}_4 = A_4 N + B_4 (T_3 - T_4) + C_4 (T_4 - T_R), \quad T_4(0) = 0;$$

$$\dot{T}_R = B_R (T_4 - T_R) + C_R T_R, \quad T_R(0) = 0,$$

where N is power; X_i are concentrations of delayed-neutron precursors; T_1 , T_2 , T_3 , and T_4 are temperature deviations in the four cells; and T_R is the coolant temperature. The reactivity has been supposed of the form

$$r_1(t) = K_1 t - K_2 T_4(t).$$

Fig. 1. SORA Reactor: Relative Powers, in Three-group Approximation, Near Stationarity

When during a transient the melting point is reached in one of the four cells, the corresponding temperature rise must stop until the fusion process is terminated. During fusion, a rise in reactivity is produced because the new liquid fuel fills the open channels. The reactivity rise has been supposed proportional to fusion energy (i.e., to the melted portion of the region). If we indicate by t_1 the time at which in region 1 the melting point is reached, the corresponding fusion energy is given by

$$E_1(t) = H_1 \int_{t_1}^{t_1+t} [A_1 N + B_1(T_1 - T_2)] dt,$$

where H_1 is a known proportionality constant. Similar expressions hold for the other cells.

The fusion process in a cell terminates when the corresponding fusion energy reaches the value corresponding to complete fusion. At the same time the temperature rises again and the growth in reactivity due to fusion energy stops. In order to solve the above-described problem by means of PINETO, we have added to system (3) four equations describing initial fusion energies in the cells:

$$\dot{E}_1 = 0, \quad [E_1(0) = 0];$$

$$\dot{E}_2 = 0, \quad [E_2(0) = 0];$$

$$\dot{E}_3 = 0, \quad [E_3(0) = 0];$$

$$\dot{E}_4 = 0, \quad [E_4(0) = 0].$$

Besides, we have introduced for reactivity the expression

$$r_1(t) = K_1 t - K_2 T_4 + K_3 [E_1 + E_2 + E_3 + E_4].$$

As soon as the melting point is reached in a cell, the equations describing temperature and fusion energy in that cell must change their form, and this is automatically done by the code. For instance, in cell 1 the new pair of equations is:

$$\dot{T}_1 = 0$$

and

$$\dot{E}_1 = H_1 A_1 N + H_1 B_1 (T_1 - T_2),$$

having as initial conditions the last values found for T_1 and E_1 . Equations of types a), b), and c) have been used for the solution of the above problem.

In Figs. 2 and 3 are shown plots obtained by PINETO, respectively, for total power and temperature deviations in one of the cells. For $t > 27.5$ sec, due to the very rapid increase of power level, some numerical indeterminacy has been encountered.

3. Finally, we will describe an application of PINETO in a problem not connected with reactors.

As is well-known, the differential equations describing the behavior of the Bessel functions $y_1 = J_0(x)$ and $y_2 = J_1(x)$ are, respectively

$$x^2 \frac{d^2 y_1}{dx^2} + x \frac{dy_1}{dx} + x^2 y_1 = 0, \quad [y_1(0) = 1; \dot{y}_1(0) = 0];$$

$$x^2 \frac{d^2 y_2}{dx^2} + x \frac{dy_2}{dx} + (x^2 - 1) y_2 = 0, \quad [y_2(0) = 0; \dot{y}_2(0) = 1/2].$$

The above system becomes first order with the usual transformations:

$$\dot{z}_1 = -\frac{z_1}{x} - y_1, \quad [z_1(0) = 0];$$

$$\dot{y}_1 = z_1, \quad [y_1(0) = 1];$$

$$\dot{z}_2 = -\frac{z_2}{x} - y_2 \frac{x^2 - 1}{x^2}, \quad [z_2(0) = 1/2];$$

$$\dot{y}_2 = z_2, \quad [y_2(0) = 0]. \quad (4)$$

Near the origin ($x=0$), equations describing z_1 and z_2 show a criticality, due to the presence of terms in $1/x$ and $1/x^2$. In order to avoid such criticality, we have substituted near the origin, in the first and third equations, terms derived by application of the L'Hopital theorem to the terms z_1/x , z_2/x , y_2/x^2 , that is, by substituting $\dot{z}_1$, $\dot{z}_2$, and $\frac{1}{2} \dot{z}_2$. The system to be solved near the origin then becomes

$$\dot{z}_1 = -\frac{y_1}{2}, \quad [z_1(0) = 0];$$

$$\dot{y}_1 = z_1, \quad [y_1(0) = 1];$$

$$\dot{z}_2 = -\frac{2}{3} y_2, \quad [z_2(0) = 1/2];$$

$$\dot{y}_2 = z_2, \quad [y_2(0) = 0]. \quad (5)$$

X=TIME Y(X,1)=ACTV (1)
 NORMAL SCALE IN ABSCISSA
 LOG SCALE IN ORDINATE
 INFORMATION ON ORIGINATE SCALE - LEFT SCALING POINT = 10.000E 00-FACTOR BETWEEN SCALING POINTS= 10.000E 00

Fig. 2. TAPIRO Reactor: Relative Power

Fig. 3. TAPIRO Reactor: Temperature Deviation ($^{\circ}\text{C}$) from Initial Value in Cell 1

PINETO solves system (5) at the beginning of calculation. Then, as soon as the condition $t > t_0$ (assigned) is fulfilled, PINETO automatically solves system (4), using as initial conditions the last values found for the corresponding variables. Equations for type c) have been used.

Figure 4 shows the output of PINETO for $J_0(x)$ and $J_1(x)$, for $0 \leq x \leq 8$. A quite satisfactory agreement with the known tabulated values of J_0 and J_1 has been obtained.

Fig. 4. Bessel Functions J_0 , J_1

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SESSION V

SPECIAL METHODS

Wednesday, May 19, 1965

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Argonne National Laboratory**

**CO-CHAIRMAN: V. Benzi
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COMPUTATIONAL PROBLEMS OF REACTOR SAFETY*

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Introduction

I am probably the last person who should give this talk, as I have never designed a computer code in my life. My work is directed toward a qualitative, or maybe semiquantitative, understanding of the complicated and interlocking phenomena affecting reactor safety. Pencil-and-paper mathematics is all that can usefully be applied to this end of the business; and if a problem ever gets to the stage where more sophisticated methods pay off, the work is transferred to mathematical experts. You may, however, enjoy hearing a broad survey of the problems of reactor safety in order to see where modern computational techniques can usefully be employed. I will try to present such a survey.

Nuclear-reactor hazards stem mainly from the possibility of dispersing fission fragments. The other hazards--such as that resulting from flying objects--are relatively minor compared to the fission-fragment hazard, or compared to similar hazards in non-nuclear plants. The largest reactor explosion actually attained so far was a deliberate destructive test of a space-propulsion reactor, and it yielded the equivalent of 100 lb of TNT, rather a small amount compared with the yield of some chemical accidents.

In almost all reactors the fissions occur in solid fuel elements, and the fission fragments are therefore normally trapped inside the solid matrix of these elements, or at least inside the cladding of the fuel. To release the fission fragments, some sort of overheating is required resulting in a phase change in the solid fuel, or in its melting, or vaporization, or in damage to the cladding. Overheating occurs when the ratio of heat production to cooling becomes unduly large. I would like to discuss, first, the case in which this results from excessive heating during a power excursion of the reactor.

Reactor Dynamics--Doppler Effect

A power excursion occurs when the population n of each neutron generation exceeds the population of the preceding generation by a fraction, called the excess reactivity k_{ex} . If τ is the lifetime of one generation,

$$\frac{dn}{dt} = (k_{ex}/\tau) n, \quad (1)$$

*Research sponsored by the United States Atomic Energy Commission under contract with the Union Carbide Corporation.

and the neutron population and reactor power increases exponentially as long as k_{ex} and τ remain constant. Actually, things are very much more complicated. In the first place, a few tenths of a percent of the neutrons are "delayed," that is, they have lifetimes that are orders of magnitude greater than the majority of the neutrons. Equation (1) then is modified, inasmuch as we have to subtract from k_{ex} a fraction corresponding to the neutrons which are delayed; however, on the right side of Eq. (1), new terms are added, corresponding to the delayed neutrons as they are formed. These terms are obtained from a set of first-order differential equations. Equation (1) and these differential equations form a system which is frequently solved by analog computers, sometimes simply involving electrical networks.

Much more fundamental modifications of Eq. (1) are caused by feedback, that is, the fact that the excess reactivity is influenced by the neutron population n . A relatively simple example of this is produced by the Doppler effect. For reasons known to many of you, the reactivity changes if the fuel temperature varies. In practical reactors the reactivity usually goes down as the fuel gets hotter, that is, we have a negative feedback. Now the temperature depends on the energy density deposited by the nuclear heating, and the energy density is the time integral of the power density, which, in turn, is essentially proportional to the neutron population n . Thus, if k_0 is the originally inserted excess reactivity,

$$k_{ex} = k_0 - \text{function of } \int^t dt' n(t'). \quad (2)$$

If we have indeed a negative feedback, this function is positive, and after a while k_{ex} goes to zero and n reaches a maximum. After this, k_{ex} becomes more and more negative and n decreases asymptotically to zero.

In case the above function is linear, an analytical solution in terms of hyperbolic functions is easily obtained, at least if Eq. (1) can be used and the delayed neutrons do not have to be considered. The latter is frequently acceptable because the excursion can be over before any appreciable amount of delayed neutrons appear. Note, that the feedback makes Eq. (1) non-linear, even if the function in Eq. (2) is linear, because n is multiplied by its own time integral.

In practice, however, the function in Eq. (2) is not linear. In the first place, the reactivity decrease per degree decreases with increasing temperature. Secondly, the heat capacity increases usually with increasing temperature so that at higher temperature less degrees are obtained for a given increase in energy density. The two nonlinearities thus aggravate each other. Furthermore, if the temperature increases are such as to constitute a safety problem, they must involve some sort of a phase change, as mentioned above; and then a violent nonlinearity is introduced by the latent heat of the phase change, which prevents a temperature increase

for a finite increase in energy density. Digital methods are used overwhelmingly in the nonlinear case though I am not absolutely sure that this is necessary.

The Doppler effect is usually regarded as "instantaneous," that is, the reactivity is usually assumed to follow the temperature or energy density without time delay. However, in some important cases even this simplification is not quite correct.⁽²⁾ For various reasons, the fissionable material, such as plutonium, is sometimes concentrated in small grains, embedded in fertile material, such as ^{238}U . The decrease in reactivity with increasing temperature comes from the fertile material. The Doppler effect of the fissionable material is small and probably goes in the other direction. In a transient, the grains of fissionable material heat up first, giving a small and probably positive reactivity change. Only after a time delay will the fertile material heat up and give the strong negative Doppler effect. This time delay is described by the heat-conduction equation, a partial differential equation of second order in the space coordinates and of first order in time. As a practical matter, the delay allows the reactor power to increase longer than would otherwise be the case, and consequently the transient becomes more violent.

It has recently been pointed out, however, that the above computational model might be misleading. If the small grains of fissionable material are to absorb, initially, almost all the energy generated, they must get very hot indeed. They will soon vaporize, and fissionable material will condense in small cracks in the fertile material, which never has exactly the maximum theoretical density. From then on, the heat transfer will be very rapid and the negative Doppler effect will terminate the transient sooner than the previous model indicated. I just mentioned this somewhat detailed argument in order to emphasize the difficulty of arriving at a suitable model, a difficulty which is superimposed on your problem of computationally describing a given model.

Other Reactivity Effects

The Doppler effect is of course not the only reactivity effect to be considered. Some reactivity change will result from the thermal expansion of the heated fuel. As long as it is a question of a metallic fuel rod that expands longitudinally as a function of its temperature, the problem is fairly straightforward, complicated only moderately by the temperature dependence of the expansion coefficient. Sometimes it is even possible to neglect the time delay connected with this expansion, since it is small compared to the time constant of some transients. However, if it is a question of a fuel rod that is constrained at the ends or elsewhere, that is "fluffed up" by the effect of many fissions, or that has many voids or cracks, the matter is usually not accessible to analytical solution. Other thermal-mechanical effects will be discussed later.

Reactivity effects are also caused by changes in coolant density, which may result from the transfer of heat from the fuel into the coolant. Here it is a question of coupling the reactor-dynamics equations with the heat-transfer equations, which involve the heat-conduction equation in several regions, coupled by boundary conditions. The great difficulty stems here from the nonlinearity, and above all, from the threshold effects such as boiling. In water-cooled reactors, the phenomena governing the heat transfer are quite different in the subcooled region and in the region where boiling is taking place. The difference also applies to the effect one unit of heat has on reactivity: if the unit is used to generate steam, it changes the reactivity much more than if it heats subcooled water.

Further reactivity effects are caused by the heating of the moderator, which again is connected to heat generation in the fuel by heat-transfer equations, involving sometimes variable contact resistances at the boundaries between regions. The moderator heating acts through a change in the low-energy spectrum of the neutrons, which interacts with the energy dependence of the cross sections in a manner that is hard to describe by analytical functions and, hence, particularly suitable for computational solutions. Furthermore, some of the nuclides with important cross-section variations in the low-energy region vary in concentration throughout the life of the reactor. For instance, ^{135}Xe , the fissionable nuclides, and some fission fragments belong in this category. For this reason, very many calculations are required, again calling for computational methods.

Advanced Topics of Reactor Dynamics

In Eq. (2) I have tacitly assumed that the reactivity is inserted as one step at low, but not extremely low, power. This assumption is frequently made because it is simple and gives pessimistic results, something required in most safety analyses. If the reactivity is inserted more gradually, the negative reactivity effects mentioned above keep up with the reactivity insertion and the reactor never gets very supercritical. Also, slower but larger reactivity effects get a chance to act. Thus, consideration of the time dependence of the reactivity addition results frequently in reduced severity of the computed transient. However, even where analytical solutions are available for the instantaneous reactivity addition, computational methods might be required for the time-dependent case of reactivity insertion. Furthermore, the postulated reactivity additions, such as rod withdrawal at maximum speed, are fairly well standardized, resulting in a large number of calculations of the same kind, which favors machine calculations.

Equation (1) breaks down if the startup occurs at extremely low power or source strength. In that case, the reactor power may fail to rise, even if the reactor is supercritical, simply because there is no neutron present to get the reaction started, or because a chain reaction, which did start, breaks off in accordance with the law of statistics. Thus

even a gradual reactivity addition may result in considerable excess reactivity and, hence, a large excursion, because there is no immediate power increase and no immediate negative reactivity effect. Codes have been written for this low-source startup.⁽³⁾

The capability of even the largest computing machines is challenged when the space dependence of the reactor excursions is taken into account. In the case of large reactors that is necessary. The point is: the power density is not the same everywhere in the reactor. Hence, the feedback effects will vary from point to point, and the reactivity distribution will change. This, in turn, distorts the power distribution. Considering that the computations usually require multigroup calculations, and that the space dependence might have to be worked out in several regions and in two or three dimensions, it is clear that one cannot be very generous with the number of groups, the number of space points, and the length of the time intervals. A procedure usually adopted is the following: First, the space-dependent problem is solved for one moment in time. This gives a power distribution, and an asymptotic reactor period. Next, for a certain time interval, the power, distributed in space as just computed, is allowed to increase exponentially with the above period. The energy density deposited during the time interval causes a space-dependent change in the local reactivity. The new reactivity distribution is used in a new space-dependent computation to obtain a power distribution and reactor period, and so on.

Quite apart from the difficulties with excessive coarseness of the space and time grid, and the possibility of computational instabilities, it is difficult to prove that the above method approximates the correct solution. In reality, of course, the power does not increase with the same period all over the reactor, something that is a basic assumption in the above method.

In some simplified cases, I have been able to obtain analytical solutions to the space-dependent problem with feedback. The solutions are based on the Weierstrass P-function, and they may be used to check the validity of some of the above computational methods. If the analytical method is applied to the multiregion case, it becomes a cumbersome system of coupled equations, involving P-functions, just as the no-feedback case becomes a system of coupled equations involving sine, cosine, and exponential functions. The system with the P-functions could presumably be coded, and that might be considerably simpler than the coding of the problem based on a grid of discrete space and time points.

Hydraulics

Overheating of the fuel elements and the resulting fission fragment release may also result from too low a coolant flow, or loss of the coolant altogether. In fact the assumed "maximum credible accident" usually

involves a break of one of the main coolant pipes, followed by the loss of the coolant through the resulting openings. Sometimes it is assumed that a coolant pump loses power, and the flow then coasts down, ultimately leaving insufficient flow for heat removal. The events immediately after the onset of the disturbance are the most important because the heat generation is largest at that time: The nuclear chain reaction has not yet quite decayed, and the afterheat from fission fragments is greatest. Basically, the problem of fluid flow involves nothing but the conservation of mass, momentum, and energy. However, the complicated nature of the problem may be understood when it is remembered that the mass flow distributes itself over several channels in series or in parallel; that the momentum equation involves friction factors in complicated channel shapes; and that the energy equations involve the pumps and frequently also gravity (such as in the case of natural convection). The matter is particularly involved when boiling is present. Here, large density changes, large accelerations, and two-phase flow enter in. Coupling with the heat-transfer equations influences the hydrodynamics, and more importantly, the flow pattern influences the heat transfer. For transient phenomena of the order of milliseconds, the interaction between heat transfer, boiling, and flow is not well understood. The situation is bad for water, and worse for other coolants. It is frequently not a question of solving the equations applicable to a specific model, but rather of finding a reasonable model.

Thermal-Mechanical Effects

I mentioned already that thermal-mechanical effects, such as fuel-element expansion or bowing, influence reactivity. They also influence fluid flow to some extent and are of particular interest with respect to possible interference with control-rod motion, etc. The interaction of time-dependent heat generation, heat transfer, and mechanics prevents solution in all cases except the simplest ones. The time-dependent equation describing the bowing of a single rod is a partial differential equation of the second order in time and the fourth order in space. Constraints in the mechanical motion, and possible creep, further complicate matters.

For really large excursions, and those are the most important ones for safety purposes, the pressure waves caused by thermal expansion or vaporization of the fuel are to be computed. The results of these pressure waves are fuel-element destruction, elastic or plastic deformation of the pressure vessel, water-hammer effects, and so on. Frequently, the fuel-element destruction and disassembly of the core are the shut-down mechanisms which ultimately terminate the nuclear excursion. The interaction between the nuclear equations and the mechanical equations is the subject of the famous AX-1 code for very large destructive transients. This code has been subject to many refinements, to take into account the Doppler effect, and two-dimensional geometry. The latter is of importance, for instance, in the case of a reactor of a shape approximating a flat cylinder.

Fission-fragment Transport

Once the above effects are assumed to conspire to release fission fragments from the reactor, or even from the fuel elements, rather simple assumptions have been made in the past as to the further fate of the fission fragments. For instance, it was postulated that 100% of the rare gases and 25% of the iodine leak out to the atmosphere. Under this assumption, the iodine is by far the dominant hazard. Practically that is unrealistic because the iodine will, to a large extent, be retained in the coolant, plate out on the containment walls, or be trapped in purposely supplied filters. Mathematical models are used to describe these effects. However, here again, we are only just on the verge of being able to understand the phenomena which have to be considered in these models. For instance, it is quite important to know what chemical form the iodine is in, and whether it is adsorbed on particulate matter or not. There is thus not much point in discussing these models in detail.

Water sprays may be used to reduce the pressure inside the containment and this leads, in a computable manner, to a reduction and final termination of any release from the containment. On the other hand, some of the postulated accidents responsible for the fission-fragment release from the fuel do not affect all the fuel simultaneously. The fuel elements in the highest flux release the fragments first; the other elements do so successively later. This, convoluted with the time function describing the release from the containment, gives an overall release more complicated, but more favorable, than the above-mentioned release fractions.

Meteorology

The leakage from the containment then represents a source term for atmospheric dispersion. Previously this dispersion had been assumed to take place according to the Sutton diffusion equation, an equation quite similar to the diffusion equation describing the neutron flux, and also to the heat-conduction equation. The meteorological equation has some wrinkles of its own, however; for instance, it is anisotropic. This relatively simple treatment neglects a few factors that reduce the computed radiation dose to an individual affected. Wind variability is one of them: it has been customary to assume that the wind has a constant direction after the incident and hence exposes a certain unfortunate group of individuals for the duration of the release. Actually, the wind rarely behaves like this, but sweeps back and forth over a larger arc. Sometimes the wind variability is neglected because of concern over the rare cases in which it does not apply, but frequently it is disregarded because of mathematical complexities which it entails. In these latter cases the convenience of computing machines may make it practical to take credit for the wind variability and similar mitigating factors.

Another example is the whole-body radiation exposure resulting from a cloud of rare gases. A simple method of computing this exposure is based on the assumption that the cloud is infinite in extent. This is far from true close to the source, and a more sophisticated calculation facilitated by computing machines⁽⁴⁾ gives more favorable, and still correct results.

To compute from given concentrations of the various fission fragments the doses to the whole body and to various organs, and to find ground and crop contamination, and other economic losses requires in any given case the performance of a large number of fairly elementary operations, something for which computers are well suited.

Concluding Remarks

I would like to mention an example of a somewhat peripheral use of computers in nuclear safety: The Nuclear Safety Information Center uses data-processing machines for the storage and retrieval of information.

In conclusion, I must apologize again for having given a talk at this meeting without understanding much about computers myself. What I tried to do was to give a survey of the problems that occur in nuclear safety, and that are suitable--to a varying degree--for solution by computational methods. This might help in establishing a background for the excellent safety-connected papers of this session. I am particularly referring to the papers by Galligani, by Blaine and Berland, by Perks, by Brickstock, Davies and Smith, by Tamagnini, and by Russell. The emphasis on reactor physics was intentional and based on the relatively advanced state of the discipline. Much of the information I presented can be found in the SIFTOR⁽¹⁾ book. I have tried to include a few examples of work done since these books were written.

Thank you.

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Discussion of Paper
Presented by Mr. Ergen

MR. VONDY (Oak Ridge National Laboratory): We make many calculations involving the time dependence of the neutron density. Would you comment on the importance of the energy spectrum of this density and its time dependence in such calculations?

MR. ERGEN: It depends on what you are trying to do. The neutron energy enters almost exclusively through the variation in the cross sections. When materials vary in cross section considerably, a given number of neutrons has a different effect if the energies differ. In this sense it does have, conceivably, a large effect. I don't have any actual numerical values to prove this, but I am quite sure that if the moderator temperature varies appreciably through the reactor, the neutron temperature also will vary. This will also give you the xenon effect to various extents in various places of the reactor.

MR. KOPP (USAEC, Division of Safety and Standards): Are there any consistent computational methods presently available for calculating any additional energy releases due to chemical reactions, such as the metal-water reaction; or are these based on experimental extrapolation?

MR. ERGEN: In pressurized-water reactors and boiling-water reactors the stored energy in the coolant is the dominant energy source and the metal-water reaction, in itself, does not add very much to the stored energy. Unless the metal-water reaction is violent, and recent indications are that it is not, then the metal-water reaction in these water reactors is not a very important effect. For the SL-1 accident and for the SPERT aluminum-plate-type-core destructive tests the total energy furnished by the metal-water reaction was of the order of 10-20%. That, probably, was added at a relatively slow rate, so the metal-water reaction is not a very important effect.

MR. OKRENT (Argonne National Laboratory): Sometimes hydrogen generation is important, even if the rate of hydrogen generation is low, if the hydrogen can possibly collect and then explode.

MR. ERGEN: Yes. In one Canadian accident there is evidence that this was an aggravating factor. This is a very important point; however, I doubt that this is subject to very easy computation.

MR. OKRENT: There is a considerable difference in the amount of hydrogen depending on whether you have a few percent of the cladding reacting, or most of it, and, in this sense, there are some problems.

Can you specify the class of reactors, and the kinds of transients, for which the spatial dependence of the rate of power change would lead to significant errors in a numerical calculation using a time-independent power distribution at each point in time, that is, in which use is made of a steady-state neutron distribution rather than of the time-dependent term.

MR. ERGEN: In the case of relatively mild excursions, excursions that may reach the vaporization of the fuel, and in reactors in which the physical dimensions are large in relation to the migration lengths, this effect might enter. In reactors that are physically small as compared to the migration length, obviously the power is fairly closely coupled and it will not change in shape very much. From work which was carried out in cooperation with General Electric we found that the peak temperature that might be reached in a large reactor is about 35% less if the calculation is made with the Weierstrass P-function than with the point model. This is subject to some doubt, because you really don't know what is assumed for average values in the point model; but in a reasonable comparison, the peak energy density comes out something of the order of 35%. If you integrate over the reactor, this is not necessarily true. The total power generation integrated over the reactor may actually be greater than what is computed from the point model. There will be a paper at the next Nuclear Society meeting in Gatlinburg on that subject. In other words, the reactor has to be large, and that's usually a water-moderated reactor because migration lengths are small and the size of the effect is something like 35% in energy density.

MR. ALWANG (Pratt & Whitney, CANEL): You say that the space dependence is not significant except in a large reactor. Would it be significant in a small reactor with a moderating reflector -- a small, fast reactor with a moderating reflector? Would you expect the AX-1 code to be valid in that case? This would be where the neutrons coming from the reflector are influenced by the moderating time in the reflector.

MR. ERGEN: You can have several generations in the core before you get the reflector neutrons back and these neutrons then act, to some extent, as delayed neutrons. This is still amenable to a point model with something equivalent to delayed neutrons. It is not quite clear that this is a question of space dependence. I think that if the whole assembly is really small compared to the migration area, which might be a little difficult to define, you could get by with a point model.

MR. ALWANG: By treating the reflected neutrons as an extra delay group?

MR. ERGEN: Yes.

MR. FISCHER (Argonne National Laboratory): Sushil Kapil and I have done slightly related calculations in connection with the Argonne concept of the coupled fast-thermal reactor, and we got some very interesting results. We could see that we were changing the prompt-neutron lifetime of the system as an accident was initiating. As disassembly began, the thermal part of the reactor, which corresponds in some degree to a reflector system, began taking a larger fraction of the total reactivity. We could see a strong influence of the magnitude of the pressure and the rate of disassembly with each time step, because the power fraction was changing and the lifetime was changing in the system.

MR. OKRENT: I would think there is a chance for an error in this calculation depending on how long it takes for neutrons to get out into the reflector, to be moderated, and to come back, compared to the time rate of change of power. I would think it depends on the amount of excess reactivity, as well.

MR. ERGEN: In the case of disassembly of a fast reactor, you, of course, get very violent changes in the constitution of the core, which is something different from what I have considered.

MR. OKRENT: In principle, you could make the observation that if you get enough excess reactivity into the fast core of the coupled reactor, or the reflected reactor described previously, you obviously have a change in the situation because it will run away with the transient, independent of what the reflector is doing; there has to be an effect. When it enters, it is subject to more analysis than we have done, apparently.

A FAMILY OF FORTRAN ROUTINES FOR THE ANALYSIS OF NEUTRON RESONANCE EFFECTS*

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INTRODUCTION

In problems connected with the evaluation of neutron resonance effects, such as resonance escape probability in homogeneous and heterogeneous media, and correlated quantities, such as reaction rates, group cross sections, fluxes, and slowing-down densities, two concurrent aspects have to be considered, which, however, are based on independent physical approaches. One is the mathematical form chosen for the actual evaluation of such quantities, the other is the choice of a physically plausible model to describe the resonance cross sections. This, in turn, has consequences on the mathematical mechanism chosen to evaluate integral properties. A family of self-consistent FORTRAN Routines for the analysis of neutron resonance effects is presented.

I. CROSS SECTIONS

A. Basic Equations

In the calculations of resonance escape probability and of reaction rates existing in the literature, the Breit-Wigner single-level formula has been used indiscriminately for resonance absorbers and fissionable elements. Many sophisticated calculations have been developed in which the resonance structure of the elements in question has been described by superpositions of single Breit-Wigner levels, complemented by a $1/v$ background. Although this method gives an adequate description of the level structure of resonance absorbers, it breaks down for fissile elements. It has been shown by several authors^(1,2) that for fissionable elements a more satisfactory description of the cross sections is attained by using the multilevel-multichannel formalism of Wigner and Eisenbud.⁽³⁾ "Multilevel" resonance parameters have been obtained by introducing simplifying assumptions, either in reducing the number of interfering channels, or in limiting the number of levels. Though physically meaningful, the multilevel parameters existing in the literature^(4,5) have a limited range of practical validity. The evaluation of the energy-temperature-dependent cross sections requires a complicated and lengthy numerical mechanism, so that their use, for practical reactor calculations, becomes cumbersome.

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With a method which has been derived elsewhere,⁽⁶⁾ the multilevel cross-section formulae can be expressed in a simplified form, which is suitable for practical reactor calculations, leaving, however, full generality to the physical content of the theory. Such formulae and related equations are used in the FORTRAN Subroutines BWSIG 1 and BWSIG 2, written for the evaluation of resonance cross sections. The equations relevant to these subroutines are given below.

The method hinges on the definition of characteristic cross-section parameters, in terms of which the cross sections are expressed as superpositions of interfering Breit-Wigner-type terms. Such an expansion has the advantage that the evaluation of temperature effects can be carried on by using existing Doppler-broadening techniques.

The outstanding difference with the single-level formula is the presence of interfering terms, corresponding to the asymmetrical line-shape function χ in all types of cross sections. The expansion obtained is theoretically defined as a summation over all the levels belonging to the same J angular momentum state. These being unlimited in number, it becomes necessary for practical calculations to break the expansion and limit it to a finite number of terms, related to the energy interval of interest. It has proved useful to take into account not only the terms of those levels which are located inside the energy range in question, but also terms arising from neighboring levels, that is, levels relatively close, although external, to the energy interval considered. Distant levels or unresolved resonance terms are, instead, approximated by suitable expansions in terms of positive and negative powers of the momentum. The equation obtained for the total cross section is of the form

$$\sqrt{E} \sigma_{nT}(E) = C \left\{ \frac{2(1 - \cos \omega)}{\sqrt{E}} + \sum_{K=1}^N \left[(GR_K^T \cos \omega + GI_K^T \sin \omega) \psi_K(E) + (GI_K^T \cos \omega - GR_K^T \sin \omega) \chi_K(E) \right] \right. \\ \left. + A_1^T + \frac{A_2^T}{E} + \frac{A_3^T}{E^2} + B_1^T E + B_2^T E^2 + B_3^T E^3 + \dots \right\}, \quad (I-1)$$

where N is the number of levels involved in the region of interest, $\psi_K(E)$ and $\chi_K(E)$ are the conventional line-shape functions evaluated at the K-th level for a given medium temperature, and ω is the hard-sphere phase shift describing the potential scattering. Equation (I-1) is also used to evaluate reaction cross sections such as fission and capture by simply setting $\omega = 0$. The corresponding expression for the scattering cross section is given by

$$\sqrt{E} \sigma_{nn}(E) = C \left\{ \frac{2(1 - \cos 2\omega)}{\sqrt{E}} + \sum_{K=1}^N \left[(GR_K^T (\cos \omega - 1) + GI_K^T \sin \omega) \psi_K(E) + (GI_K^T (\cos \omega - 1) - GR_K^T \sin \omega) \chi_K(E) \right] \right. \\ \left. + \sum_{K=1}^N \left[GR_K^R \psi_K(E) + GI_K^R \chi_K(E) \right] + A_1^R + \frac{A_2^R}{E} + \dots + B_1^R E + \dots \right\}, \quad (I-2)$$

where the parameters GR_K^n , GI_K^n are related to the GR_K^T , GI_K^T parameters of σ_{nT} by a dispersion relation and can be obtained from them directly.

B. Theoretical Background

Basically, these equations are derived from the multilevel-multichannel formalism by diagonalization of the Wigner level matrix.⁽⁷⁾ Complex eigenvalues, $C_K = \mu_K - i\nu_K$, are obtained, which define level energy μ_K and half-width ν_K . Complex partial widths $\tilde{\Gamma}_{Kc}$ are derived from the Wigner-Eisenbud partial widths $\Gamma_{\lambda c}$:

$$(\tilde{\Gamma}_{Kc})^{1/2} = \sum_{\lambda} S_{\lambda K} \sqrt{\Gamma_{\lambda c}}; \quad (I-3)$$

here $S_{\lambda K}$ is the element of the orthogonal complex transformation S diagonalizing the level matrix, and $\Gamma_{\lambda c}$ is the (real) partial width describing the decay of the λ -th level into the channel c . In particular, one defines for each level K a reduced neutron width

$$\tilde{\Gamma}_{Kn}^0 \equiv \alpha_K^0 + i\beta_K^0 = \sum_{\lambda \lambda'} S_{\lambda K} S_{\lambda' K} \sqrt{\Gamma_{Kn}^0 \Gamma_{K'n}^0}, \quad (I-4)$$

from which the corresponding characteristic parameters for the total cross section are obtainable:

$$GR_K^T = \alpha_K^0 / \nu_K; \quad GI_K^T = \beta_K^0 / \nu_K. \quad (I-4')$$

For reaction cross sections it is useful to define intermediate matrices connecting a given channel c to the interfering levels K and K' :

$$N_{KK'}^{(c)} = (\tilde{\Gamma}_{Kn} \tilde{\Gamma}_{K'n}^* \tilde{\Gamma}_{Kc} \tilde{\Gamma}_{K'c}^*)^{1/2}; \quad (I-5)$$

$$\frac{2g}{\sqrt{E}} N_{KK'}^{(c)} \equiv \phi_{KK'}^{(c)} + i\sigma_{KK'}^{(c)}. \quad (I-5')$$

Similar matrices related to the generic reaction (x) are defined as

$$\phi_{KK'}^{(x)} + i\sigma_{KK'}^{(x)} = (\tilde{\Gamma}_{Kn}^0 \tilde{\Gamma}_{K'n}^{0*})^{1/2} \sum_{c(x)} (\tilde{\Gamma}_{Kc} \tilde{\Gamma}_{K'c}^*)^{1/2}, \quad (I-6)$$

where $c(x)$ are all those channels which contribute to the (x) reaction. From (I-6) one derives, finally, the characteristic parameters for the (x) reaction:

$$GR_K^{(x)} = \frac{1}{\nu_K} \sum_{K'=1}^N \frac{(\nu_K + \nu_{K'}) \phi_{KK'}^{(x)} + (\mu_K - \mu_{K'}) \sigma_{KK'}^{(x)}}{|\rho_{KK'}|^2}; \quad (I-7)$$

$$GI_K^{(x)} = \frac{1}{\nu_K} \sum_{K'=1}^N \frac{(\nu_K + \nu_{K'}) \sigma_{KK'}^{(x)} - (\mu_K - \mu_{K'}) \phi_{KK'}^{(x)}}{|\rho_{KK'}|^2}; \quad (I-8)$$

$$\text{where } |\rho_{KK'}|^2 = |C_K^* - C_{K'}|^2,$$

and N represents the totality of the levels taken into account. In Eqs. (I-7) and (I-8), (x) can refer to fission (F), capture (γ), as well as scattering (n).

The corresponding single-level parameters, needed to calculate cross sections with the same Eqs. (I-1) and (I-2), are deducible from (I-4), (I-7), and (I-8) under the conditions $S\lambda_K = \delta_{\lambda K}$ (i.e., diagonal level matrix) combined with the assumption that

$$\sum_{c(x)} \sqrt{\Gamma_{Kc} \Gamma_{K'c}} = \delta_{KK'} \Gamma_{K(x)}, \quad (I-6')$$

leading to the obvious consequence that $GI^{(x)} = 0$. Useful relations between the characteristic parameters appearing in (I-1) and (I-2) (consistent with the unitarity of the collision matrix):

$$\begin{aligned} GR^T &= GR^{(n)} + GR^{(\lambda)} + GR^{(F)}; \\ GI^T &= GI^{(n)} + GI^{(\lambda)} + GR^{(F)}, \end{aligned} \quad (I-9)$$

permit the derivation of the parameters of one of the four cross sections (usually σ_γ) when three of them are known. In effect, σ_F and σ_T are sufficient for the purpose, because the parameters GR^n and GI^n are derivable from those of σ_{nT} .

C. Computational Methods

There exist two possible sources of information from which the characteristic parameters useful for Eqs. (I-1) and (I-2) are obtainable:

(1) Existing compilations of multilevel-multichannel resonance parameters:

These parameters provide essentially the reciprocal of the Wigner level matrix. The computational complications connected with its inversion, at each energy point, and with the cross-section evaluation can be overcome with the diagonalization method outlined in this paper, provided

one has a suitable method to calculate the transformation S . For this purpose, a perturbation procedure⁽⁸⁾ has been formulated so as to obtain with relatively short computing time the elements of the complex orthogonal matrix S as a function of the multilevel-multichannel resonance parameters. With the same perturbation procedure, the eigenvalues C_K are calculated and, finally, the characteristic parameters given by Eqs. (I-4'), (I-7), and (I-8) are derived. This type of calculation is performed in the first part of the subroutine BWSIG 1. A separate branch of this subroutine provides also single-level parameters in a form suitable for use in Eqs. (I-1) and (I-2).

(2) Experimental cross-section data:

Wherever fission and total cross-section data are available, a least-squares-fit analysis of the data using Eq. (I-1) as a trial function provides characteristic resonance parameters for either cross section. The least-squares analysis (PROGRAM CODILLI) is carried on by guessing initially the values for μ and ν for each level.

The routine fits in this case the linear parameters GR and GI. Improvements can be obtained in two different manners: either by successive linear fits, using improved guesses for μ and ν , as obtainable by comparison between calculated and experimental curves; or in continuation with the initial linear fit, by fitting together with GR and GI the nonlinear parameters μ and ν . In this case the program uses the well-known Gauss method of linearization of nonlinear equations. With a linear fit one can handle a maximum of 42 resonances; with the nonlinear branch the maximum is 21.

A typical running time on the IBM 7094 for a linear fit with 19 resonances is about 35 sec. The characteristic parameters obtained for σ_F and σ_T , and the set of level parameters μ and ν , which are output for the Program CODILLI, are made available to subroutine BWSIG 2. The first part of this subroutine evaluates from total and fission parameters the corresponding parameters for scattering and capture cross sections. An independent option permits obtaining corresponding parameters for single-level calculations, whenever wanted.

Both subroutines BWSIG 1 and BWSIG 2 are set up to handle simultaneously five different "resonance elements" (fissile and resonance absorbers) with a maximum of 50 levels for each element. In the following section it will be discussed how the calculations can be set up to account for a practically unlimited number of levels.

The energy-dependent, temperature-dependent cross sections given by Eqs. (I-1) and (I-2) are calculated in the second part of either subroutine BWSIG, as superpositions of ψ and χ line-shape functions. At this stage multilevel and single-level cross sections are handled identically. At each energy step, the energy-dependent set of cross sections, for each wanted element, is returned to the main program. The entire computation is performed in the fast memory of the IBM 7094 of the University of Illinois. This convenient feature of this family of routines is mainly achieved by virtue of the fast algorithm used for the evaluation of the line-shape functions ψ and χ , calculated in the subroutine SHAPE.

D. Line-shape Functions--Subroutine SHAPE

The well-known line-shape functions⁽⁹⁾

$$\psi(x, t) = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{\infty} \frac{dy}{1+y^2} e^{-(x-y)^2/4t}; \quad (\text{I-10})$$

$$\chi(x, t) = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{\infty} \frac{y dy}{1+y^2} e^{-(x-y)^2/4t}$$

are evaluated by three different approximations, depending on the value of $|x|$: Taylor expansion, asymptotic expansion, and a complex integration

- a) For $|x| \ll 1$, the Taylor expansion⁽⁹⁾ converges rapidly.
- b) For $|x| > 1$, the well-known asymptotic expansion⁽⁹⁾ is calculated.
- c) In the intermediate region, the exponential in the integrand of Eqs. (I-10) and (I-11) is approximated by a polynomial.⁽¹⁰⁾ The resulting integral can be evaluated analytically, by means of the Cauchy integral formula,⁽¹¹⁾ and ψ and χ are then expressed as simple functions of x and t .

The choice between these branches of the subroutine is made within the subroutine. Considering a parameter plane with the axes $x/\sqrt{2t}$ and $1/\sqrt{2t}$, one can easily see that the expansion (a) applies in a quadrant near the origin, while the expansion (b) is suitable outside a circle around the origin of the parameter plane. In the intermediate region, the polynomial expansion provides a good approximation.

The number of terms to be included to reach a given accuracy with the asymptotic or Taylor series expansions depends on the values of the parameters x and t . To attain an accuracy of 0.00001,

eight terms have to be retained in these expansions. Computing times needed to calculate ψ and χ together range between 1 and 3.7 msec for the expansions a) and b), and are of the order of 3.45 msec for the polynomial approximation, which is, however, less accurate (0.00005). These computing times apparently compare favorably with those obtained in other integration schemes.^{(12),(13)}

II. SLOWING-DOWN CALCULATIONS IN HOMOGENEOUS MEDIA

With the availability of large computers it has become possible to solve numerically the integral Boltzmann equation for homogeneous media in exact form (i.e., without auxiliary approximations) for an arbitrarily large number of resonance absorbers or (and) fissile elements, by substituting a difference equation for the integral equation. The method, developed originally by Nordheim⁽¹²⁾ for the case of neutron slowing down in presence of one resonance only, has been enlarged to encompass five resonance absorbers with two nonhydrogen moderators and hydrogen. No assumption is made here regarding the flux in the moderator, but all elements are treated by the same numerical method. The step-by-step integration is obtained by increments, in a way such that accumulations of errors arising from the substitution of finite sums for integrals are minimized.

The point at which the choice of cross-section model becomes critical is at the stage of stating the initializing conditions for the integral equation. In handling one resonance at the time, the implicit assumption is made that at energies much larger and much lower than the location of the energy level, the flux be "flat," i.e., behaves as a $1/E$ function. The assumption corresponds to ignoring any absorptions above and below the level of interest. Numerical tests concerning this assumption show that the approximation is valid only for high dilution. For the case of the two thorium resonances at 21 and 23 eV, for example, it can be shown that the spacing between the two levels is not large enough to permit a full recovery of the flux, the effect becoming larger the higher the medium temperature. This elementary example indicates that in solving the Boltzmann equation for neutron slowing down, the presence of levels physically existing above and below the energy range of interest influences the results. In particular, the presence of absorptions above the energy of interest modifies the analytical structure of the initializing solutions.

The integral Boltzmann equation for homogeneous media is given by

$$G(u) = H_0 + \int_0^u G(u') S_H(u') du' + \sum_i \int_{u-\gamma_i}^u G(u') S_i(u') du', \quad (\text{II-1})$$

where $G(u) = F(u)e^u$ and, in standard notations, $F(u)$ indicates the collision density and u the variable lethargy. The subscript i indicates

the i -th element of the mixture, and the elements are ordered by increasing atomic mass number A_i with $A_i > 1$, the subscript H referring to hydrogen. The terms containing the cross sections explicitly are

$$S_i(u) = \frac{\Sigma_{si}(u)}{\alpha_i \Sigma_{\text{tot}}(u)} \quad \text{with } \Sigma_{si} = \begin{array}{l} \text{macroscopic scattering cross} \\ \text{section of the } i\text{-th species,} \end{array} \quad (\text{II-2})$$

where

$$\alpha_i = \frac{4A_i}{(A_i + 1)^2}, \quad (\text{II-3})$$

and

$$S_H(u) = \frac{\Sigma_{sH}(u)}{\Sigma_{\text{tot}}(u)} \quad \text{with } \Sigma_{sH} = \begin{array}{l} \text{macroscopic scattering cross} \\ \text{section of hydrogen.} \end{array} \quad (\text{II-4})$$

In (II-1),

$$\gamma_i = \ln \frac{1}{1 - \alpha_i},$$

and

$$H_0 = \int_{u^*}^0 S_H(u') G(u') du' + S_H(u^*) q(u^*) e^{u^*},$$

where $u = 0$ is the reference lethargy at which the integration begins, while u^* represents the fission lethargy from which the virgin neutron contribution $S_H(u^*)q(u^*)e^{u^*}$ arises.

Numerically (II-1) is solved by forward integration in lethargy, initiating the integration from an energy region above the resonance region where the solution $G(u)$ is known. In all practical cases, such a region is so far below the fission region that one can initialize the calculation with a known asymptotic solution of the Boltzmann equation. The width of the initializing region must be chosen at least as wide as the largest γ , in this case γ_1 . In conventional slowing-down calculations, the chosen initializing solution is of the form

$$G_{as}(u) = G_0 e^u. \quad (\text{II-5})$$

This corresponds to constant cross sections in a purely scattering medium.

Rigorously, (II-5) can be used only if the resonances in question are so far below in energy, and so peaked, that no tails from the absorption cross section can reach the asymptotic region. In particular, for calculations involving single-level cross sections with a compensating $1/v$ absorption background, as used with Monte Carlo techniques,⁽¹⁴⁾ (II-5) would provide a misrepresentation of $F(u)$ at least for the first interval after the asymptotic region.

In calculations for mixtures containing fissile elements treated with the multilevel parameters, (II-5) would definitively distort the results, the more the lower is the dilution.

To account for the absorption in the asymptotic region in a simple manner, it is assumed that the cross sections can be considered there as constant, so that the asymptotic solution is given by

$$G(u) = G_0 e^{\rho u}. \quad (\text{II-6})$$

The constant ρ is the solution of the transcendental equation

$$\rho = S_H + \sum_i S_i (1 - e^{-\rho \gamma_i}), \quad (\text{II-7})$$

and in the presence of hydrogen

$$G_0 = H_0 \rho / S_H, \quad H_0 \text{ arbitrary};$$

for no hydrogen, G_0 is arbitrary.

The program EXACTQ can handle mixtures of two nonhydrogen moderators, hydrogen, and at most five resonance absorbers and fissile elements. The cross sections for EXACTQ are evaluated by subroutine BWSIG. The initial part of the program establishes the initializing solution and stores in memory locations the first arrays of known integrands, thus preparing the calculation to handle moderators and resonance elements numerically in the same manner. The lethargy steps are chosen as integer fractions of γ_1 . Each array, e.g., for the i -th element of the mixture, contains values of $S_i(u) G(u)$ at each of the lethargy steps contained in the corresponding width γ_i .

The second part of program EXACTQ performs the forward integration in lethargy by calculating the increment of $G(u)$ from u to $u + \Delta u$ rather than calculating $G(u + \Delta u)$ directly.

Using (II-1) at $u + \Delta u$, and at u and subtracting, one has

$$G(u + \Delta u) - G(u) = \int_u^{u+\Delta u} S_H(u') G(u') du' + \sum_i \left[\int_u^{u+\Delta u} G(u') S_i(u') du' - \int_{u-\gamma_i}^{u+\Delta u-\gamma_i} G(u') S_i(u') du' \right]. \quad (\text{II-8})$$

Because the lethargy intervals Δu are chosen to be always much smaller than the smallest resonance width, it is permissible to replace with two terms of a trapezoidal integration the integral

$$\int_u^{u+\Delta u} G(u') [S_H(u') + \sum_i S_i(u')] du'$$

appearing in (II-8). The equation solved in EXACTQ for $G(u + \Delta u)$ is therefore

$$G(u + \Delta u) \left\{ 1 - \frac{\Delta u}{2} \left[S_H(u + \Delta u) + \sum_i S_i(u + \Delta u) \right] \right\} = G(u) \left\{ 1 - \frac{\Delta u}{2} \left[S_H(u) + \sum_i S_i(u) \right] \right\} - \sum_i \int_{u-\gamma_i}^{u+\Delta u-\gamma_i} G(u') S_i(u') du'. \quad (\text{II-9})$$

The integrals of the form $\int_{u-\gamma_i}^{u+\Delta u-\gamma_i}$ are evaluated by parabolic interpolation

(since $u + \Delta u - \gamma_i$ and $u - \gamma_i$ do not necessarily coincide with the established subdivision in equal parts of γ_i , using the values of the integrand at the points

$$u - (M_i + 1) \Delta u, \quad u - M_i \Delta u, \quad u + \Delta u - M_i \Delta u,$$

where $M_i \Delta u = \gamma_i - \epsilon_i$; $\epsilon_i < \Delta u$.

As the solution at $u + \Delta u$ is obtained, EXACTQ shifts the stored arrays forward by one step in lethargy, thus "forgetting" the existing values at $u - (M_i + 1) \Delta u$ and acquiring into the location previously designed for u the obtained values for $u + \Delta u$.

This method is economical from the point of view of memory storage, and it eliminates as far as possible all those numerical errors which would arise from the explicit evaluation of the right-hand side of (II-1) as a sum of

step-by-step integrals. It also permits propagation of the integration from one energy interval to a subsequent one. Practically this is obtained by use of an index which indicates if at the first input value of $E_{\min}$ the integration stops, or if a new energy interval has to be expected, for which the old $E_{\min}$ becomes the new $E_{\max}$, and a new value for $E_{\min}$ is read in. Automatically, the last stored arrays provide the new initializing solution.

Consistently, BWSIG reads in a new set of resonance parameters connected with the subsequent energy interval. Thus, any number of resonance levels can be handled in this type of calculation. The output results of EXACTQ are: $F(u)$, $\phi(u)$, $\phi(E)$, $Q(u)$, and, by option, either the values of the total absorption and scattering cross sections of the mixture of resonance elements at each energy step, or the reaction rates. The quantity $Q(u)$ is the value at u of the slowing-down density for the mixture:

$$Q(u) = 1 - \frac{1}{q(0)} \int_0^u \frac{\Sigma_a(u')}{\Sigma_{\text{tot}}(u')} F(u') du'. \quad (\text{II-10})$$

Thus $Q(u)$ corresponds to the physical definition of resonance escape probability, though in conventional calculations $p(u)$ is defined in terms of a resonance integral.

This program is written in FORTRAN, and it uses only the fast memory of the IBM-7094 of the University of Illinois

As regards typical running time, 16 Doppler-broadened resonances in a mixture of Th and U^{233} with one moderator require 1.3 min.

III. HETEROGENEOUS CALCULATIONS

A method has been developed for calculating resonance effects in nuclear reactor lattices without either of two widely used assumptions:^(15,16) (1) that the neutron flux is spatially independent within each region of the lattice cell, (2) that the flux recovers an asymptotic $1/E$ form between resonances. The neutron slowing-down problem is formulated in terms of a Boltzmann integral equation, and the correct transport kernel is derived for a Wigner-Seitz equivalent cell with isotropic scattering in the laboratory system. A new method of polynomial approximations is then used to reduce the transport problem to matrix form. From this there results a set of integral equations in lethargy for the neutron flux at a number of discrete ordinates. These equations are numerically integrated to obtain the neutron flux as a function of space and energy. The mathematical basis for these calculations is derived elsewhere.⁽¹⁷⁾

Resolved resonance integrals have been calculated for a number of U^{238} -graphite lattices with both metal and oxide rods. Where comparisons are made, the results are in excellent agreement with accurate Monte Carlo calculations. Two computer codes, PRELIM and ILLINI, have been written in FORTRAN for calculating flux distributions and reaction rates in simple cylindrical reactor lattices, consisting of a fuel region surrounded by a moderator region. The nuclear species in the fuel region may include up to five resonance absorbers or fissile elements, and up to five moderators.

The moderator region can include up to five elements with constant cross sections.

The slowing-down problem is first reduced to a set of coupled integral equations in lethargy by using a discrete ordinate approximation for the space dependency. The coupling coefficients depend on the lattice geometry and the optical path lengths between the discrete ordinates, that is, on the cross sections which vary rapidly with energy in the fuel region. The solution of the coupled integral equation proceeds exactly as described above for the program EXACTQ. The energy-dependent cross sections for fissile and fertile elements are again evaluated by the subroutine BWSIG.

Because the resonance cross sections vary very rapidly with lethargy, the lethargy mesh used in the numerical integration must be very fine. The direct calculation of the coupling coefficients is therefore much too time-consuming to be done at each lethargy step. Therefore, an interpolation scheme is used which is based on the fact that for a lattice in which the cross sections of the moderator region are energy independent, the coupling coefficients are functions only of the total cross section of the fuel region.

For a particular lattice geometry it is thus possible to perform the time-consuming calculation of the coupling coefficients for a relatively few, well-chosen values of the total fuel cross section, and then to set up an appropriate interpolation scheme.

The data for the interpolation scheme are obtained in the routine PRELIM. This routine calculates the coupling coefficients for a given lattice for a set of values of the fuel cross section. The resulting interpolation coefficients from which the coupling coefficients can be calculated are permanently recorded on punched data cards, which are then used as part of the input of Program ILLINI.

Specifically, these coefficients are used by the Subroutine HETRO to reconstruct the coupling coefficients at every step of the lethargy integration.

With this method, changes in the fuel composition, resonance structure, or fuel temperature are taken care of by the same set of interpolation coefficients, without the need of repeating the calculations of Program PRELIM.

Although Program ILLINI has not been optimized, running times on the IBM-7094 are of the order of 15 min, whereas comparable Monte Carlo calculations require about 35 min.

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Discussion of Paper
Presented by Mr. F. T. Adler

MR. ROY (Babcock & Wilcox): Would you care to comment on the errors introduced in assuming or ignoring overlap in flux recovery in the doublet in thorium? Have you examined thorium at 22 eV?

MR. ADLER: Yes. The influence is there and very noticeably in the thorium doublets.

COMPUTATION OF SCATTERING CROSS SECTIONS FOR USE IN THERMAL-NEUTRON TRANSPORT CALCULATIONS

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(Paper presented by P. Hutchinson)

ABSTRACT

In the past, the inelastic scattering cross sections for use in thermal-neutron transport calculations have, basically, been calculated in two stages. First, the "scattering law" $S(\alpha, \beta)$ is computed from data which give details of the chemical binding of the moderator atoms which affect the thermalizing properties, and then the required Legendre coefficients $\sigma_l(E' \rightarrow E)$ of the cross sections $\sigma(E' \rightarrow E, \mu)$ are obtained by numerical integration over the variable α . This procedure has several drawbacks. Unless great care is taken, serious numerical errors occur in the results, especially for high incident neutron energy.

To overcome these difficulties, a FORTRAN code, SCAT, has been written, which uses a specially designed integration routine to evaluate the cross sections $\sigma_l(E' \rightarrow E)$ directly from the data used in the calculation of $S(\alpha, \beta)$, without the intermediate step of evaluating $S(\alpha, \beta)$ itself.

The method of computation for a complex distribution, $\rho(\beta)$, compares favorably in computer time with previous methods for the evaluation of scattering matrices, and is believed to be generally of much greater numerical reliability.

Details of calculations with SCAT are given, together with a general discussion of the numerical problems associated with the evaluation of thermal scattering cross sections.

1. Introduction

The computer code SCAT described in this paper is designed to compute inelastic scattering cross sections for use in thermal-neutron transport calculations.

It is by now well-known (1, 2) that the cross section $\Sigma(E' \rightarrow E, \mu)$ for the scattering of a thermal neutron from an initial energy E' to final energy E , through an angle $\cos^{-1} \mu$, can be expressed in terms of a "scattering law" which is a function only of the energy change of the

neutron, and its momentum change, and which is determined by the thermal motion of the atoms of the scatterer. The scattering law $S(\alpha, \beta)$ is conventionally written as a function of the dimensionless variables α and β :

$$\alpha = \frac{1}{AkT} [E' + E - 2\mu(E, E')^{1/2}]; \quad \beta = (E' - E)/kT, \quad (1)$$

where kT is the moderator temperature in energy units and A the ratio of the mass of the moderating atoms to that of the neutron (if more than one nuclear species is affecting the moderation, then A is usually taken as the dominant scatterer).

For a single nuclear species $\Sigma(E' \rightarrow E, \mu)$ is given in terms of $S(\alpha, \beta)$ by

$$\Sigma(E' \rightarrow E, \mu) = \frac{N\sigma_b}{2kT} \left(\frac{E}{E'} \right)^{1/2} S \left(\frac{1}{AkT} [E' + E - 2\mu(E, E')^{1/2}] \frac{1}{kT} (E' - E) \right) e^{(E' - E)/2kT}, \quad (2)$$

where N is the number of atoms per unit volume, and σ_b is the bound-atom scattering cross section.

SCAT is concerned only with the "incoherent Gaussian" contribution to the scattering law⁽²⁾. Thus, $S(\alpha, \beta)$ consists of a sum of terms for each nuclide present, weighted with the relative number density and bound-atom cross section. For each term $S(\alpha, \beta)$ has the form

$$S(\alpha, \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} I(\alpha, t) e^{-i\beta t} dt; \quad (3)$$

$$I(\alpha, t) = \exp[-\alpha W(t)], \quad (4)$$

where $W(t)$, the "width function," is a real, even function of t which contains information related to the thermal motions of the moderator atoms, and is usually specified in terms of an energy-distribution function $\rho(\epsilon)$. The relation between $W(t)$ and $\rho(\epsilon)$ is:

$$W(t) = \int_0^{\infty} \rho(\epsilon) d\epsilon \frac{\cosh \frac{\epsilon}{2kT} - \cos \frac{\epsilon}{kT} t}{\frac{\epsilon}{kT} \sinh \frac{\epsilon}{2kT}}. \quad (5)$$

We take $\rho(\epsilon)$ normalized to unity:

$$\int_0^{\infty} \rho(\epsilon) d\epsilon = 1. \quad (6)$$

If, for a thermal-neutron-distribution calculation, the full angular dependence of the scattering must be taken into account, then $S(\alpha, \beta)$ has to be computed for the entire range of α and β required for the calculation. This can be done by the methods described in Ref. 2, and programs to do this have been in use for some time. (It might nevertheless be the case that the use of the numerical method described in this paper is more reliable, although this has not yet been investigated). However, for very many calculations, it is only considered necessary to use the isotropic or, at most, a few terms in the Legendre polynomial expansion of the cross sections. In many other calculations, one is restricted by reasons of practicality to the same approximation.

What is required, therefore, is not $S(\alpha, \beta)$ itself, but the angular averages $\Sigma_{\ell}(E' \rightarrow E)$, defined by

$$\Sigma_{\ell}(E' \rightarrow E) = \int_{-1}^1 \Sigma(E' \rightarrow E, \mu) P_{\ell}(\mu) d\mu. \quad (7)$$

The right-hand side, of course, involves an integral of $S(\alpha, \beta)$ for $\alpha_- \leq \alpha \leq \alpha_+$, with

$$\alpha_{\pm} = \frac{1}{AkT} \left(E^{1/2} \pm E'^{1/2} \right)^2. \quad (8)$$

In the past, it has been customary to obtain $\Sigma_{\ell}(E' \rightarrow E)$ through the two stages of (a) tabulating $S(\alpha, \beta)$ at a large number of values of α and β , and (b) then computing $\Sigma_{\ell}(E' \rightarrow E)$ numerically by the appropriate integration over α .

This procedure has several drawbacks; unless great care is taken, serious numerical errors can be introduced, particularly at high incident neutron energy. This is because (a) at high neutron energy, there is strong angular correlation between angle of scattering and energy transfer [in the limit $E \gg kT$, we have $S(\alpha, \beta) \rightarrow \delta(\alpha - \beta)$] so that the numerical integration over α is very difficult, and (b) it is necessary to interpolate and extrapolate in the table of $S(\alpha, \beta)$ where the function is varying rapidly.

A point here is that, if only a few energy moments are required, the advantage gained by expressing the cross section basically in terms of only two variables α and β is largely illusory, since the number of points at which $S(\alpha, \beta)$ should be tabulated must be greater than the number of energy points required.

The purpose of SCAT is to compute $\Sigma_g(E' \rightarrow E)$ directly, taking advantage of the fact that by use of (4) the angular integration may be performed analytically, leaving only the t -integration to be carried out numerically. In order to do this, it is necessary to have an accurate tabulation of $W(t)$ at a large number of points. In SCAT this is done by fitting $\rho(\epsilon)$ by a set of analytic functions, for which (5) may be evaluated analytically. This avoids errors which might arise in a numerical evaluation from a table of $\rho(\epsilon)$. This procedure also allows one to make use, not only of experimentally determined values of $\rho(\epsilon)$, which are themselves subject to error, but also of such parameters as the thermal average scattering cross section (see Ref. 3).

2. Parametric Fitting of the Width Function

The function $\rho(\epsilon)$ which determines the width function $W(t)$ represents an energy spectrum of excitations of the moderator atoms. Its general features are illustrated in Fig. 1, where water is taken as an example.

Fig. 1. $\rho(\epsilon)$ for Room-temperature Water

For fluid (gas and liquid) moderators, $\rho(\epsilon)$ has a peak at the origin, the intercept $\rho(0)$ being proportional to the coefficient of self-diffusion of the atoms.⁽²⁾ In solid moderators $\rho(0) = 0$; hence $W(t)$ is bounded for all t .

For simple solids and in molecular liquids, there is a range of ϵ for which $\rho(\epsilon)$ is continuous and may have one or more broad peaks, corresponding to the frequency distributions of acoustic and broad optical

modes (in the solid) or hindered molecular rotations (in liquids). For molecular substances there may also be sharp peaks in $\rho(\epsilon)$ at higher energies, corresponding to internal molecular vibrations (or narrow optical bands in solids).

In the present form of SCAT these three types of motion are each represented by a specific functional form of $\rho(\epsilon)$ and $W(t)$. These are summarized in Table 1 and below.

Table 1
SCATTERING-LAW MODELS

Model	Parameter	$\rho(\beta)^*$	$W(t)$
Gas	-	$2 \delta(\beta)$	$t^2 + 1/4$
Fluid	$\emptyset$	$\left[\frac{4}{\pi \emptyset^2} \left(1 + \frac{\emptyset^2}{4} \right)^{1/2} \sinh \frac{\beta}{2} \right] K_1 \left[\frac{1}{\emptyset} \left(1 + \frac{\emptyset^2}{4} \right)^{1/2} \beta \right]$	$\frac{2}{\emptyset^2} \left\{ \left[1 + \emptyset^2 (t^2 + 1/4) \right]^{1/2} - 1 \right\}$
Gauss	θ	$\left(\frac{1}{2\pi} \right)^{1/2} \frac{2\beta}{\theta^3} \left\{ \exp \left[-\frac{2}{2\theta^2} \left(\beta - \frac{\theta^2}{2} \right)^2 \right] - \exp \left[-\frac{1}{2\theta^2} \left(\beta + \frac{\theta^2}{2} \right)^2 \right] \right\}$	$\frac{2}{\theta^2} \left\{ 1 - \exp \left[-\frac{\theta^2}{2} (t^2 + 1/4) \right] \right\}$
Oscillator	ω	$\delta(\beta - \omega)$	$\frac{1}{\omega \sinh \frac{\omega}{2}} \left\{ \cosh \frac{\omega}{2} - \cos \omega t \right\}$

* $\beta = \epsilon/kT$.

We write $\rho(\epsilon)$ as

$$\rho(\epsilon) = [\sum_i a_i \rho^{(1)}(\theta_i, \epsilon) + \sum_j b_j \rho^{(2)}(\omega_j, \epsilon) + c \rho^{(3)}(\phi, \epsilon)] / (\sum_i a_i + \sum_j b_j + c), \quad (9)$$

and $W(t)$ as

$$W(t) = [\sum_i a_i \Theta(\theta_i, t) + \sum_j b_j \Omega(\omega_j, t) + c \Phi(\phi, t)] / (\sum_i a_i + \sum_j b_j + c). \quad (10)$$

(a) $\rho^{(3)}$ represents fluid effects and is characterized by the parameter ϕ . If the moderator consists of a dilute gas of noninteracting molecules, then $\phi = 0$ and $\Phi = (t^2 + 1/4)$. In a solid, c must be set equal to zero.

(b) $\rho^{(1)}$ represents a broad phonon distribution, any number of which are allowed. We refer to this as a Gaussian frequency distribution.

(c) $\rho^{(2)}$ represents vibrational levels.

The forms of ρ are illustrated in Fig. 2.

Fig. 2
Types of $\rho(x)$ Employed
for Fitting Procedure

3. Integration Procedure

The detailed description of the integration procedure given here will be confined to the calculation of the isotropic part of the cross section ($L = 0$). The generalization of these procedures to higher moments will be briefly described at the end of this section.

The problem of evaluating the transfer cross section divides naturally into two parts once the width function has been specified in parametric form; these are, respectively, the angular integration of Eq. (7) and the integration of Eq. (3) over time. Combination of Eqs. (2), (3), and (7) results in

$$\Sigma(E' \rightarrow E) = \frac{N\sigma b}{4\pi kT} \left(\frac{E}{E'} \right)^{1/2} \exp \left\{ \frac{E' - E}{2kT} \right\} \int_{-\infty}^{\infty} dt e^{-i\beta t} \int_{-1}^1 d\mu \exp \left\{ -\frac{W(t)}{AkT} \left[E' + E - 2\mu (EE')^{1/2} \right] \right\}. \quad (11)$$

Integration over angle leads to

$$\Sigma(E' \rightarrow E) = \frac{AN\sigma b}{4\pi E'} \exp \left\{ \frac{E' - E}{2kT} \right\} \int_0^{\infty} dt \frac{1}{W(t)} \left(e^{-\alpha_- W(t)} - e^{-\alpha_+ W(t)} \right) \cos \beta t, \quad (12a)$$

where

$$\alpha_{\pm} = (E'^{1/2} \pm E^{1/2}) / AkT \quad (12b)$$

and

$$\beta = (E' - E) / kT. \quad (12c)$$

For a fluid the integrand of Eq. (12a) approaches zero for large t , and no special treatment is necessary. For a solid, however, the width function has a finite asymptotic limit, and this gives rise to a delta function term of the form

$$\Sigma_{el}(E' \rightarrow E) = \Sigma_{el}(E) \delta(E' - E), \quad (13a)$$

where

$$\Sigma_{el}(E) = N\sigma_b \frac{AkT}{4EW_\infty} \left[1 - \exp\left(\frac{-4EW_\infty}{kT}\right) \right] \quad (13b)$$

and

$$W_\infty = \lim_{t \rightarrow \infty} W(t) = 2 \sum_i \frac{a_i}{\theta_i^2} / \sum_j a_j. \quad (13c)$$

Furthermore, the asymptotic part must now be subtracted from the integrand of Eq. (12a). For delta functions in a solid, $\Sigma(E' \rightarrow E)$ is highly singular, and SCAT cannot deal with this situation at present. However, neither can any general neutron transport code, and such a facility is of no use to the reactor physicist!

It is thus clear that we are concerned with the numerical evaluation of integrals of the form

$$I(\alpha, \beta) = \int_0^\infty \frac{1}{W(t)} e^{-\alpha W(t)} \cos \beta t \, dt. \quad (14)$$

The numerical procedure used is a generalization of the method originally proposed by Filon⁽⁴⁾ for the evaluation of trigonometric integrals. This procedure treats the trigonometric term as a weight function and has the advantage that errors are slowly dependent on β . In the case under review here the integration range is split into a series of small intervals, over each of which a linear fit is made to the multiplicative term, $1/W(t)$, and the $W(t)$ term in the exponent of Eq. (14). Equation (14) then takes the form

$$I(\alpha, \beta) = \sum_{i=0}^{\infty} I^{(i)}(\alpha, \beta), \quad (15a)$$

where

$$I^{(i)}(\alpha, \beta) = \int_{\tau_i}^{\tau_{i+1}} (A_i + B_i t) \exp \left[-\alpha (a_i + b_i t) \right] \cos \beta t \, dt. \quad (15b)$$

The coefficients which appear in Eq. (15b) are determined by the values of the width function at the limits of integration; in particular,

$$b_i = \frac{W_{i+1} - W_i}{\tau_{i+1} - \tau_i}; \quad (16a)$$

$$B_i = \frac{-b_i}{W_{i+1} W_i}. \quad (16b)$$

Evaluation of the integral in (15b) and use of the relations (16) result in a quadrature formula of the form

$$I^{(i)}(\alpha, \beta) = \left[\frac{e^{-\alpha W(t)}}{(\alpha^2 b_i^2 + \beta^2) W(t)} \left\{ \left(\alpha b_i - \frac{b_i W(t)}{W_i W_{i+1}} \frac{\alpha^2 b_i^2 - \beta^2}{\alpha^2 b_i^2 + \beta^2} \right) \cos \beta t \right. \right. \\ \left. \left. - \left[\beta - \frac{2 \alpha \beta b_i^2 W(t)}{W_i W_{i+1} (\alpha^2 b_i^2 + \beta^2)} \right] \sin \beta t \right\} \right]_{\tau_{i+1}}^{\tau_i}. \quad (17)$$

A subroutine in the code evaluates the integrals $I^{(i)}(\alpha, \beta)$ for the necessary values of α and β . The step length in any given calculation is fixed by the parametric specification of the width function and the α value.

The α dependence of the error may be illustrated by considering the evaluation by a similar method of the integral

$$\int_a^b x e^{-\frac{1}{2} \alpha x^2} dx.$$

Linear interpolation of the exponent gives rise to a value for the fractional error of the form

$$\frac{4}{\alpha(a+b)^2} \approx \frac{b-a}{b+a} \coth \left[\frac{\alpha}{4} (b^2 - a^2) \right].$$

For small α the error depends on the square of the step length, and even for large α this is only increased to a linear dependence.

The truncation of the sum in Eq. (15a) is arranged so that the maximum truncation error is less than 0.1% of the value to be calculated. This is done by requiring that the value of $I^{(i)}(\alpha, \beta)$ should be less than $8h \cdot 10^{-4}$ of the value of the sum already calculated, over an interval in which $\cos \beta t$ is a maximum.

A significant saving in time may be made by noticing that $I(E,E)$ always contains the constant term

$$C = \int_0^{\infty} \frac{1}{W(t)} dt. \quad (18)$$

This term has the slowest asymptotic decay and is evaluated once and for all in the early stages of the code.

When a diffusive damping mode of the effective width type occurs, the integral (12a) has a logarithmic singularity. This integral, and hence the singularity, contribute only to the forward scattering; since this is indistinguishable from unscattered neutrons, the singularity is neglected. This procedure is satisfactory provided that care is taken, when performing a transport calculation, to evaluate all the scattering terms in a consistent way. It should also be stressed that consistency in the numerical evaluation of the in-scatter and out-scatter terms, in a transport calculation, is most important, as otherwise spurious "source" and "capture" terms appear.

For higher-order Legendre moments of the cross section, it may easily be seen from Eq. (7) that the integrals to be evaluated take on the form

$$I_{\ell}(\alpha, \beta) = \int_0^{\infty} Q_{\ell+1}\left(\frac{1}{W(t)}\right) e^{-\alpha W(t)} \cos \beta t dt, \quad (19)$$

where $Q_{\ell}(x)$ is a polynomial in x of order ℓ , e.g.,

$$I_1(\alpha, \beta) = \int_0^{\infty} \left\{ \frac{1}{W(t)} \pm \frac{AkT}{2(EE')^{1/2}} \left[\frac{1}{W(t)} \right]^2 \right\} e^{-\alpha W(t)} \cos \beta t dt. \quad (20)$$

In this case the same linear fit is made to the inverse of the width function, and this again leads to an integral which may be evaluated analytically to give an appropriate quadrature formula. The delta function elastic term may again be dealt with analytically. The highest-order Legendre moment available will be the third.

4. The Code in User Form

The basic form of the code in user form is shown in the flow diagram, Fig. 3. The general divisions are as follows:

1. Read moderator parameters.
2. Tabulate and list the width and frequency functions.
3. Read the energy mesh.
4. Integration procedure.
5. Output.

Fig. 3
General Flow Diagram
for SCAT

These sections will now each be dealt with in more detail.

1. The moderator parameters consist of the parametric fit to the frequency function, the free-atom cross section, the mass, and the temperature. The moderator parameters are given in units of eV, i.e., temperature independent, and are immediately scaled by the code relative to temperature. Each of the data decks is preceded by a descriptive title card to provide a boundary and a reminder of the contents of the cards.

2. First of all the minimum t interval is calculated, and the width function listed over an adequate range. The frequency function is then calculated and listed. At this point any integrals over the frequency or width functions may be calculated and printed, e.g.,

$$\bar{T} = \frac{1}{2} \int_0^{\infty} \beta \rho(\beta) \coth(\beta/2) d\beta$$

is currently calculated. These calculations precede the intake of the energy mesh so that the code may be used for these relatively simple tasks if required, and will automatically halt when no energy mesh is provided.

4. The integration procedure forms the bulk of the code, and a fairly detailed flow diagram is given in Fig. 4. As may be seen, if a perfect-gas calculation is specified for the zeroth Legendre moment, a special subroutine calculates the values from an analytic expression.

5. The output consists of a print-out of the remaining parameters, i.e., temperature, mass of scatterer, free-atom cross section, and order of Legendre moment. These are followed by a print-out of the energy mesh and the scattering matrix. The scattering cross section and delta function elastic terms then appear. Finally, a statement of the total execution time is given. A graph-plotting routine for an SC 4020 is to be added to the code; this will allow selected rows of the scattering matrix, the cross section, frequency, and width functions to be obtained in graphical form. A further facility to be added will allow the transfer cross sections to be evaluated for mixtures.

5. Conclusions

First, some general remarks about execution time should be made. As the width function is tabulated once and for all in the early stages of the calculation, the time for execution of the code is virtually independent of the complexity of the frequency function. An additional virtue of this feature is that there is no loss of accuracy when more than one delta function is present. This was not the case with older methods which limited the number of delta functions which could be taken into account without loss of accuracy.

It is difficult to give precise estimates of execution times as, for instance, the truncation point of the sum (15a) is clearly quite sensitive to the energy values. However, for the purposes of comparison and checking the operation of the code, several perfect-gas calculations were done by numerical evaluation of the integrals. A typical example is that described below for a perfect gas of unit mass. The total time required was 466 sec for an energy mesh of thirty points running between 10^{-3} and 1 eV.

In Table 2 are shown comparative approximate and analytic results for $\Sigma(E' \rightarrow E)$ of a perfect gas of unit mass. The values are given in units

Table 2

VALUES OF $\Sigma(E' \rightarrow E)$ FOR PERFECT GAS OF UNIT MASS ($T = 300^\circ\text{A}$)

$E'_0 \backslash E$	1.0×10^{-3}	1.0×10^{-2}	1.0×10^{-1}	1.0
1.0×10^{-3}	2.138×10^2 2.191×10^2			
1.0×10^{-2}	2.191×10^1 2.191×10^1	6.155×10 6.209×10		
1.0×10^{-1}	2.190 2.191	6.207 6.209	9.893 9.946	
1.0	2.190×10^{-1} 2.191×10^{-1}	6.206×10^{-1} 6.209×10^{-1}	9.941×10^{-1} 9.945×10^{-1}	9.947×10^{-1} 1.000

of Σ_f , and only one-half of the matrix is shown, as the detailed balance condition is sufficient to define the rest. The upper number in each box is that obtained by numerical evaluation of the cross section; the lower number is the result given by the analytical formula. As may be seen, the largest percentage error occurs when E' and E are both 10^{-3} eV. This is due to the fact that heavy cancellation occurs in this position as α_+ and α_- are relatively close to each other. Even so the error here is only $2\frac{1}{2}\%$, and elsewhere the total error is 1% or less.

A comparison of the results for Nelkin water as given by SCAT and GAKER is shown in Table 3. Again the value given by SCAT is the upper figure in each box. As is clear, the results for the off-diagonal terms agree well, but the values on the diagonal show significant disagreement for energies of 0.1 eV and above. A test may be applied to the general behavior of the function on the diagonal. Rearrangement of (12a) gives

$$E \Sigma(E \rightarrow E) = \frac{AN\sigma_b}{4\pi} \int_0^\infty \frac{1}{W(t)} \left(1 - e^{-4EW(t)/AkT}\right) dt. \quad (21)$$

This shows that $E \Sigma(E \rightarrow E)$ should be a monotonically increasing function of energy with an asymptotic value

$$E \sum_{as} (E \rightarrow E) = \frac{NA\sigma_b}{4\pi} \int_0^\infty \frac{1}{W(t)} dt. \quad (22)$$

Table 3

VALUES OF $\Sigma(E' \rightarrow E)$ FOR NELKIN WATER ($T = 293^\circ\text{A}$)

$E' \backslash E$	1.0×10^{-3}	1.0×10^{-2}	1.0×10^{-1}	1.0
1.0×10^{-3}	8.487 x 10 ² 8.337 x 10 ²			
1.0×10^{-2}	2.376 x 10 2.357 x 10	2.550 x 10 ² 2.592 x 10 ²		
1.0×10^{-1}	6.752 x 10 ⁻¹ 6.995 x 10 ⁻¹	3.393 3.331	4.185 x 10 3.362 x 10	
1.0	1.007 x 10 ⁻¹ 1.009 x 10 ⁻¹	3.123 x 10 ⁻¹ 3.137 x 10 ⁻¹	8.494 x 10 ⁻¹ 8.273 x 10 ⁻¹	4.253 1.220

A comparison of the diagonal terms is shown in Table 4. Clearly the behavior of SCAT conforms with that to be expected from Eq. (21), whereas that of GAKER does not. As a consequence, we believe the results from SCAT to be more reliable.

Table 4
COMPARISON OF $E \Sigma(E \rightarrow E)$ FROM SCAT
AND GAKER FOR NELKIN WATER

E, eV	$E \Sigma(E \rightarrow E), \text{eV}/\Sigma F$	
	GAKER	SCAT
1.0×10^{-3}	8.337×10^{-1}	8.487×10^{-1}
1.0×10^{-2}	2.592	2.550
1.0×10^{-1}	3.362	4.185
1.0	1.220	4.253
2.0	1.231	4.253
3.0	1.252	4.253

In general, SCAT gives good accuracy for small masses, but accuracy becomes worse for larger masses. This is due to the fact that the difference between the exponents in the α_+ and α_- integrals decreases with increasing mass, and thus leads to heavy cancellation.

Finally, it should be stressed that one of the most significant advantages of SCAT is that it will in general be possible to use the code without a detailed knowledge of the physical properties of the moderator for which cross sections are required.

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Discussion of Paper
Presented by Mr. Hutchinson

MR. JARVIS (Chalk River): We seem to be using a similar sort of model. I have the same sort of components for liquids, and so on, but we have slightly different objectives. I am after transfer cross sections for spectrum calculations. Above about 1 eV I was getting too much round-off error and I had to go to other methods. I notice you seem to have stopped at 1 eV.

MR. HUTCHINSON: Results are available above 1 eV. What happens is that, as long as you stay around the diagonal where the absolute values are significantly large, you are safe. As soon as the absolute values become small, you lose.

MR. JARVIS: Right. I was trying to fill in off-diagonal terms, but it's a law of diminishing returns. You said you might fit to the $\rho(\beta)$, the generalized frequency distribution. Experiment really doesn't go very high in this. For instance, when you showed your slide, you had a nice delta function way up high, but that's not out of experiment I think.

MR. HUTCHINSON: No. This is one of those things that the experimentalists supply which isn't always due to experiment.

MR. JARVIS: Yes. Experiment only goes to about 10 beta, and so you don't even see a delta function or a spike. There is then difficulty in deciding the relative magnitude of these components. I believed I had to fit $S(\alpha, \beta)$, which is a lot more difficult, because $S(\alpha, \beta)$ must be calculated and then the parameters tuned. I don't know how many parameters you tune, but I have two: the area of the delta function and the position of the solid-type term. Everything else can be more or less obtained from the experiment or by hand waving, but it is very difficult to fit $\rho(\beta)$. I quizzed our experimentalists very hard on this. They back off very hurriedly if you say, "Well, does the $\rho(\beta)$ curve really look like this?" There are large experimental errors.

MR. HUTCHINSON: Our water model is time-dependent.

EXTENSIONS OF THE POWER-CONTROL METHOD FOR SOLUTION OF LARGE INHOMOGENEOUS REACTOR PROBLEMS

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Introduction

The Power-Control Method⁽¹⁾ was developed for solution of steady-state neutron diffusion-theory problems for boiling water reactors (BWR) in which spatial variation of the coolant-moderator density influences the nuclear properties. The method involves fixed eigenvalue iterations in which the control absorber distribution is varied to converge to a critical condition which is consistent with specified constraints on the control rod distribution. Rapid convergence for large, low-leakage reactor problems which are slow to converge with usual iterative methods is an advantage of the method. A weakness is that no single unique solution exists because, just as in the actual reactor, many possible control absorber distributions satisfy a critical condition. A unique solution is defined by an optimum control rod distribution such as one which provides maximum thermal capability.

The usual iterative approach for solution of BWR problems is shown in Fig. 1. A power or source distribution is assumed; the spatial distributions of the voids, fuel temperature, xenon and nuclear properties are calculated; the neutron flux equations are solved by conventional eigenvalue methods; a new power distribution is calculated, and the process is repeated until convergence is achieved. For a large reactor in which the neutron leakage and the split in the first and second eigenvalues are small, the neutron flux converges very slowly, the spatial shape is sensitive to small errors, and many iterations are usually required.

Fig. 1
Conventional Solution

The solution is complicated further by the necessity for distribution of the control rods so that the reactor is just critical. It is also desirable that the control rods be distributed to achieve an optimum operating state, such as minimum peak-to-average power or maximum MCHFR (minimum critical heat flux ratio) or ratio of allowable to actual heat flux. The latter two requirements place a heavy computing burden on the conventional iterative approach shown in Fig. 1.

Harker and Steward⁽²⁾ previously developed the "Backwards Method" for solution of this problem. Their method, which has been applied in use of the BORE code, involved the use of a desired power shape to calculate an approximate control distribution which satisfied that shape. The calculated control distribution was smoothed to satisfy constraints and then used as a starting point for the usual iterative process. This method greatly aided representation of large reactor operating states, but suffered from the necessity for the conventional "forward" iteration process, and the difficulties of achieving simultaneous convergence of the spatial variation of the nuclear properties and the neutron flux in a large reactor.

Power-Control Method

The Power-Control method is illustrated by Fig. 2. A desired power distribution is specified and the spatially variant voids, xenon, Doppler, and nuclear properties are calculated. Usual numerical techniques are used to determine the fast flux, with the reactor assumed to be critical. A control absorber distribution is calculated which exactly satisfies the desired power

Fig. 2
Power-Control Method

distribution and the critical condition. The control absorber distribution is modified to satisfy physical constraints, such as the direction which the control rods enter the reactor. A new power distribution which satisfies the physically realizable state is approximated from the revised control absorber distribution and is accelerated by Chebyshev extrapolation. The neutron multiplication is tested for criticality, and if the specified convergence is not satisfied, the preceding process is repeated with the revised power shape as a starting point. If there are no constraints on the absorber distribution only one pass is required.

The following will be limited to discussion of a one-dimensional axial BWR in a few-group representation. Space-dependent coupling between neutron flux and power, moderator steam voids, Doppler, xenon, and moderator density-dependent control rod worth are included in the iterative approach.

Steady-state fast-neutron diffusion is described by

$$\nabla \cdot D_1(z) \nabla \phi_1(z) - \Sigma_1(z) \phi_1(z) + \frac{\nu(z) \epsilon(z) P(z)}{1 + F(z) \nu(z)} = 0, \quad (1)$$

where D_1 and Σ_1 are the pointwise-varying diffusion coefficient and removal, respectively. Further, $F(z)$ defines the spatially dependent fissions per virgin neutron from nonfast fission, $\epsilon(z)$ is the number of neutrons slowing down past the fast fission threshold per virgin neutron from nonfast fission, and $\nu(z)$ is the average number of neutrons produced by nonfast fissions. The desired power distribution $P(z)$ is fixed. The void, fuel temperature, and xenon distributions are functions of $P(z)$ and, therefore, the nuclear properties have a fixed spatial shape for a fixed $P(z)$ distribution. It is assumed that the control rods do not have significant absorption in the first group.

Equation (1) is solved with a 3-point difference scheme. The difference equations are derived by integrating over a double interval with Simpson's rule. It is assumed that the spatially variant properties are continuously differentiable so that

$$\int_{i-1}^{i+1} \nabla \cdot D \nabla \phi \, dz = D \nabla \phi \big|_{i+1} - D \nabla \phi \big|_{i-1}. \quad (2)$$

The leakage contribution to the difference equations is evaluated by expanding the flux in a Taylor series about the points $i+1$ and $i-1$, and choosing the coefficients so that the second-derivative terms vanish. In one dimension a single forward elimination backwards substitution sweep is required to obtain $\phi_1(z)$.

The power is related to the neutron flux by

$$P(z) = \left[1 + F(z) \nu(z) \right] \sum_{g=1}^G \Sigma_{fg}(z) \phi_g(z), \quad (3)$$

which can be transformed to

$$\sum_{g=2}^G \Sigma_{fg}(z) \phi_g(z) = \frac{P(z)}{1 + F(z) \nu(z)} - \Sigma_{f1}(z) \phi_1(z), \quad (4)$$

where $\Sigma_{f1}(z)$ is defined to be the fission cross section for fissions below the fast-fission threshold but above the bottom of the first group.

For the two-group case the thermal flux is given directly in terms of the fast flux and the power:

$$\phi_2(z) = \frac{1}{\Sigma_{f2}(z)} \left[\frac{P(z)}{1 + F(z) \nu(z)} - \Sigma_{f1}(z) \phi_1(z) \right]. \quad (5)$$

The thermal flux is also related to the fast flux by

$$\nabla \cdot D_2(z) \nabla \phi_2(z) - \Sigma_2(z) \phi_2(z) + p(z) \Sigma_{s1}(z) \phi_1(z) = 0. \quad (6)$$

Equation (6) is solved for the control absorber distribution:

$$C(z) = \frac{p_0(z) \Sigma_{s1}(z) \phi_1(z) - [\Sigma_{a2}(z) + \Sigma_{aXe}(z)] \phi_2(z) + \nabla \cdot D_2(z) \nabla \phi_2(z)}{\Sigma_p(z) [\phi_2(z) + \gamma_c(z) p_0(z) \Sigma_{s1}(z) \phi_1(z)]}, \quad (7)$$

where $C(z)$ represents the fractional control inserted in a plane of the reactor for one-dimensional axial representation, $\Sigma_p(z)$ is the effective thermal control rod absorption cross section, $\gamma_c(z)$ is a void-dependent term in the resonance escape probability of the control rod, and $p_0(z)$ is the resonance escape probability, excluding control.

The most important spatially variant quantities in a BWR are the fast-neutron flux, the voids, and the control absorption. Therefore, the calculations can be speeded by replacing $\nabla \cdot D_2(z) \nabla \phi_2(z)$ in Eq. (7) with $-D_2(z) B_2^2(z)$, converging the most important quantities, and then introducing the exact thermal-leakage dependence in a final set of iterations. This works particularly well in axial representation of a BWR because control rods and voids in the bottom and top reflectors, respectively, result in little thermal-neutron flux spike at the core-reflector interfaces.

After the control absorption distribution has been calculated, the specified constraints are applied. Options allow specification of the maximum and minimum values of the fractional control rod absorption (C), bottom- or top-entry control rods, step-varying control, or arbitrary control distribution with no constraints. If the control distribution does not satisfy the constraints, it is modified. For example, for bottom-entry control rods the fractional control insertion must decrease with distance from the bottom of the reactor, and if valleys exist they are filled in.

The first-iteration, fractional control rod insertion for 1-D vertical representation of a large BWR with bottom-entry control rods is shown by the dashed line in Fig. 3, along with the requested power shape. A revised control absorption distribution (C') is used to estimate the power distribution which should have been requested, as follows:

The ratio of thermal-to-fast flux is

$$\alpha'(z) = \left(\frac{\phi_2(z)}{\phi_1(z)} \right)' = \frac{P_0(z) \Sigma_s \ell_1(z) [1 - \gamma_c(z) \Sigma_p(z) C'(z)]}{\Sigma_2(z) - [\nabla \cdot D_2(z) \nabla \phi_2 / \phi_2(z)] + \Sigma_p(z) C'(z)}. \quad (8)$$

The revised power shape is estimated from the unperturbed fast flux:

$$P'(z) = \phi_1(z) [\Sigma_{f1}(z) + \Sigma_{f2}(z) \alpha'(z)] [1 + \nu(z) F(z)]. \quad (9)$$

This is accelerated by Chebyshev extrapolation:

$$P_{\ell+1} = P_{\ell-2} + \alpha_{\ell+1} [P_{\ell-1} - P_{\ell-2} + \Gamma(P_{\ell}^i - P_{\ell-1})]. \quad (10)$$

Fig. 3. Spatial Power and Control on First and Last Iterations

The coefficients are generated recursively, as described by Curtis and Trylor:⁽³⁾

$$\alpha_{\ell+1} = \frac{4(2 - \mu)^2}{4(2 - \mu)^2 - \alpha_{\ell} \mu^2} \quad (11)$$

and

$$\Gamma = \frac{2}{2 - \mu}. \quad (12)$$

Optional linear acceleration has been provided, but has been found to converge less slowly.

As a test of convergence the overall multiplication factor is calculated;

$$k = \frac{\int \nu(z) \epsilon(z) [\Sigma_{f1}(z) + \Sigma_{f2}(z) \alpha'(z)] \phi_1(z) dV}{\int [\Sigma_1(z) \phi_1(z) - \nabla \cdot D_1(z) \nabla \phi_1(z)] dV}. \quad (13)$$

If k is not within the specified deviation from 1.0, a new void distribution and space-dependent cross sections are calculated, and the iteration process is repeated as shown in Fig. 2. The final converged control and power distributions are shown relative to the initial requested power distribution in Fig. 3.

For a reactor with many control rods which are not operated in a bank, no single unique solution exists because there are many control rod positions which satisfy the condition that the reactor must be exactly critical. Thus, the solution represents the true operating state in which a similar condition prevails.

Typical rates of convergence of the Power-Control Method are plotted in Fig. 4 for one-dimensional, two-group description of a large BWR with approximately 2 per cent neutron leakage. These cases represent different operating states of a 12-ft-diameter, 12-ft-long BWR. In steady-state starting calculations for dynamics studies,^(4,5) convergence of the pointwise multiplication to within 10^{-10} of 1.0 is achieved in less than 30 iterations (an iteration consists of steps 2 to 5, above). Xenon, Doppler, voids, and control rod positions are varied in each iteration. Similar speed and degree of convergence are not achievable with conventional methods. In one-dimensional, large-core test comparisons for a fixed control rod position and an assumed void content (spatial xenon and Doppler ignored), the WANDA and AIM flux solutions would not converge the power shape to 1 per cent in 100 iterations.

Fig. 4. Rate of Convergence of Power-Control Iteration Method for Various Test Problems

Near the end of a fuel-cycle interval, when few control rods remain in the reactor, the convergence rate depreciates. This can be accounted for by varying the acceleration factor μ on the basis of the average fraction of control rods inserted in the core. It has also been observed that the rate of convergence is a function of the negative power coefficient. A large negative power coefficient aids convergence. In BWR applications special provisions are made to vary the reactor power, the inlet flow, or the inlet temperature to simulate control of the reactor with these variables, or to achieve convergence in cases in which movement of the control rods will not converge the reactor multiplication to 1.0 in a specified maximum number of iterations.

Representation of Neutron Cross Sections

In representing the combined effects of voids, control rods, and long-term fuel irradiation, it is important to include void history dependence in the neutron cross sections. The dependence of the cross sections on moderator void history is particularly important because of the appreciable effect of voids on plutonium production and U^{235} destruction. A detailed analysis of an assumed separable reactor cell is a source for the cross-section data. The spectrum is calculated, and microscopic cross sections are energy- and space-weighted to obtain few-group macroscopic cross sections.

The cross sections are represented as polynomials in fuel exposure, isotopic composition, and relative water density defined as $U(z) = \rho(z)/\rho_{\text{sat}}$, where ρ is the effective water density including steam slip and subcooled boiling.

The isotopic compositions are represented as polynomials in the exposure-weighted relative water density, $UB(z)$, and fuel exposure. For example, the U^{235} concentration is expressed as

$$N_{25}(z) = \exp \left\{ a_0 + \frac{1}{1 + UB} (a_1 + a_2 E \cdot UB) + E [a_3 + a_4 UB^2 + E(a_5 + a_6 \cdot UB)] \right. \\ \left. + \frac{1}{1 + E} \left[\frac{a_7 \cdot UB}{1 + UB} + a_8 E + \frac{1}{1 + E} (a_9 + a_{10} \cdot UB) \right] + \frac{a_{11}}{UB^3} \right\}, \quad (14)$$

where E is the fuel exposure. This expression is accurate to a few tenths of a per cent for most BWR lattices.

As an additional example, the average thermal-fission cross section is expressed as

$$\Sigma_f = b_0 + b_1 U + \frac{b_2}{1 + U}, \quad (15)$$

where

$$b_0 = c_0 + N_{25}(c_1 N_{Pu} + c_2) + \frac{c_3}{(1 + N_{25})(1 + N_{Pu})} + \frac{c_4}{1 + E} \\ + \frac{c_5 N_{Pu}}{1 + FPU} + \frac{c_6}{(1 + N_{Pu})^2} + c_7 FPU^2; \quad (16)$$

$$b_1 = c_8 N_{25}; \quad (17)$$

$$b_2 = c_9 N_{25} + c_{10} N_{Pu}, \quad (18)$$

and where N_{Pu} and FPU are the total plutonium concentration and fissile plutonium fraction, respectively, which are represented by polynomials in UB and E .

The resonance capture is divided into fertile, nonfertile, and control rod components, which are represented by polynomials in the isotopic concentrations, voids, and exposure. The temperature dependence of Doppler broadening of U^{238} is represented by a third-order polynomial in $(\sqrt{T_{fuel}} - \sqrt{T_0})$.

Optimization Procedure

An optimization procedure has been developed to determine the optimum control rod positions to minimize the peak-to-average power or maximize the MCHFR (minimum critical heat flux ratio). Parameters describing the input power shape are varied to achieve the optimum condition. The points are successively added to a least-squares quadratic fit which is differentiated to predict the optimum shape-describing parameters.

Several input power-shape forms are allowed. A skewed, truncated sine power shape is one alternate. In this case the extrapolated distance becomes the parameter which is varied to achieve optimum conditions.

Optimizations are carried out either at a fixed level of fuel exposure or with variation of the fuel irradiation. The results of a constant fuel irradiation CHF optimization of a large, high steam quality BWR is shown in Fig. 5. Because of the steam-quality dependence of the CHFR, the optimum power shape is skewed to the bottom of the core.

In irradiation-dependent optimizations, a number of fuel-irradiation histories are followed to determine the optimum sequence of control rod withdrawal. On each fuel-irradiation trajectory the control rods are moved in an attempt to maintain a constant power distribution. The optimum for a BWR occurs when the fuel irradiation is spatially distributed so as to compensate for withdrawal of the bottom-entry control rods and provide limiting thermal conditions which are approximately independent of fuel irradiation.

Fig. 5. Large BWR, Constant Fuel-exposure Optimization

The results of a fuel-irradiation optimization are shown in Fig. 6, which illustrates the dependence of limiting thermal conditions on core-averaged fuel exposure. The method converges to a pattern of control rod withdrawal which results in an average axial peak-to-average that is independent of fuel irradiation and a CHF_R (B/O Ratio) which varies slightly because of the position of the peak.

The MCHF_R is difficult to optimize because of steam-quality dependence which makes it power-shape sensitive. The MCHF_R variations in a typical exposure-dependent optimization are shown in Fig. 7. Trajectory B is the typical result of distributing the fuel exposure incorrectly, early in fuel irradiation history.

A typical optimum end-of-life power shape with most of the control rods withdrawn is shown in Fig. 8.

In three dimensions the perturbations caused by the control rods make exposure-independent thermal conditions difficult to achieve. However, the one-dimensional optimization provides a guide for optimal spatial distribution of the control rods in three-dimensional analyses.

The method has also proven useful for spatial xenon transient analyses. Special provisions have been made to maintain criticality with recirculation flow, inlet temperature, or reactor power. A Lagrangian interpolation polynomial is used to converge on values of these parameters which produce a critical condition.

Acknowledgment

The author wishes to thank W. H. Wolf for his assistance in programming the Power-Control Method for computer solution.

Fig. 6. Fuel-exposure-dependent Optimization

Fig. 7. CHF-exposure Trajectories from Optimization

Fig. 8. End of Cycle Power Distribution with Most Control Rods Withdrawn

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Discussion of Paper Presented by Mr. Crowther

MR. SHAFTMAN (Argonne National Laboratory): My first question relates to the definition of k in one of your figures. Was that done just for convenience without any adjoint-weighting, or is it simply some sort of a convergence parameter rather than the multiplication factor?

MR. CROWTHER: The actual multiplication is given as

$$k = \frac{\int_{v \in} \sum_g \Sigma_{fg} \phi_g \, dv}{\int (\Sigma_{R_1} \phi_1 - \nabla \cdot D_1 \nabla \phi_1) \, dv},$$

which is just the solution of the diffusion equation.

MR. SHAFTMAN: I don't think that is the way k is normally defined. The other question relates to this matter of getting a trajectory, locally in time, optimized. If you locally optimized, you might be very far off the optimum trajectory. Are there some ways that control where they come closer together, that is, where the local optimization comes closer to the optimum trajectory?

MR. CROWTHER: By local, do you mean the optimization at any point in time?

MR. SHAFTMAN: Yes.

MR. CROWTHER: This depends on the specific characteristics of the reactors of concern. You'd like to select the average, the one which divides the maximum power capability of the reactor, considering all time.

MR. SHAFTMAN: Do you find, in general, that locally optimizing gives you a very poor approximation to the overall optimum trajectory?

MR. CROWTHER: Normally this is true. The entire radiation history should be examined before selecting the optimum. I think this is the normal way of defining the eigenvalue in the solution of diffusion equations: set the norm, for which there is no problem. I don't see where the adjoint comes in.

MR. SHAFTMAN: This is an overall neutron balance where no distinction is made between neutrons of different energies. Normally, this is where the adjoint would come in. You can define it in this way for a bare reactor, but in your case, where you do not have a shape which is independent of neutron-group index, I don't think that is the proper definition.

MR. CROWTHER: This integral is carried out only over the region in which it is nonzero. I think it is the normal way of defining it.

A COMPUTER CALCULATION OF THE ENERGY YIELD PRODUCED BY A HYPOTHETICAL FAST REACTOR ACCIDENT

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(Paper presented by L. M. Russell)

1. Introduction

There is at Aldermaston a zero-energy fast reactor, VERA, which is used in various integral experiments and can accommodate a variety of cores. In the consideration of the safety aspects of this reactor and the possible yield from an excursion, some calculations were done using Bethe-Tait⁽¹⁾ theory. However, it was felt that these should be confirmed by more accurate calculations. Accordingly a computer code, later called COOT, was put together. The code is written in the S2 language,⁽²⁾ the AWRE dialect of Fortran II for the IBM-7030. In general principles the code is similar to the AX-1 code⁽³⁾ and is at the moment still a little unsophisticated in its overall control, owing to the manner in which it was put together. However, this has enabled us to gain some experience with the factors which should be taken into account. We have been able to investigate the effect of changing the equation of state used for the core material. This is important since it can affect greatly the amount of kinetic energy produced, as well as changing the total energy yield.

2. The Code

In a coupled hydrodynamic-neutronic code there is a problem in that the hydrodynamics requires knowledge of the energy-release rate as a function of time, which is derived by the neutronics, whereas the neutronics requires knowledge of the material density as a function of radius, which is obtained by the hydrodynamics.

In COOT this problem is solved by predicting the neutronic state at some future time, using this prediction to advance the hydrodynamics up to this time, and then calculating the actual neutronic state. This process completes a (neutronic) time step, and the code then proceeds on to the next step. For the prediction we assume that α , the time constant or inverse period, is a quadratic function of t , the time. The quadratic, obtained by fitting to the last three calculated values of α , is then used for two purposes. Firstly, the neutronic time step is chosen by solving the equation

$$\Delta G = \int_{t_a}^{t_b} \alpha(t') dt' , \quad (1)$$

where t_a is the time at the beginning and t_b the time at the end of the time step. The ΔG need not be all the same, are part of the data for the problem, and can be chosen by the user. Thus, the neutron population is allowed to rise (or fall) by a factor $\exp(|\Delta G|)$ in a time step. Secondly, the quadratic is used to extrapolate the energy-release rate $\dot{E}(t)$ forward over the time step:

$$\dot{E}(t) = \dot{E}(t_a) \exp \left\{ \int_{t_a}^t \alpha(t') dt' \right\}. \quad (2)$$

The energy-release rate is then used to advance the hydrodynamics to the end of the step so that the neutronics can be calculated. This gives a calculated value of α which is used together with the two previous calculated values of α to form a new quadratic and, hence, a calculated ΔG_C . Thus the neutron population at the end of the time step is known, and by comparing ΔG and ΔG_C , the accuracy of the prediction can be checked.

The difference equations used for the hydrodynamics conserve energy, in the sense that for any cell the sum of the internal energy, the kinetic energy, and the net work done by the cell on its neighbors will exactly equal the energy released into that cell by fission. The equations are given in detail in the Appendix.

The equations are solved in a natural order. All data at the beginning of the time step is known. By means of a guessed pressure the acceleration is calculated, and from that the velocity and radius of the mesh point are obtained. When all mesh points have been processed, the cell density is calculated, and also the work done on the cell. Hence, the internal energy is known, and the material pressure is obtained from the equation of state. Should the cell be in the process of being compressed, the viscous pressure can be calculated and added to the material pressure to give the total pressure. In order to achieve consistency and accuracy (but not energy conservation), the pressure obtained from the equation of state should be the same as that used in obtaining the specific internal energy. Therefore the whole set of equations is iterated until the pressure converges. This, in fact, only takes one or two iterations. The iteration must comprise the whole set of equations, since an iteration round the energy equation alone would not preserve the correct balance between kinetic and internal energy. Similarly, if no iteration were allowed, the kinetic and internal energies could be calculated using pressures with large errors. It will be noticed from the equations that shocks are treated by using the well-known technique of Richtmeyer and von Neumann⁽⁴⁾ of smearing them out by including a pseudo-viscous term.

The control scheme allows the hydrodynamics to take more than one step while proceeding from one neutronic calculation to the next should it desire to do so. By examining the behavior of errors during the pressure

iteration, a criterion can be obtained which determines the maximum time step for which the iteration will converge. This is the equivalent of a stability condition for noniterative procedures. It is found that the time step must satisfy either

$$a \Delta t < \Delta r$$

if no viscous term is present or

$$a^2 \Delta t^2 + b^2 \Delta u^2 \Delta t^2 + 4b^2 \Delta u \Delta r \Delta t < \Delta r^2$$

if there is a viscous term. Here a is the velocity of sound and b the coefficient of the viscous term. The first condition is seen to be identical with the normal Courant stability condition.

The neutronics is calculated by the S_n method.⁽⁵⁾ The version of the equations used includes the modification⁽⁶⁾ which ensures conservation of neutrons as they travel outwards. Delayed neutrons are neglected. The usual assumption of isotropic scattering is made. The nuclear data used are obtained from UKAEA nuclear-data file,⁽⁷⁾ being put into group-constant form either by CANDY⁽⁸⁾ or its successor GALAXY,^(9,10) and taken by COOT from the standard binary tape used by other AWRE multi-group codes. The radial mesh used for the neutronics calculation need not be the same as that used for the hydrodynamic calculation. A certain amount of interpolation has therefore to be done in order to interchange information between the two parts of the code. But this does mean that, for instance, the neutronic mesh can be fine if needed without causing the hydrodynamics to take small time steps or, alternatively, some hydrodynamic phenomenon can be observed in detail without increasing the machine time spent computing in the neutronics. Both neutronic and hydrodynamic mesh points are regarded as being fixed in the material, so that material interfaces always remain at the same mesh point.

3. The Model

VERA is a zero-energy reactor and is not subject to the same modes of failure as a power reactor. In this investigation into the size of the energy yield from an excursion, it was envisaged that the excursion would occur because of a continual addition of reactivity by control rod movement of 0.2 dollar per second. Since this rate of addition is low, delayed neutrons are important in the early stages of the excursion, which could not therefore be calculated by COOT. A simpler code was therefore used to calculate the interval between delayed and prompt critical, and the COOT calculations normalized to start with the period and power given by the simpler code.

To give the rate of increase of reactivity the whole system was given an initial velocity so that it was compressing uniformly. The velocity is

maintained until the pressure generated by the energy released from fission starts the disassembly process. The material density at the time the disassembly process starts is thus greater than in the initial state, but the difference is negligible.

4. Equations of State

The code requires an equation of state in the form

$$P = P(e, \rho),$$

where e is the specific internal energy and ρ the material density. During an excursion the overall density at a given point will not change greatly, but the pressure can reach several kilobars. At the peak pressure the core may be either partially vaporized or a compressed liquid, according as the energy is less or greater than that given by the saturation curve at that density. It is assumed that the saturation curve can be represented in the energy-density plane by a series of straight lines, and two lines appeared to be adequate in this case.

For energies below the saturation curve the liquid and vapor phases coexist, and the temperature and pressure are related by the Clausius-Clapeyron equation

$$\frac{dP}{dT} = \frac{L\rho_1\rho_2}{T(\rho_1 - \rho_2)}, \quad (3)$$

where P is the saturation pressure, T the temperature, L the latent heat of vaporization, and ρ_1 and ρ_2 the densities of the liquid and vapor phases, respectively. The vapor can be regarded as a perfect gas whose density is small compared with the density of the liquid. The latent heat is assumed constant. With these assumptions Eq. (3) can be integrated to give

$$P = P_0 \exp\left\{\frac{L}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right\}, \quad (4)$$

where P_0 and T_0 are a corresponding pressure and temperature. If T_0 is the boiling point, P_0 is one atmosphere.

If α is the mass fraction of material in the vapor phase, then

$$\frac{1}{\rho} = \frac{1 - \alpha}{\rho_1(T)} + \frac{\alpha}{\rho_2(T)} \quad (5)$$

and

$$\begin{aligned} e &= (1 - \alpha) e_1(T) + \alpha e_2(T) \\ &= e_1(T) + \alpha(L - RT), \end{aligned} \quad (6)$$

where subscripts 1 and 2 refer to the liquid and vapor phases as before. These equations would normally have to be solved simultaneously but, since only a small amount of material will be in the vapor phase,

$$e = e_1(T) \quad (7)$$

is a good approximation to Eq. (6), and Eq. (5) is then redundant. For liquid metals it is usually assumed that specific heat is constant, so that $e_1(T)$ is a linear function of T . This assumption is not true in the solid phase, but the properties of this phase are not important in an excursion. The thermodynamic data given by Stull and Sinke⁽¹¹⁾ have been used. Grosse and his co-workers have shown that the densities of many liquid metals, and in particular of uranium,⁽¹²⁾ are linear functions of the temperature. This fact together with the assumed constancy of the specific heat justify the linearity of the saturation curve for the range in which it is actually used. Oben, Sandenow, and Herrick's data⁽¹³⁾ were used for the density of liquid plutonium.

When the energy is greater than that on the saturation curve, an equation of the Grüneisen form is used for the pressure:

$$P = \gamma \rho \{e - f(\rho)\} + P_2(T), \quad (8)$$

where $f(\rho)$ is the energy on the saturation curve and $P_2(T)$ is the vapor pressure from Eq. (4), with T the solution of

$$e_1(T) = f(\rho). \quad (9)$$

5. Results of Calculations

The core of VERA consists of steel and graphite as well as fissile material, and a certain amount of voidage. Two simplified cores were considered with fissile materials 93% enriched uranium and plutonium, respectively. For the uranium core two equations of state were used; one assumed that heat produced in the uranium is distributed locally between the component materials in a time short on the time scale of the excursion; the other equation of state goes to the other extreme and assumes that there is no heat conducted out of the uranium, and the steel and graphite remain cold. The second is, in fact, much more realistic. The assumptions change not only the specific heat, but also the position of the saturation curve.

For the equation of state with perfect local heat conduction, the total energy yield was 2.93×10^8 Joules, of which 76% came before the disassembly process started and only one part in a million went into kinetic energy. None of the core materials reached boiling point, and the excursion was terminated by the expansion filling the voids and then pushing the core apart. The pressures, although comparatively high, act only for a short time, and so the kinetic energy is low.

When the second equation of state is used, the uranium boils before the voids close and the excursion is terminated by the vapor pressure. The total energy yield is lower, 1.14×10^8 Joules, 64% of which came before the disassembly process began. At the end of the calculation the kinetic energy was still increasing. In this case the pressures did not rise to such high values, but acted for a long time and at the end of the calculation were still acting.

Owing to the assumption that the mass fraction in the vapor phase is negligibly small, both the effect that expansion would have on the vapor pressure and also the energy absorbed as latent heat have been ignored. Therefore, if the calculation were continued after the cessation of the nuclear energy release, the equation of state would become invalid. The continuation would also require the use of a large amount of computer time. However, the following simple theory enables the final amount of kinetic energy to be estimated.

The specific entropy s is the weighted average of the specific entropies of the liquid and vapor, s^l and s^v :

$$\begin{aligned} s &= (1 - \alpha) s^l + \alpha s^v \\ &= s^l + \alpha(s^v - s^l) \\ &= s^l + (\alpha L/T). \end{aligned}$$

Along an adiabat the total entropy is constant, so that

$$\begin{aligned} \frac{\alpha_2 L_2}{T_2} - \frac{\alpha_1 L_1}{T_1} &= s_1^l - s_2^l \\ &= \int_2^1 \frac{C_{sat}^l}{T} dT, \end{aligned} \tag{10}$$

where the subscripts 1 and 2 denote initial and final states, respectively. Here C_{sat}^l is the specific heat of the saturated liquid, defined as

$$C_{\text{sat}}^{\ell} \equiv T \left(\frac{\partial s^{\ell}}{\partial T} \right)_{\text{sat}} = C_P^{\ell} - T \left(\frac{\partial v^{\ell}}{\partial T} \right)_p \frac{dp_{\text{sat}}}{dT}.$$

If initially all the material is liquid and if also the thermal expansion coefficient of the liquid is sufficiently small, Eq. (10) simplifies to

$$\alpha_2 = \frac{T_2}{L_2} C_P^{\ell} \ln \left(\frac{T_1}{T_2} \right). \quad (11)$$

The change in internal energy which accompanies this drop in temperature and production of vapor follows from Eq. (6). It is

$$e_2 - e_1 = \int_1^2 C dT + \alpha_2 (L_2 - RT_2),$$

where

$$\begin{aligned} C &\equiv \left(\frac{\partial e^{\ell}}{\partial T} \right)_{\text{sat}} \\ &= C_P^{\ell} - p \left(\frac{\partial v^{\ell}}{\partial T} \right)_p - \frac{dp_{\text{sat}}}{dT} \left[p \left(\frac{\partial v^{\ell}}{\partial p} \right)_T + T \left(\frac{\partial v^{\ell}}{\partial T} \right)_p \right]. \end{aligned}$$

Approximately,

$$e_2 - e_1 = C_P^{\ell} (T_2 - T_1) + \alpha_2 (L_2 - RT_2). \quad (12)$$

The first term on the right-hand side of Eq. (12) is just numerically equal to the energy absorbed by the core when its temperature rose from T_2 to T_1 . However, during the subsequent adiabatic expansion, only a fraction, f say, of this energy is released, the remainder being absorbed by the vapor produced. From Eqs. (11) and (12),

$$f = 1 - \left(1 - \frac{RT_2}{L_2} \right) \frac{T_2 \ln(T_1/T_2)}{T_1 - T_2}. \quad (13)$$

Only this fraction of the energy which was needed to heat the core up to the temperature T_1 can appear as destructive work. Fortunately, a reactor core exploding in this manner is a rather inefficient heat engine, and the fractions involved turn out to be small. The factor $[1 - (RT_2/L_2)]$ is slowly varying and has a value 0.917 for uranium when T_2 is the boiling point (4200°K). Therefore, only 2.1% of the energy generated in the core by fission can appear as kinetic energy in the core and reflector.

For the plutonium core, only the form of the equation of state which assumes no heat conduction was used. The total energy yield was 2.6×10^7 Joules, of which 55% came before the plutonium boiled. The final amount of energy which could appear as kinetic energy was estimated by the theory above as 0.36% of the total fission energy yield. The lower energy yield from this core arises because the mass of fissile material is smaller and the energy needed to reach boiling point of the plutonium is less than that required for uranium.

6. Acknowledgment

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APPENDIX

Hydrodynamic Difference Equations

In the equations

r_i = radius of the mesh point i

u_i = velocity of the mesh point i

$\dot{u}_i$ = acceleration of mesh point i

$P_{i+1/2}(1)$ = guessed or predicted pressure in cell $i + 1/2$ (the cell between mesh points i and $i + 1$)

$P_{i+1/2}(2)$ = calculated pressure in cell $i + 1/2$

$V_{i+1/2}$ = volume of cell $i + 1/2$

$\rho_{i+1/2}$ = density of cell $i + 1/2$

$M_{i+1/2}$ = mass of cell $i + 1/2$

$M_i = (M_{i-1/2} + M_{i+1/2})/2$

$W_{i+1/2}$ = work done on cell $i + 1/2$

$e_{i+1/2}$ = specific internal energy in cell $i + 1/2$

$F_{i+1/2}$ = fission energy released in cell in the time step

δt = time step

Superscripts 0 and 1 denote values at the beginning and end of the time step, respectively.

The equations are solved in the order given starting with the acceleration equation:

$$M_i \dot{u}_i^1 = 4\pi(r_i^1)^2 \{P_{i-1/2}^1 - P_{i+1/2}^1\}$$

$$u_i^1 - u_i^0 = \{A_i \dot{u}_i^0 + B_i \dot{u}_i^1\} \delta t$$

$$A_i = \frac{r_i^0 + 2r_i^1}{3(r_i^0 + r_i^1)}$$

$$B_i = \frac{2r_i^0 + r_i^1}{3(r_i^0 + r_i^1)}$$

$$r_i^1 - r_i^0 = [(u_i^0 + u_i^1)/2] \delta t$$

$$W_{i+1/2} = 4\pi P_{i+1/2}^0 \{A_i(r_i^0)^2(r_i^1 - r_i^0) + A_{i+1}(r_{i+1}^0)^2(r_{i+1}^1 - r_i^0)\} \\ + 4\pi P_{i+1/2}^1 \{B_i(r_i^1)^2(r_i^1 - r_i^0) + B_{i+1}(r_{i+1}^1)^2(r_{i+1}^1 - r_i^0)\}$$

$$e_{i+1/2}^1 - e_{i+1/2}^0 = \frac{W_{i+1/2} + F_{i+1/2}}{M_{i+1/2}}$$

$$V_{i+1/2}^1 = \frac{4\pi}{3} \{(r_{i+1}^1)^3 - (r_i^1)^3\}$$

$$\rho_{i+1/2}^1 = M_{i+1/2} / V_{i+1/2}^1$$

$$P_{i+1/2}^1(2) = P(e_{i+1/2}^1, \rho_{i+1/2}^1) + Q_{i+1/2},$$

where $P(e, \rho)$ is the equation of state, and

$$Q_{i+1/2} = b^2 \rho_{i+1/2}^1 (u_i^1 - u_{i+1}^1)^2 \quad \text{if } u_i^1 > u_{i+1}^1 + 1 \\ = 0 \quad \text{if } u_i^1 < u_{i+1}^1 + 1$$

Discussion of Paper
Presented by Mr. Russell

MR. FISCHER (Argonne National Laboratory): When you go to the vapor phase you have available, perhaps, only about 10% more volume than the solid occupies. Since the interatomic distance is so very short, I wonder about the validity of using the Clausius-Clapeyron equation at this very critical time in the history of the accident. Could you comment?

MR. RUSSELL: We thought it was alright.

MR. FISCHER: At Argonne we tried using the Van der Waals gas model in this kind of a situation. We made the mistake of putting in a few check points to see whether we could believe the applicability of the Van der Waals model, and it was embarrassing.

For the liquid phase you used the Grüneisen equation, as I have also tried. What confidence do you put in your determination of the coefficient? How do you go about it? It's a simple harmonic oscillator model; if you use the coefficients of the cold crystal then you are, probably, very far off from where you should be.

MR. RUSSELL: Yes, it is difficult, particularly for our mixture of three different materials. We do have a fair degree of confidence.

MR. OKRENT (Argonne National Laboratory): You mentioned that one chooses this step in change in power between new neutronic calculations. Is this something that is input information?

MR. RUSSELL: Yes, that is, at the moment, input information. This is not satisfactory.

MR. OKRENT: I was curious how one made this satisfactory without knowing the course of the accident.

MR. RUSSELL: We stop the calculation occasionally. I think it should be possible to automate this.

MR. OKRENT: I think the feature of guessing ahead the way alpha will be changing is an improvement over the previous codes. I wasn't quite sure how you would make this feature work.

MR. GRIMES (Reactor Licensing, USAEC): If there is no further comment on this paper I would like to comment on an earlier paper for which we ran out of discussion time. The first paper this morning treated only the computational problems involved in reactor transients. We have another accident of current concern which is the coolant-loss accident, initiated by a primary system break. Some of the computational problems associated with the accident are: the determination of the initial temperature of the fuel elements after the blow-down, and incorporation in the calculation of the metal-water reaction along with the resultant heat contribution to the core heatup. The degree of metal-water reaction will depend on steam availability to the core, which will depend on the geometry of the system and the position of the break. A third problem is the transfer of the core heat to the containment. This can be by a core spray mechanism or, perhaps, by the core slumping into a pool of water in the bottom of the primary vessel. An associated problem is the hydrogen evolution from the metal-water reaction and how it is distributed or burned in the containment. An IDO document by the Phillips Company is forthcoming, I believe, which considers the metal-water reaction and associated computational problems, in some detail. I believe this was undertaken by Phillips for the LOFT project.

SESSION VI

MONTE CARLO COMPUTATIONS

Wednesday, May 19, 1965

CHAIRMAN: L. H. Underhill
UKAEE, Winfrith--United Kingdom

CO-CHAIRMAN: Robert R. Coveyou
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THE PROCESSING OF NUCLEAR DATA FOR REACTOR CALCULATIONS

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ABSTRACT

The nuclear data used in reactor calculations are outlined, particular emphasis being given to neutron cross sections. Problems involved in converting nuclear physics measurements and calculations into a form suitable for use in reactor calculations are discussed. The need for computer processing of the data is demonstrated. Examples of existing punched card/magnetic tape libraries of microscopic neutron cross sections and associated computer processing codes are described. The desirability of international cooperation in the exchange of libraries and processing codes is discussed as a logical consequence of the scale of effort involved. The concept and development of the Evaluated Nuclear Data File at Brookhaven National Laboratory as an effort in this direction is described. The paper concludes with a discussion of likely developments during the next few years.

1. INTRODUCTION

1.1 Classification of Nuclear Data Used in Reactor Calculations

The vast variety of measured and calculated quantities which can be classified as nuclear data can be seen from the directory to nuclear-data tabulations published by Gibbs and Way.⁽¹⁾ Many quantities such as magnetic moments are of little or no importance in reactor calculations, but the amount of data that must be considered is still formidable, including, as it does, the following:

- neutron cross sections - including cross sections for neutron transmission, production, disappearance, etc., and for the production of photons;
- photon cross sections;
- fission product yields;
- delayed-neutron yields;
- nuclidic abundances, masses, and binding energies;
- energy levels and decay schemes;
- penetration of charged particles through matter.

A casual inspection of the standard data tabulations for any of these quantities reveals a vast amount of material whose handling by manual means is a daunting task. It is therefore not surprising that during the last few years there has been a trend towards computer handling of the large amounts of data involved. This trend would doubtless have occurred even if nuclear physics had no practical applications. In fact, the rapid development of computers has, in turn, led to a rapid increase in the size and complexity of neutronics and other reactor calculations, and this in turn has created a demand for the large amounts of data input which many of the more sophisticated reactor codes require.

It is important to distinguish between nuclear data which are measured and/or calculated by nuclear physicists and those which are input to reactor codes. The former are limited by the current capabilities of experimental techniques and theory. In the latter case a minimum amount of data must be provided or the code will fail to function, and where measurements or calculations do not exist then input numbers must be estimated in some way. This difference is most clearly seen in the case of neutron cross sections. In a Monte Carlo calculation of, say, the slowing down of 14-MeV neutrons in uranium, it is possible for collisions to occur at all energies from 14 MeV down to thermal, and sufficient data must be available not only to determine the chance of a collision for a neutron of any energy between thermal and 14 MeV, but also to determine (statistically) the number, direction of motion, and energy of secondaries in a collision at any incident neutron energy. Much of the necessary data may be very poorly determined, or may not have been measured or calculated at all.

Nuclear data can then be classified as follows for the purposes of reactor calculations:

- (a) results of individual measurements or calculations;
- (b) compilations - being collections of all measurements and/or calculations in a particular field - results being given in essentially the same form as in the original reference;

- (c) partial evaluations in which numbers of related measurements have been analysed and synthesised to produce self-consistent "best" values in some sense complete;
- (d) complete evaluations which are intended as direct or indirect input to reactor codes and in which values are given for all input parameters required by the particular code(s). Some values may have been obtained by interpolation, "guesstimating," and so on;
- (e) processed data, the result of processing fully-evaluated data into a form (differing from the basic nuclear physics form) more convenient for use in reactor codes. A well-known example of processed data is neutron group cross sections for use in transport-theory codes. Fully evaluated microscopic neutron cross sections in essentially the same form as the original experimental measurements are averaged over energy to give group cross sections.

Computers are used in deriving and/or handling all five classes of nuclear data. In this paper it is possible to discuss in detail only a limited part of the field, namely, neutron cross sections and, in particular, the handling of evaluated neutron cross-section data. However, it is in just this area that the application of computers is probably most advanced, and so this specialization is less restrictive than might first appear.

1.2 Handling and Processing of Neutron Cross-section Data

It is useful to outline the application of computers to the five classes of neutron cross-section data distinguished in Section 1.1.

The use of on-line computers in making neutron cross-section measurements is spreading rapidly and was the subject of a conference held at Karlsruhe in July 1964.⁽²⁾ The pioneering work of A. B. Smith and co-workers at Argonne National Laboratory deserves special mention. The calculation of neutron cross sections on the basis of the optical model and statistical theories of the nucleus is well known. Computer codes such as LOKI,⁽³⁾ SCAT,⁽⁴⁾ ABACUS,⁽⁵⁾ and HFS⁽⁶⁾ have been widely used to fill gaps in our knowledge of the variation of neutron cross section with energy in the low-MeV range. Other codes have been developed to analyze experimental data and derive resonance parameters.

The compilation of neutron cross sections has been undertaken at Brookhaven National Laboratory and at Lawrence Radiation Laboratory, Livermore, for many years. The rapid increase in the amount of data available has led to the setting up of the ENEA Neutron Data Compilation Center at Saclay. Most workers in this field are now using computers to handle

the vast amount of data involved. At Livermore Howerton has transferred his library of experimental neutron cross sections⁽⁷⁾ and angular distributions⁽⁸⁾ (1 keV to 14.5 MeV) to magnetic tape, and developed searching and retrieval codes for particular types of data. The Sigma Center at Brookhaven is developing SCIRS⁽⁹⁾ ("Sigma Center Information Storage and Retrieval System") for storing measured and calculation neutron cross section data on magnetic tape. Again searching and retrieval routines are available. The Saclay center is likely to adopt this or some similar system.

The work of compilation centers is of great importance for the evaluation of neutron cross sections. At best they provide a vast amount of the numerical data involved in a compact and ordered form. Further information is often available in the literature, and CINDA⁽¹⁰⁾ ("Computer Index Neutron Data") has been developed by Goldstein, Kalos, and co-workers to provide an ordered, mechanized bibliography of the literature which neutron cross-section evaluators need to consult. Briefly, details of appropriate references are written on punched cards by numbers of readers covering different areas of the literature. The cards are transcribed to magnetic tape, and listings ordered by nuclide and reaction type are prepared by search codes. The evaluations of neutron cross sections which are available differ greatly in quality and quantity, but good evaluations may provide complete information on the interactions of neutrons with a nuclide in the energy range from 0.001 eV to 15 MeV. Large amounts of data are concerned, and the repeated input of this data to neutronics codes by manual methods is very inefficient. As a result, many evaluations have been represented on punched cards/magnetic tape in a form convenient for further processing. A number of mechanized neutron cross-section libraries are reviewed in Section 2.

Processed data in the neutron cross-section field generally means group-averaged cross sections. Even when available on magnetic tape evaluated microscopic neutron cross sections are not necessarily directly usable in reactor calculations. Although Monte Carlo and certain other calculations can use the contents of the evaluated libraries directly, most deterministic methods of solving the neutron transport equation involve the use of group approximations, and it is necessary to calculate weighted energy averages of the continuously varying microscopic cross sections. These calculations may involve large numbers of neutron-energy groups and complex weighting prescriptions, and the use of large computers to calculate group cross sections is increasing rapidly.

The brief discussion given above should make clear that if the reactor designer desires to make not only sophisticated calculations, but correct sophisticated calculations, then considerable effort must be expended on collecting, evaluating, handling, and processing nuclear data. Several steps are required to go from a measurement of a neutron cross section to a parameter which can be used directly in a design calculation. The methods

of the forties and fifties for handling nuclear data are just not appropriate any longer. This is already largely recognized in the field of cross-section measurement where EANDC coordinates a large program of work at many laboratories. It is increasingly recognized in the evaluation field, although many data-evaluation and processing problems remain to be solved.

It is now appropriate to discuss some existing nuclear data libraries and processing codes in more detail.

2. REVIEW OF EXISTING MECHANIZED NUCLEAR-DATA LIBRARIES

2.1 General

Many laboratories have developed mechanized nuclear-data libraries. Their contents are mostly evaluated neutron cross sections, but in some cases other data are included. Unfortunately for any reviewer, details of many systems have not been published, and a balanced discussion is therefore impossible. However, it is possible to bring out the advantages and limitations of mechanized nuclear-data libraries by describing the main features of a few systems. It seems likely that some 10 to 20 different systems are currently in use, and some of these are used at several laboratories.

The main features of any library can be described under the following headings:

- (a) methods used to evaluate the data;
- (b) format for representation of the data;
- (c) ancillary codes for checking, copying, revising, and general handling of data in the library format;
- (d) processing of data in the library format to give the input to reactor codes.

The methods used to evaluate the data will not be discussed further. A summary of UKAEA practice is given by Story et al.⁽¹¹⁾

The precise choice of punched card/magnetic tape format is of great importance. It must allow for the entry of data in a relatively simple way and yet provide an economical means of feeding the many ancillary and processing codes which are likely to be developed. Experience suggests that input/output operations are crucial as far as computer time is concerned, and while the use of BCD (binary coded decimal) mode makes card-to-tape transfer simple, the availability of an alternative binary-mode representation can often result in substantial saving of machine time needed to operate ancillary and processing codes.

The development of ancillary codes is essential if the handling of library material is to be a manageable task. The detection of random punching errors should be done mechanically in so far as possible.

As already mentioned, processing codes are generally needed if the library data are to be put to real use.

An important corollary of the foregoing discussion is that the inauguration and efficient use of a mechanized library of microscopic neutron cross sections is a formidable and time-consuming task, requiring an immense effort before the system becomes usable in any way. This no doubt accounts for the fact that many laboratories have fought shy of entering this field and have settled for the simpler, but less flexible, approach of using standard sets of group cross sections. Unfortunately, this approach renders difficult any appraisal of the effect on calculations of errors in the basic microscopic cross sections. Given a mechanized library and a flexible group-cross-section-formation code, one can more easily study the effect of group structure in any particular calculation and separate the uncertainties due to use of the particular group approximation from those due to the use of poor neutron cross sections. The comparison of basic data libraries is also much easier than the comparison of group-cross-section libraries. The authors are convinced that group cross sections should be derived in a precise, reproducible way from specified comparable libraries of microscopic neutron cross sections, so that the assessment of calculation results can be done in a much more precise way.

There follows an outline of four existing mechanized libraries which illustrate many of the principles and difficulties involved. The following discussion (see Sections 2.2-2.6) relates past experience to some present and possible future developments described in Sections 3 and 4.

2.2 The UKAEA Nuclear Data Library

A concise description of the UKAEA Nuclear Data Library and its associated ancillary and processing codes was given by Story *et al.*⁽¹¹⁾ The library formats and conventions have been developed from 1961 onwards and supersede the earlier AWRE Punched Card Library of Neutron Cross Sections.⁽¹²⁾ It is interesting that the binary representation of data and use of machine language (IBM-704/709/7090) codes has been replaced by a BCD representation of data used in conjunction with FORTRAN codes.

A full description of the format has been given by Parker.⁽¹³⁾ It is sufficiently flexible to allow the inclusion of many different kinds of reaction data in point-by-point tabulations or in parametric forms. Three-dimensional arrays may be included, such as the scattering law $S(\alpha, \beta)$ considered as a function of temperature. Data are first classified into thirteen general classes, which include cross sections for neutrons and photons,

angular distributions and energy spectra of secondaries, neutron resonance parameters, statistical parameters for the unresolved resonance range, and thermal scattering laws. Next, there is a particular classification by reactions so that, for example, the neutron total cross section is distinguished from that for the $(n,2n)$ reaction.

Every set of data in the library constitutes a file organized into several sections of which the first is an index to the nature and number of data in that file. Most files contain some redundant information designed to facilitate checking. Each file is labeled with a data file number; when a revised set of data is prepared for the same substance, then a new data file number is used. It is generally desirable to keep both sets in the library for a considerable time so that reactor physicists can make comparative calculations.

While the library still consists mostly of point value tabulations, increasing use is being made of parametric forms from which point values can be obtained by means of subsidiary codes. Firstly, many parametric forms, such as resonance parameters, represent the natural output of nuclear physics experiments and, secondly, the use of parametric forms can yield a great saving of storage space within the library. Against these advantages must be set the disadvantage of having to write codes which will take parametric data and generate secondary data libraries containing only point values for particular material temperatures; alternatively, it is necessary to develop more complicated processing codes for the production of group cross sections, collision probabilities, and the like. A number of codes for handling parametric data are associated with the UKAEA Library. These include LEAP⁽¹⁴⁾ and PIXSE⁽¹⁵⁾ for handling thermal-scattering-law data, and GENEX, which is used to calculate Doppler-broadened cross sections from resonance data input in the library format; a subsidiary code RESP is used to sample for resonance parameters in the unresolved region by use of statistical data. GENEX is the subject of another paper presented at this meeting.⁽¹⁶⁾

The day-to-day administration of the library and the handling of data requests are greatly facilitated by the availability of a number of ancillary codes written in FORTRAN language.

EDITOR⁽¹⁷⁾ permits the reordering of data files on magnetic tape with the option of adding further data files from punched cards. Although the translation from cards to tape can be accomplished by standard peripheral equipment, EDITOR is of great use in meeting requests for particular selections of data files and in economizing in the use of magnetic tape.

IDA⁽¹⁸⁾ modifies the contents of a library tape by adding, subtracting, or altering records, and is used to correct data which have already been copied from cards to tape.

REFORM⁽¹⁹⁾ accepts point values of cross sections prepared in a simplified format for ease of punching and reproduces them on punched cards in the library format.

CHECK⁽²⁰⁾ applies a great variety of logical and arithmetical tests to the contents of a given data file. For example, the sum of partial cross sections is compared with the total cross section at each energy point, the energy points are checked for monotone increase, and the index is checked against the contents of the file. Large numbers of punched cards are used in preparing a file, and a number of punching errors must be expected. It is far better to check the accuracy and self-consistency of the data before use rather than to experience frustrating halts in the processing codes. The average number of errors found by CHECK is about 5 per 1000 cards.

NDF PRINT⁽²¹⁾ prepares annotated listings of library data in an easy-to-read form. Output is on magnetic tape in BCD format, and prints can be obtained at will on peripheral equipment. They are of great help to users who wish to make a detailed study of the data in tabular form.

GROD⁽²²⁾ is a code used with an IBM-7030 and an associated SC 4020 high-speed microfilm recorder to obtain a graphical representation of data presented in tabular form in the library format. The output is thus complementary to that of NDF PRINT; examples are given in a report on the data file for titanium.⁽²³⁾

A number of processing codes use the UKAEA data library as input. The rather specialized codes RESP, GENEX, and PIXSE have already been mentioned. GALAXY and DICE are rather more general codes designed in conjunction with the library to satisfy the input requirements of multigroup neutronics codes and of Monte Carlo codes, respectively. In both cases the aim is to make full use of all the data in the library and to develop very flexible output facilities. Thus, GALAXY is designed to prepare data for diffusion theory (CRAM),⁽²⁴⁾ transport theory (STRAINT)⁽²⁵⁾ and Winfrith (DSN),⁽²⁶⁾ and perturbation (DUNDEE)⁽²⁷⁾ codes. A detailed account of GALAXY is given by Pull⁽²⁸⁾ at this meeting, and DICE has been described by Kerr.⁽²⁹⁾

Space does not permit a more detailed description of the UKAEA effort in this field. Reference 11 should be consulted both for more details and for further references. Summarizing, it seems fair to claim that it represents the most comprehensive and systematic attack so far made on the problem of using nuclear data in reactor calculations. The fact that many of the workers involved in the effort are far from satisfied with the achievements to date only underlines the magnitude of the task remaining.

2.3 The Hanford RBU Basic Cross Section Library

The following description of the RBU Basic Cross Section Library and associated codes is based on a paper presented by M. R. Egan to the Reactor Mathematics and Computation Division of the American Nuclear Society Panel Meeting on "Master Cross Section Libraries" held in New York July 19, 1963. Originally developed for the RBU (Reactor Burnup) project, the library was later used as a data source for other projects, both at Hanford and elsewhere. The library contains microscopic elastic, inelastic, capture, and fission data; special provisions are made for resolved and unresolved resonance data, inelastic scattering spectra, anisotropic elastic scattering data, and transmutation chain (descendant) data. The energy range is 0-10 MeV.

In contrast to the UKAEA Nuclear Data Library, considerable emphasis is placed on compacting data by allowing mixed representations of the same quantity (point values and resonance values for cross sections) and by using different interpolation procedures ($1/v$, linear-linear, constant, etc.) in different energy ranges. This compacting appears to be achieved only by a loss of simplicity in data input and by making checking very difficult. Additionally, processing codes need complicated routines to read the library tapes. This is a general point which will be returned to later.

The original library occupied about 25,000 (BCD) records on magnetic tape, and was converted into binary and written on a second tape by use of the RBU Pre-Input code. This binary tape can be input to the codes UPDATE when data changes are to be made or to BARNS when the user wishes to obtain specific subsets of data in a directly usable form.

The binary library tape is arranged as a series of physical records. Record 1 contains complete descendant data for all isotopes in the library, and record 2 contains tables of inelastic spectra and resonance parameters. Each table relates to a particular nuclide and is numbered for easy reference as part of the data for that nuclide in a subsequent record. The remaining records are in pairs. Each odd-numbered record contains cross-section data for an isotope, and the following even-numbered record contains the burnup (descendant) data for this isotope. The isotopes are entered roughly as they appear on a Chart of Nuclides.

The descendant data are constructed so that fission yields and decay constants (if any) are available for as many fission product isotopes as one pleases. Inelastic-scattering tables for these nuclides where the evaporation model is inappropriate take the form of cumulative probability distributions for various excitation levels. Resolved and unresolved resonance parameters can be given, and there is provision for superimposing point values of the cross section and values calculated from the single level s-wave Breit-Wigner formula.

Records 3, 5, ..., contain cross-section information for an arbitrary number of energy ranges covering 0-10 MeV. Associated with each range is an index indicating the cross-section behavior over the range. This may be linear in energy, constant, $1/v$, or as given by the single level Breit-Wigner formula, and may be different for different cross sections so that, for example, the frequently occurring combination of a constant elastic cross section and a $1/v$ capture cross section can be represented in a very economical way. Angular distributions for elastic scattering are represented by the first five Legendre coefficients (up to P_4 , that is) in the laboratory system. Great emphasis is placed on economy of storage. For instance, the same storage is used for point values of the elastic cross section or neutron widths for resonances according to the representation used in a particular energy range. In this way a vast amount of information can be presented very compactly, but at the expense of excluding certain types of information, such as cross sections for $(n,2n)$ reactions.

A listing of the library data has been published by Liikala.⁽³⁰⁾ The quality and quantity of data vary considerably from nuclide to nuclide. The library has been used to provide data input to a number of codes, including GAM-1,⁽³¹⁾ TEMPEST,⁽³²⁾ and THERMOS.⁽³³⁾ BARNs⁽³⁴⁾ is a group-cross-section code for use with the Hanford library. Greenborg⁽³⁵⁾ has described the use of this code and others to calculate 31- and 15-group cross sections for use in shielding codes.

2.4 Atomics International Cross Section Analysis and Applications Project

This project is very similar in its aims to that leading to the creation of the UKAEA Nuclear Data Library. The principal features of the project described by Alter and Lorenzi⁽³⁶⁾ are

- (a) literature searching leading to an automated reference system⁽³⁷⁾ designed to aid work on cross-section evaluation;
- (b) compilation and evaluation of neutron cross sections;
- (c) production of a magnetic-tape library of neutron cross sections and associated FORTRAN-handling codes;
- (d) analysis and application of resonance-parameter data;
- (e) analysis and application of thermalization data;
- (f) production of multigroup cross-section libraries for use in engineering applications.

The format of the tape together with details of MOMUS (a code which can make a tape, list selected elements, update a tape, make a copy tape containing selected elements, and provide graphical displays of any or all cross-section parameters for any or all elements) has been described by

Blaine,⁽³⁸⁾ and CRT plots of the data for 21 elements and nuclides have been given by Alter and Lorenzi.⁽³⁹⁾

The Atomics International Library has been used in the calculation of processed data. GRAVE⁽⁴⁰⁾ is an IBM-7094 FORTRAN II code which calculates group-averaged cross sections. Resonance-region cross sections are produced by use of ARES II,⁽⁴¹⁾ while a separate code, PRISM,⁽⁴²⁾ calculates transfer matrices for elastic and inelastic scattering. The elastic-scattering data can also be processed into a form suitable for Monte Carlo calculations.

It is inappropriate here to go into details of the format, for which the references should be consulted, but it is very pertinent to the discussion to note the way in which this project follows the general pattern set out in Section 2.1. The efforts of various laboratories suggest that there is a very wide measure of agreement on the general pattern to be followed, but the vast effort involved in relation to even the largest laboratory's resources means that all existing systems are capable of substantial improvement in many ways.

2.5 The Martin Company General Nuclear Data Tape

A report by Hubner⁽⁴³⁾ describes the comprehensive system of neutron cross-section handling developed by the Martin Company Nuclear Division and used also at General Electric Nuclear Materials and Propulsion Operation at Cincinnati. The associated codes are in FORTRAN II for the IBM-7090. Features of the system include:

- (a) the mechanical reading of cross-section curves through use of a Benson-Lehner machine, followed by conversion to digital form and automatic replotting, so that accuracy may be checked by overlaying original and replotted curves;
- (b) the use of alternative methods of storing point values of neutron cross sections: (log energy, log cross section), (log energy, cross section), (energy, log cross section), and (energy, cross section) pairs can all be dealt with;
- (c) the use of many error-detection routines in the computer codes;
- (d) the use of the single-level Breit-Wigner formula to generate capture fission and scattering cross sections in the resonance region;
- (e) the construction of a basic group-cross-section library at 100 fixed energy values from which fewer group-cross-section data can be constructed;

- (f) the restricted use of elastic-scattering angular-distribution data. Only the average cosine of the scattering angle and the average logarithmic energy decrement are calculated by the processing codes.

2.6 Discussion

There is now available sufficient experience with mechanized nuclear-data libraries to enable some kind of general philosophy to be set out. The fundamental problem is to reconcile the generally conflicting virtues of simplicity and comprehensiveness. Some libraries have been developed with simplicity as the keynote, and it has proved difficult to add new types of data which have become important later. Other libraries have a flexible format, but insufficient effort has been available to achieve a desirable degree of completeness for some types of data. Resonance data are often included in a very incomplete form, and processing codes for their use are relatively few. Many of these difficulties arise from manpower difficulties in that systems have often been developed as part of a tightly scheduled and financed reactor-development program, so that desirable generalizations have generally been ignored. The authors believe that the mechanized handling of neutron cross sections for reactor calculations should be dissociated from any particular design project as far as possible. Development should aim to serve the needs of a wide range of projects. The manpower and computer implications are fairly obvious, but are generally outside the scope of this paper. However, one major implication that must be mentioned is that the field is potentially fruitful for interlaboratory cooperation. This has begun, but there is plenty of room for further progress.

The major factors in the mechanized handling of neutron cross sections appear to be:

- (a) the format. This must facilitate entry and checking of the data and the use of the data. Use of the data includes its entry into processing codes, and its transmission and dissemination to other laboratories;
- (b) computer capability. Present experience suggests that a substantial increase in the availability of cheap high-speed storage would be of greater help than decreases in arithmetic times;
- (c) standardization of input to neutronics codes. At present a great deal of coding effort is needed to meet the requirements of the many neutronics codes which are in use;
- (d) general flexibility. The format and other features should as far as possible be capable of handling new types of data as these become of importance in practical calculations.

Some attention has been given to these points in existing libraries. By combining the best features of these libraries in an internationally available system, it should be possible to make a substantial advance in the present position.

3. SECOND-GENERATION MECHANIZED NUCLEAR DATA LIBRARIES

3.1 General Requirements for a Second-generation Nuclear Data Library

Several meetings were held between July 1963 and May 1964 to discuss existing libraries and requirements for future libraries. These meetings, sponsored by the Mathematics and Computation Division of the American Nuclear Society, were attended by some thirty-four people representing twenty laboratories. These meetings were characterized by great differences of opinion (because of the different requirements of each laboratory) and by equally great unanimity of opinion that something can and ought to be done to standardize libraries. Most people who attended these meetings were more concerned with using the data in reactor calculations than in the collection and evaluation of data. Hence, the attitudes and opinions were admittedly those of the reactor physicist. These will compensate to some extent for the prevailing opinions of the nuclear physicists.

There are a number of requirements for a workable nuclear-data library:

- (a) quantities of good data to put on the library;
- (b) a set of card formats for recording the data;
- (c) computer programs to process these cards and store them on magnetic tape, to retrieve data from the master tapes for distribution or to make up more efficient working tapes, to take data from the working tapes and reduce data to the form required for a reactor calculation;
- (d) a center charged with the maintenance of the library and associated computer programs, and with the collection and distribution of the data.

Let us consider each of these requirements.

The data file is obviously only as good as the data that exist on it. The main sources of evaluated data are the libraries that now exist. If the standard format were sufficiently flexible, these libraries could be converted to the standard format by means of a simple computer program. The quality of the existing data varies widely, and it might appear to be

wasteful to convert all of these data. This argument is countered by the user's desire to select which data he considers to be the best and by the necessity of doing comparative calculations with various sets of data. Thus, it appears to be desirable to be able to translate many, if not all, existing libraries into a standard format. The other sources of evaluated data are the nuclear-model calculations and measurements which will be done in the future. A second-generation library should be able to incorporate these data with a minimum of inconvenience and delay. Unfortunately, there is much unknown about the formats, arrangement, and quantity of these data, so that again flexibility is necessary.

The second requirement for a nuclear-data library is a set of card formats for recording the data. Undoubtedly too much discussion has already been devoted to card formats, and the arguments about simplicity versus flexibility will never be settled. Flexibility is required for the conversion of existing libraries, and this will be the dominant factor in the next-generation library. Simplicity may be obtained later by using a selected subset of the standard formats. Computer programs can also be written which will convert data presented in a simple format to the more complex format, and thus simplify the preparation of data.

The third requirement for a nuclear-data library is a series of computer programs to manipulate and process the data. A great variety of programs is required, some quite simple, and some very complex (particularly if the card formats are not simple). There would be considerable wasted effort if each installation had to write its own set of programs. Interlaboratory cooperation is needed here. Differences between computers and computer systems rule out complete program compatibility, but much can be done to reduce the difficulties. Nearly all computers have a FORTRAN compiler, so that all programs should be written in FORTRAN II (avoiding Boolean and any special features included in the local version).

Finally, there must be one center which will be primarily responsible for development and maintenance of the library. The center must serve as a clearing house for data and computer programs.

3.2 The ENDF System

Following many of the recommendations made at the panel meetings, work was started at BNL on a second-generation system called the ENDF (Evaluated Nuclear Data File). Formats and several computer programs have been completed.⁽⁴⁴⁾ The Sigma Center at BNL will be responsible for the collection and distribution of data.

The basic unit contained in the ENDF is called a Data Record and is defined as the data associated with:

- (a) a particular isotope, i.e., U^{235} ;
- (b) a particular reaction, i.e., elastic scattering;
- (c) the type of data given, i.e., angular distributions;
- (d) a particular energy range, i.e., 0.1-15 MeV;
- (e) a particular evaluation, i.e., taken from the smooth curves in BNL 400.

The ENDF is a collection of these Data Records on magnetic tape. We now trace the path of a Data Record from its origin to its use in a reactor calculation.

The Data Record may have originated from the results of new measurement and evaluation of a particular cross section, from a nuclear-model calculation, or from an existing library. The Data Record is sent to the ENDF center at BNL as card images on magnetic tape. Upon receipt by the center, the Data Record is assigned an acquisition number and added to the master library tapes. The acquisition number is in the form of an alphabetic character and a 4-digit number, i.e., A0269 or B1596. The master library tapes are ordered by acquisition number. Periodically the center will send out a newsletter describing recent additions. Interested users can then request Data Records from the master library and receive them as card images on magnetic tape. Probably the user will add these Data Records to his personal master library.

Up to this point the ENDF is just a random collection of blocks of data. The ENDF can be visualized as a "do-it-yourself library kit." The reactor physicist must now select the blocks he desires and (with a sort-and-merge program) place them on a working library tape. The order here will be first by isotope, second by reaction type, and third by the type of data given.

A retrieval program can next be used to read the working library and process the data into the form desired. The user would instruct the retrieval program as to what Data Records are to be used. This request might be of the form

0.001 A1137 2.0 A0986 1.0×10^5 A1631 1.5×10^7 ,

which reads: use Data Record A1137 from 0.001 to 2.0 eV, use Data Record A0986 from 2.0 to 1.0×10^5 eV, etc.

Nearly all existing libraries consider a much larger basic unit. This unit (an isotope file) is generally a complete set of data for a particular element and includes all cross-section types for the full energy range in a predetermined order. This is the most convenient unit for the retrieval

program but has several disadvantages. The first disadvantage is that data will rarely be received in this form. New evaluations will frequently be made of a particular cross section over a particular energy range. This data could not be distributed unless it were made part of an existing isotope file. The old data plus the new part would form a new isotope file and could be distributed. Obviously, this is unnecessarily restrictive and costly in storage capacity. Under the ENDF system of "building blocks," an isotope file is specified by a series of energy ranges and acquisition numbers. New data received can be easily incorporated.

The "building block" structure of the library has several other advantages. The storage requirements are reduced since the data in each block can be represented in a manner best suited to that data without regard for the other blocks. Alternative evaluations are also stored economically, since only that data which is different need be stored. Finally, the reactor physicist must know the contents of each block before he can put them together in an intelligent manner. The ENDF system will not reduce the physics and judgment required to put together a new library, but it will reduce the physical effort and data handling. This will be viewed by some reactor physicists as an advantage and by others as a disadvantage.

3.3 Structure of a Data Record

A Data Record is a complete unit describing particular data for a particular cross section for a particular isotope and a given energy range. The various elements of a Data Record are:

- (1) heading cards - These cards give a complete description of the cross section, isotope, type of data given, energy range, units, and source of the data in three forms;
 - (a) a Hollerith card which can easily be read both by a human and by a computer;
 - (b) the numerical equivalents (via a dictionary) of the Hollerith data. This will be easier for some computers to read than the Hollerith;
 - (c) comment cards, readable only by the human, which further describe the source of the data, evaluation methods, references, etc.
- (2) control cards - These cards describe the quantity and arrangement of the data;
- (3) the data cards.

We will not go into any further detail concerning the control and data cards, but merely list some of the types of data that can be included.

- (a) tabulated multidimensional cross-section data in various arrangements with various interpolation methods;
- (b) various analytic representations of multidimensional cross-section data;
- (c) combinations of the above two items;
- (d) resolved and unresolved resonance parameters;
- (e) isotope decay and fission product yield data.

3.4 Retrieval Programs

The retrieval programs select the desired Data Record from the working library tape and process the data into a form required for reactor calculations. Since the Data Record formats are quite flexible, the retrieval programs will be rather complex. We hope that it will be necessary for only one program to be written, and if it is written in a simple version of FORTRAN II that it can be used on almost all computers. The program will be in the form of a subroutine with a list of arguments. The user will then write a control program which processes the data from the retrieval program into the form required for the particular application. Generally this final processing will consist only of reordering and suitable output operations.

Specifications for a retrieval program have not been completed but the argument list will resemble the following:

- (1) a description of what Data Records are to be used and in what energy ranges; a scale factor for each Data Record may also be provided;
- (2) a description of what information is desired. The request might be for:
 - (a) the data as they stand;
 - (b) values at given energies, angles, etc.;
 - (c) averages (weighted) over intervals;
- (3) input data to the retrieval subroutine. When required, this would be energies, angles, intervals, weighting functions, etc.;
- (4) information about where and in what order to store the results.

The user will generally not need to know the details of how the data appears in the Data Record. If he requests $\sigma_{\text{elastic}}(E)$ at various E and the Data Record contains $\sigma_{\text{elastic}}(E, \mu_{\text{CM}})$, both the transformation from CM to laboratory system and the integration will be done automatically.

4. NUCLEAR-DATA PROCESSING IN THE FUTURE

In Section 2 some existing neutron cross-section libraries and processing codes have been described, while in Section 3 the development of the ENDF as an attempt to promote the greater use and exchange of evaluated neutron cross sections in a mechanized form has been described. The following past and present experience seems pertinent to any attempt to forecast future developments:

(a) Experimental and calculated values of neutron cross sections are becoming available in greater and greater numbers. If the naturally-occurring isotopes and the neutron-energy range 0.0001 eV-15 MeV are considered, it seems quite possible that within 20 yr some information will be available on nearly every interaction of importance. Additionally, there will be much information available on unstable nuclides.

(b) At present the increase in the amount of data available often adds to existing confusion. There are many inconsistencies among different measurements of the same cross section, and it is difficult to see any major application of computers to resolution of these discrepancies. Much patient experimental and theoretical work seems to be needed here, and it is debatable as to how much effort should be devoted to mechanizing the measurement of new cross-section points and how much to resolving the known discrepancies. Certainly one good answer is worth more than a dozen bad ones.

(c) A related point is the disparity between the number of physicists involved in measuring cross sections or in making theoretical calculations and the number involved in evaluation. It seems fair to say that at present there is made available in a usable form to the reactor physicist only a small fraction of the store of nuclear data which is available.

(d) While people have been struggling to improve the quality of basic neutron cross-section libraries, reactor physicists have been developing increasingly complicated methods of dealing with the effects of self-shielding, molecular binding, and temperature variation. Currently, it is hard to see any practical method of dealing with the combination of these effects in a comprehensive manner. The design trend towards a softer spectrum in "fast" reactors and a harder spectrum in "thermal" reactors means that many more calculations must be made for that energy range (1 eV-100 keV, say) for which calculations are most difficult. This requires not only good values of resonance parameters, strength functions, etc., but also much more sophisticated processing codes.

(e) As data libraries have increased in size, acute storage problems have been encountered in the various computers used. The large increases in the arithmetical speed of computers during the past 10 yr do not seem to

have been matched by a similar increase in the availability of cheap high-speed storage. While backing stores, such as random-access discs, are useful, there seems little doubt that a large increase in high-speed central-core storage would be of major benefit to future development of both data libraries and processing codes. The amount of data to be handled is also such as to place a high premium on the reliability of punched cards, magnetic tape, etc., and the associated handling equipment.

(f) Large resources are now needed to deploy a flexible range of modern reactor codes in any one laboratory, and even the largest laboratories find difficulty in keeping in the forefront in all fields. The position is particularly acute for data libraries and processing codes, and this field seems ripe for increasing interlaboratory cooperation.

We then expect that the likely developments in the future include:

- (a) computers with large amounts of cheap fast storage of high reliability;
- (b) greater international cooperation with the development of evaluated cross-section request lists, etc.;
- (c) a trend towards one standard format - first for exchange, then for input to processing codes;
- (d) greater exchange of processing codes through the Argonne and Ispra centers;
- (e) a comprehensive attack on processing for thermal scattering data and resonance-region cross sections;
- (f) more comprehensive manuals describing formats, etc. These will be increasingly produced by automated methods (as for CINDA);
- (g) a decrease in the ratio of people producing new data by experiment or calculation to those engaged in putting them in a form suitable for use in reactor calculations.

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Discussion of Paper
Presented by Mr. Honeck

MR. UNDERHILL (AERE, Winfrith): I would like to put in one word to avoid a chance of a Civil War in England; the nuclear data file is not now called the AWRE nuclear data file. It is the United Kingdom Atomic Energy nuclear data library.

MR. HUMMEL (Argonne National Laboratory): Consider, for instance, the U^{238} capture cross section. In the fast region the points pepper around pretty much on the appropriate page of BNL-325, in which no attempt is made to assign weights to the various experimental results; nor is there any least-squares fitting of the data. I would like to have, since I'm not an experimenter and it's hard for me to tell whose data is better than someone else's, some complete listing of what data are available, together with some form of value-weighting. Although this mechanization is very important, I believe that it is most necessary to have some way to judge the data and to arrive at a reasonable average to use.

MR. HONECK: I agree. The one thing that will help in this direction is that with different sets in the same format, comparative calculations can be done.

MR. RAVETS (Westinghouse Astronuclear Laboratory): Exactly what do you intend to do, if anything, on temperature dependence? Also, do you have any detailed plans for the thermal range and the different scattering kernels?

MR. HONECK: Yes. All of these quantities, such as cross sections, can be put in as temperature-dependent quantities. The data file is set up as a mathematical device, allowing the expression of multidimensional functions. The file is set up to be able to take all of these various forms; however, the thermal scattering law $S(\alpha, \beta)$, being a somewhat different animal, required special provisions. It can be handled.

MR. RAVETS: Was this included in the Aldermasten or Howerton's data?

MR. HONECK: It is certainly included in the Aldermasten format. There is a special provision for $S(\alpha, \beta)$.

REACTOR SHIELDING CALCULATIONS BY THE MONTE CARLO METHOD

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ABSTRACT

This paper outlines Monte Carlo techniques for the numerical solution of the energy-dependent Boltzmann equation for neutrons or gamma rays, which significantly reduce the computer time required for Monte Carlo shielding calculations. This reduction is a maximum for calculations involving multi-energy source and/or interaction spectra and complicated source, shield, and system geometries. The Monte Carlo techniques include the use of energy-independent biasing functions, energy-dependent samples which span the entire energy range of interest, and analytic integrations of the energy dependence of the differential angular-energy interaction cross sections.

Typical numerical results obtained from the Douglas Monte Carlo computer program SOBER are presented to demonstrate the accuracy, flexibility, and computational speed achieved through the use of these techniques.

1.0 INTRODUCTION

The Monte Carlo method, when applied to the numerical solution of the energy-dependent Boltzmann equation for neutrons or gamma rays, provides a powerful technique for treating the complicated source, shield, and system geometries encountered in proposed applications of nuclear reactors in space. In theory, the Monte Carlo method is capable of yielding solutions of any desired accuracy. In practice, however, the repeated sampling required to insure the convergence and to decrease the variance of the solution results in large computer-time requirements which have often discouraged the use of Monte Carlo programs.

Several techniques are available for decreasing the number of samples and the corresponding computer time required to obtain a given accuracy. These include the use of biased sampling and the use of analytic rather than random sampling techniques, whenever feasible. By proper choice of analytic and random sampling techniques, it is possible to reduce the random sampling to the selection of position vectors and direction vectors

for the Monte Carlo samples. This reduction is accomplished through the use of energy-independent biasing functions, energy-dependent samples which span the entire energy range of interest, and analytic integrations of the energy dependence of the differential angular-energy interaction cross sections.

Several significant benefits accrue from this formulation when applied to transport problems involving multi-energy source and/or interaction spectra:

a) The elimination of many similar geometric calculations, since a multitude of mono-energetic samples can be represented by a single energy-dependent sample. This result has the greatest significance for complicated geometries where ray-tracing calculations usually require a large proportion of the computer time.

b) The elimination of involved sampling techniques commonly employed for the independent source and the various transport and interaction kernels.

c) The simultaneous treatment of all possible interactions at each scattering point, thereby eliminating the variance resulting from the random selection of a single event for the usual mono-energetic sample, and also resulting in solutions with smoother spectra.

d) The ability to treat cross-section data in more conventional forms; the need for discrete interaction probability tables is eliminated. In fact, this method invites the use of the multigroup constants commonly employed in the S_n method for neutrons.

The net result of this formulation is a significant reduction in the computer time required for Monte Carlo verification of reactor shield designs and generation of basic shielding data.

These techniques have been used in the Douglas Monte Carlo computer program SOBER,⁽¹⁾ which is written in FORTRAN IV. SOBER solves the energy-dependent transport equation for neutrons using multigroup constants or basic cross sections, and for gamma rays using basic cross sections. This program treats independent sources with spatial distributions ranging from points to rectangular, cylindrical, or spherical volumes, and with angular distributions ranging from mono-directional to angular. The solution is obtained for a geometric system described by quadric surfaces and consists of point, surface-averaged, and/or volume-averaged number and energy fluxes and currents. A calculation of the variance of the number flux is included to provide the necessary information on the convergence and accuracy of the solution, and several arbitrary number-flux-response functions are also calculated.

Typical results obtained from SOBER are presented to demonstrate the accuracy, flexibility, and computational speed achieved through the use of these Monte Carlo techniques.

2.0 THE MONTE CARLO METHOD

Although the Monte Carlo method permits exact treatment of time-dependent transport problems, it is not necessary in most shielding calculations to explicitly include this time dependence. Moreover, the usual forms of the Boltzmann equation^(2, 3) do not provide the best framework for describing the random sampling techniques employed in solving neutron and gamma-ray transport problems. It is more desirable to approach these problems by examining the integral equations satisfied by the average particle densities.

2.1 Particle Density Integral Equation

For this description the basic particle coordinates are the position vector $\vec{r}$, the direction vector $\vec{\Omega}$, and the energy E . The particle densities are expressed as the number per unit phase space $d\vec{r} \cdot d\vec{\Omega} \cdot dE \cdot dt$ and are related to the number of interactions which the particles or their precursors have experienced since being emitted by the independent source. Thus, $S_i(\vec{r}, \vec{\Omega}, E)$, the i th source density, is the number of particles per unit phase space coming out of the i th interaction at $\vec{r}$ in the direction $\vec{\Omega}$ with energy E . In particular, $S_0(\vec{r}, \vec{\Omega}, E)$ is the independent source. The contribution to the differential flux from the i th source density is obtained from the integral equation:

$$\phi_i(\vec{r}, \vec{\Omega}, E) = \int_0^\infty S_i(\vec{r}-s\vec{\Omega}, \vec{\Omega}, E) e^{-\int_0^s \Sigma^t(\vec{r}-s'\vec{\Omega}, E) ds'} ds, \quad (1)$$

where s is the distance between a source point and the flux point, and $\Sigma^t(\vec{r}, E)$ is the total cross section at $\vec{r}$ for particles of energy E . For points $\vec{r}$ which are located in nonvoid regions, the $(i+1)$ th collision density is

$$C_{i+1}(\vec{r}, \vec{\Omega}, E) = \Sigma^t(\vec{r}, E) \phi_i(\vec{r}, \vec{\Omega}, E), \quad (2)$$

and the $(i+1)$ th source density is given by the integral equation

$$S_{i+1}(\vec{r}, \vec{\Omega}, E) = \iiint_{4\pi} \phi_i(\vec{r}, \vec{\Omega}', E') \frac{d^2 \Sigma^s}{d\Omega dE}(\vec{r}; \vec{\Omega}', E' \rightarrow \vec{\Omega}, E) dE' d\Omega', \quad (3)$$

where $(d^2\Sigma^S/d\Omega dE)(\vec{r};\vec{\Omega}', E' \rightarrow \vec{\Omega}, E)$ is the total differential angular-energy interaction cross section including isotropic and anisotropic elastic scattering, inelastic scattering, n-xn, and fission for neutrons, and Compton scattering for gamma rays.

2.2 Monte Carlo Techniques

The Monte Carlo method utilizes random discrete values of the particle coordinates in the solution of the Boltzmann equation, thereby reducing both the computer storage and the computing time required for iterative solution of the above equations. For the techniques being described, the discrete coordinates of a given sample at the i th interaction point consist of the position vector $\vec{r}_i$ and the direction vector $\vec{\Omega}_i$. The corresponding Monte Carlo source density sample "weight" $W_i^S(E)$ can be visualized as a packet of particles in a manner analogous with the correspondence made between mono-energetic samples and individual particles.

The Monte Carlo samples are traced from the independent source through the shield and system geometries in a random manner, utilizing various biasing functions in the selection of interaction points and direction vectors. Biasing functions are usually introduced to reduce the variance of Monte Carlo calculations,⁽⁴⁾ but by requiring energy-independence, their use also permits the elimination of many similar geometric calculations and the analytic integration of the energy-dependence of the differential angular-energy interaction cross section.

These biasing functions are probability density functions, and they are chosen so that if: x is a random variable, e.g., the distance between interaction points or the cosine of the scattering angle, $p(x|E)$ is the conditional probability density function (pdf) for x ; $w(x, E)$ is some function of x , e.g., the particle density; and $p^*(x)$ is an arbitrary biasing function, then the average value $\bar{w}(E)$ of $w(E, x)$ is

$$\bar{w}(E) = \int_{-\infty}^{\infty} w(x, E) p(x|E) dx = \int_{-\infty}^{\infty} y(x, E) p^*(x) dx, \quad (4)$$

where

$$\begin{aligned} y(x, E) &= w(x, E) p(x|E)/p^*(x), \\ p^*(x) &= 0 \text{ only if } p(x|E) = 0. \end{aligned} \quad (5)$$

Stated more explicitly, random sampling of the biasing function rather than of the actual pdf will yield the correct average particle density if the sample weight is adjusted according to Eq. (5). For the techniques being described,

the biasing functions may be given any spatial and angular dependence. Sampling of the biasing functions utilizes numbers, ξ , drawn at random from the rectangular distribution:

$$\begin{aligned} p(\xi) &= 1 & 0 \leq \xi \leq 1 \\ &= 0 & \text{otherwise.} \end{aligned} \quad (6)$$

The biasing functions used in SOBER have been chosen to permit the calculation of each random variable x from the equation

$$\xi = P(\xi) = \int_0^{\xi} p(\xi') d\xi' = P^*(x) = \int_{-\infty}^x p^*(x) dx. \quad (7)$$

2.2.1 The Independent Source

In the most general problem, the initial position and direction vectors are calculated in the following manner:

$$\text{obtain } \vec{r}_0 \text{ at random from } p^*(\vec{r}), \text{ where } \iiint_{\substack{\text{source} \\ \text{volume}}} p^*(\vec{r}) d\vec{r} = 1; \quad (8)$$

$$\text{obtain } \vec{\Omega}_0 \text{ at random from } q^*(\vec{\Omega}|\vec{r}_0), \text{ where } \iint_{4\pi} q^*(\vec{\Omega}|\vec{r}_0) d\Omega = 1. \quad (9)$$

Then the initial source sample weight is given by

$$W_0^s(E) = \frac{S_0(\vec{r}_0, \vec{\Omega}_0, E)}{p^*(\vec{r}_0) q^*(\vec{\Omega}_0|\vec{r}_0)}. \quad (10)$$

For most reactor shielding problems, the assumption of separable variables simplifies these source-sampling procedures without appreciably affecting the accuracy of the calculations. Moreover, this assumption eliminates the need for using auxiliary storage such as magnetic tapes for the initial sample coordinates, since they may be generated with relative ease as required during the calculations.

In SOBER, this procedure is applied to an independent source of one particle per second so that the spatial, angular, and energy distributions become probability density functions:

$$S_0(\vec{r}, \vec{\Omega}, E) = \left[\prod_{\ell=1}^5 p_{\ell}(v_{\ell}) \right] n(E), \quad (11)$$

where $n(E)$ is the normalized differential number spectrum. The first three variables are used to represent the spatial distribution: $(v_1, v_2, v_3) = (x, y, z)$, (r, θ, z) , or (ρ, θ, μ) for rectangular, cylindrical, or spherical source geometries. The last two variables are used to represent the azimuthal angle ($v_4 = \Theta$) and the cosine of the polar angle ($v_5 = \cos \phi$) of the angular distribution. Each of these variables is given either a continuous distribution or a single discrete value, and the biasing functions are given a corresponding distribution or value so that the initial source sample weight is given by

$$W_0^S(E) = \left[\prod_{\ell=1}^5 \frac{p_{\ell}(v_{\ell})}{p_{\ell}^*(v_{\ell})} \right] n(E). \quad (12)$$

2.2.2 The Transport Kernel

Assuming that the Monte Carlo calculations have proceeded to the i th interaction point $\vec{r}_i$, and that the direction vector and sample weight are $\vec{\Omega}_i$ and $W_i^S(E)$, then the calculations continue with the determination of the next interaction point $\vec{r}_{i+1}$. From Eqs. (1) and (2), the conditional probability density function for the particle collision density is related to the distance s from $\vec{r}_i$, measured along $\vec{\Omega}_i$, by

$$\begin{aligned} u(s|\vec{r}_i, \vec{\Omega}_i, E) &= \Sigma^t(\vec{r}_i + s\vec{\Omega}_i, E) e^{-\int_0^s \Sigma^t(\vec{r}_i + s'\vec{\Omega}_i, E) ds'} \\ &= -\frac{d}{ds} \left[e^{-\int_0^s \Sigma^t(\vec{r}_i + s'\vec{\Omega}_i, E) ds'} \right]. \end{aligned} \quad (13)$$

In order to force the same interaction point for all particle energies, the random sampling proceeds as follows:

$$\text{obtain } s_{i+1} \text{ at random from } u^*(s|\vec{r}_i, \vec{\Omega}_i), \text{ where } \int_0^\infty u^*(s|\vec{r}_i, \vec{\Omega}_i) ds = 1. \quad (14)$$

By requiring this last condition, the sample is restricted to interaction points within the geometric system. The interaction point $\vec{r}_{i+1}$, collision density $W_{i+1}^C(E)$, and element of the differential flux $W_i^\phi(E)$ are given by

$$\vec{r}_{i+1} = \vec{r}_i + s_{i+1} \vec{\Omega}_i; \quad (15)$$

$$W_{i+1}^c(E) = W_i^s(E) \frac{u(s_{i+1} | \vec{r}_i, \vec{\Omega}_i, E)}{u^*(s_{i+1} | \vec{r}_i, \vec{\Omega}_i)}, \quad (16)$$

$$W_i^\phi(E) = \frac{W_{i+1}^c(E)}{\Sigma^t(\vec{r}_{i+1}, E)} = W_i^s(E) \frac{e^{-\int_0^{s_{i+1}} \Sigma^t(\vec{r}_i + s' \vec{\Omega}_i, E) ds'}}{u^*(s_{i+1} | \vec{r}_i, \vec{\Omega}_i)}. \quad (17)$$

To avoid numerical and convergence difficulties, the biasing function for particle transport should be chosen similar to the actual pdf:

$$\begin{aligned} u^*(s | \vec{r}_i, \vec{\Omega}_i) &\propto \Sigma^*(\vec{r}_i + s \vec{\Omega}_i) e^{-\int_0^s \Sigma^*(\vec{r}_i + s' \vec{\Omega}_i) ds'} \\ &= -\frac{d}{ds} \left[e^{-\int_0^s \Sigma^*(\vec{r}_i + s' \vec{\Omega}_i) ds'} \right]. \end{aligned} \quad (18)$$

To enable a variety of biasing possibilities, the value of $\Sigma^*(\vec{r}')$ can be given any angular or spatial dependence. In SOBER, the values of $\Sigma^*(\vec{r}')$ are:

$$\begin{aligned} \Sigma^t(\vec{r}', E) = 0: \quad \Sigma^*(\vec{r}') &= 0 \\ \Sigma^t(\vec{r}', E) \neq 0: \quad \Sigma^*(\vec{r}') &= a, a + b\alpha_i, a + b\beta_i, a + b\gamma_i, a + b\vec{\Omega}_i \cdot \vec{\Omega}_p, \\ &\text{or } a + b\vec{\Omega}_i \cdot \frac{(\vec{r}' - \vec{r}_p)}{|\vec{r}' - \vec{r}_p|}, \end{aligned} \quad (19)$$

where a and b are constants, $|b| < a$, $(\alpha_i, \beta_i, \gamma_i)$ are the direction cosines of $\vec{\Omega}_i$, $\vec{\Omega}_p$ is an arbitrary direction, and $\vec{r}_p$ is an arbitrary point.

The evaluation of the actual and biasing probability density functions for particle transport requires a knowledge of the partial path lengths measured from $\vec{r}_i$ along $\vec{\Omega}_i$. In SOBER, the material densities, and therefore the total cross sections, are assumed constant within each geometric region used to describe the geometry, and the ray-tracing or path-length calculations are performed by the Douglas computer subroutine QUAD⁽⁵⁾ for quadric surface region boundaries of the form

$$A_0 + A_1x + A_2y + A_3z + A_4x^2 + A_5y^2 + A_6z^2 + A_7xy + A_8yz + A_9zx = 0. \quad (20)$$

2.2.3 The Interaction Kernel

Once the interaction point $\vec{r}_{i+1}$ is determined, the next step in the calculations involves a determination of the scattered direction $\vec{\Omega}_{i+1}$ and the $(i+1)$ th source density. The probability that a particle will survive the $(i+1)$ th interaction is $\Sigma^s(\vec{r}_{i+1}, E') / \Sigma^t(\vec{r}_{i+1}, E')$, where

$$\Sigma^s(\vec{r}_{i+1}, E') = \iiint_{4\pi}^{\infty} \frac{d^2 \Sigma^s}{d\Omega dE} (\vec{r}_{i+1}; \vec{\Omega}_i, E' \rightarrow \vec{\Omega}, E) d\Omega dE. \quad (21)$$

Having survived the interaction, the conditional probability density function for the number of particles proceeding in the direction $\vec{\Omega}$ is

$$v(\vec{\Omega} | \vec{r}_{i+1}, \vec{\Omega}_i, E') = \frac{\int_0^{\infty} \frac{d^2 \Sigma^s}{d\Omega dE} (\vec{r}_{i+1}; \vec{\Omega}_i, E' \rightarrow \vec{\Omega}, E) dE}{\Sigma^s(\vec{r}_{i+1}, E')}. \quad (22)$$

The scattered direction is calculated in the following manner:

obtain $\vec{\Omega}_{i+1}$ at random from $v^*(\vec{\Omega} | \vec{r}_{i+1}, \vec{\Omega}_i)$,

$$\text{where } \iint_{4\pi} v^*(\vec{\Omega} | \vec{r}_{i+1}, \vec{\Omega}_i) d\Omega = 1. \quad (23)$$

Therefore, the $(i+1)$ th source density is given by

$$W_{i+1}^s(E) = \int_0^{\infty} W_i^{\phi}(E') \frac{\frac{d^2 \Sigma^s}{d\Omega dE} (\vec{r}_{i+1}; \vec{\Omega}_i, E' \rightarrow \vec{\Omega}_{i+1}, E) dE'}{v^*(\vec{\Omega}_{i+1} | \vec{r}_{i+1}, \vec{\Omega}_i)}, \quad (24)$$

since several cross-section terms cancel. This procedure forces particles of all energies in the same direction.

In the actual calculation of the scattered direction vector, the scattering angles, say (θ', ϕ') , may be chosen with respect to an arbitrary axis and then rotated to determine the corresponding angles (θ, ϕ) used to define $\vec{\Omega}_{i+1}$ in the reference system, since the Jacobian $J(\theta', \phi' / \theta, \phi) \equiv 1$. This fact is used in SOBER to permit angular biasing in the x, y, or z direction, radially for cylinders or spheres, or in the original direction for scattering which may be predominantly forward, e.g., Compton scattering for $E > 0.1$ MeV, and neutron scattering in hydrogenous materials.

The techniques used in SOBER for describing the differential angular-energy interaction cross sections are too involved for a complete discussion here. In general, the following procedures are used:

- a) multigroup constants for neutrons--used in the standard S_n terminology, except for hydrogen, which is treated exactly,
- b) basic cross sections for neutrons--constant over arbitrarily defined groups, isotropic and anisotropic scattering in the center-of-mass coordinate system, exact treatment of energy losses, n - n' and n - xn matrices by element,
- c) basic cross sections for gamma rays--total cross sections constant over arbitrarily defined groups, exact treatment of Compton scattering.

2.2.4 Flux Estimators

There are a variety of techniques which can be used in conjunction with the Monte Carlo samples and their coordinates to estimate the scalar flux and the current. Program SOBER uses these samples in conjunction with analytic estimation to calculate point, surface-averaged, and volume-averaged fluxes. The numerical techniques used in estimating the scalar fluxes for a given Monte Carlo sample include:

- a) point detector at $\vec{r}_d$:

$$\phi(\vec{r}_d, E) = \sum_{i=1}^{\infty} N_i(E) \frac{e^{-\int_0^s \Sigma^t(\vec{r}_i + s' \vec{\Omega}, E) ds'}}{s^2 + f(s)}, \quad (25)$$

where

$$s = |\vec{r}_d - \vec{r}_i|;$$

$$\vec{\Omega} = (\vec{r}_d - \vec{r}_i)/s;$$

$f(s)$ = a function used to prevent a singularity at $s = 0$,

i.e., $f(0) > 0$;

$$i = 0, N_0(E) = \frac{S_0(\vec{r}_0, \vec{\Omega}, E)}{p^*(\vec{r}_0)};$$

$$i > 0, N_i(E) = \int_0^\infty W_{i-1}^\phi(E') \frac{d^2 \Sigma^S}{d\Omega dE} (\vec{r}_i; \vec{\Omega}_{i-1}, E' \rightarrow \vec{\Omega}, E) dE';$$

b) surface detector:

$$\phi^A(E) = \frac{1}{A} \sum_{i=0}^{\infty} W_i^S(E) \frac{e^{-\int_0^S \Sigma^t(\vec{r}_i + s' \vec{\Omega}_i, E) ds'}}{|\vec{\Omega}_i \cdot \vec{n}|}, \quad (26)$$

where

A = area of the surface;

s = distance from $\vec{r}_i$ to the surface;

$\vec{n}$ = normal to the surface at $\vec{r}_i + s \vec{\Omega}_i$;

c) volume detector:

$$\phi^V(E) = \frac{1}{V} \sum_{i=0}^{\infty} W_i^S(E) e^{-\int_0^S \Sigma^t(\vec{r}_i + s' \vec{\Omega}_i, E) ds'} g(\rho, E), \quad (27)$$

where

V = volume of the detector;

s = distance from $\vec{r}_i$ to the volume;

ρ = path length in the volume;

$g(\rho, E) = \rho$ if the volume is void

$$= \frac{1 - e^{-\rho \Sigma^t(\vec{r}^1, E)}}{\Sigma^t(\vec{r}^1, E)} \text{ if not void;}$$

$\vec{r}^1$ = any point in the volume (constant cross sections).

3.0 NUMERICAL RESULTS

The Monte Carlo techniques just outlined are equally applicable to the generation of basic shielding data and to the evaluation of reactor shield designs. Before applying SOBER to any of these problems, however, a comparison was first made with moments-method data for point, isotropic neutron and gamma-ray sources. This comparison had a two-fold purpose: to gain experience in the selection of biasing functions; and to determine the applicability of multigroup constants to neutron-penetration calculations.

Typical dose-attenuations for prompt fission-spectrum gamma rays are shown in Fig. 1. These results were obtained with the use of the National Bureau of Standards tabulation of cross sections.⁽⁶⁾ As a result there is a significant deviation of the cross sections used for lead from those used in the original moments-method calculations, and this deviation is sufficient to account for the higher Monte Carlo results.

All neutron-penetration calculations to this date have been performed with the use of the LASL⁽⁷⁾ (16-group) and GAM⁽⁸⁾ (top 20-group) multigroup cross sections and the transport approximation, i.e., isotropic scattering with corrections for forward scattering. Typical results obtained for these cross sections are also shown in Fig. 1. Almost all of these calculations show marked deviations from moments-method results at deep penetrations, due in part to insufficient sampling. For penetrations up to 7 relaxation lengths, however, agreement within a factor of two was achieved even with nonoptimum biasing parameters.

Each of these calculations involved a minimum of 100 to a maximum of 500 Monte Carlo samples, significantly less than would be required by the usual Monte Carlo techniques which treat mono-energetic samples. The computing time per sample increased, of course, due to the simultaneous treatment of approximately 20 energy groups for each sample. Typical running times (with the IBM-7094) were on the order of 3 min per 100 samples for neutron calculations, and 1.5 min per 100 gamma-ray samples.

The accuracy obtained in these calculations was sufficient to warrant the analysis of an idealized description of the KIWI-B test reactor using program SOBER. The reactor description included a carbon retainer, a beryllium reflector, axial LiH and stainless steel shielding, and an aluminum pressure vessel. In addition, the axial and radial power profiles were used in describing the independent source. Results are tabulated in Table 1 for 7 point detectors positioned around the reactor. The fission-spectrum neutron calculation involved 100 Monte Carlo samples and required less than 7 min of computer time. For the prompt fission-spectrum gamma-ray source, 500 samples were used, requiring approximately 7 min of computer time. A point-kernel calculation for the same reactor and detectors,

PROMPT FISSION SPECTRUM GAMMA RAYS

FISSION SPECTRUM NEUTRONS

FISSION SPECTRUM NEUTRONS

Fig. 1. Point Isotropic Sources in Infinite Media

Table 1

POINT-DETECTOR RESULTS, KIWI-B REACTOR

Distance from Core Center, ft	Angle from Core ϕ , degrees	Rad Neutron	Standard Deviation	Rad Gamma Ray	Standard Deviation
15	0	4.7(-17)	1.2(-17)	5.0(-19)	1.3(-19)
15	45	5.9(-17)	0.7(-17)	2.9(-17)	0.5(-17)
15	90	9.8(-17)	0.8(-17)	6.6(-17)	1.1(-17)
15	135	1.6(-16)	0.3(-16)	2.4(-17)	0.2(-17)
15	180	2.5(-16)	0.5(-16)	1.8(-17)	0.2(-17)
10	90	2.3(-16)	0.2(-16)	1.5(-16)	0.2(-16)
20	90	5.4(-17)	0.5(-17)	3.6(-17)	0.5(-17)

involving one-group removal theory for neutrons and five-group attenuation with buildup for gamma rays, required about 1 min of computer time. A single scattering-point-kernel calculation would require approximately 15 min of computer time by standard numerical-integration techniques.

4.0 CONCLUSIONS

The Monte Carlo techniques presented in this paper are superior in many respects to the conventional techniques. Positive features include:

- a) consistent use of biasing functions,
- b) elimination of involved random sampling techniques including "splitting" and "Russian Roulette,"
- c) simultaneous treatment of all particle energies,
- d) elimination of many geometric calculations,
- e) simplified data-handling procedures, especially for cross sections,
- f) analytic integrations of the differential angular-energy interaction cross sections, and
- g) significant reduction in computer-time requirements.

The maximum benefit is derived from these techniques for problems involving multi-energy source and/or interaction spectra.

The use of multigroup constants in the transport approximation has a limited, but useful, range of applicability in neutron-penetration calculations. This range of applicability should be extended by including the P_1 Legendre scattering coefficients.

The use of point detectors in Monte Carlo reactor shielding calculations is desirable, and by the techniques described here, these calculations require approximately the same computer time as a "single scattering" point-kernel calculation.

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Discussion of Paper Presented by Mr. Jordan

MR. LEIMDORFER (Research Institute of National Defense, Stockholm): I wonder if you have compared your deep-penetration calculations with those of Kalos which were published in Nuclear Science and Engineering in 1963. He got some very nice spectra at a penetration of about 2400 gm/cm² in hydrogen.

MR. JORDAN: The calculations they have been doing with hydrogen have been run for specific detectors. I have been trying to achieve good results over a range of attenuation values. Their technique devised for point detectors gives very good agreement at quite deep penetrations; however, this technique isn't really applicable to the shielding-type calculation in which we treat many detectors for a given one-run calculation.

MR. KELLMAN (United Nuclear Corporation): With the use of the SANE or SAGE programs in which we do do the energy-dependent weight and sampling, we're not treating specific detectors. The biasing is both energy and spatially dependent. Have you attempted to compare your code with one of these?

MR. JORDAN: No. This was done during original check-out. I had available some original moments data which covered a good range of attenuation ranges, probably sufficient for anything that would be involved in a nuclear vehicle study. I don't think I am going to run into any problems with 400-gm/cm² penetration.

MR. LEVITT (Atomics International): How did you obtain the standard deviation in the angular measurements?

MR. JORDAN: I used the most straightforward treatment. Everything that I got from one sample, that is, from the initial source point, until I dropped it off at some arbitrary weight cutoff, I treated as one random sample and used standard equations.

MR. UNDERHILL (AERE, Winfrith): Does the method extend to calculations with a continuous energy dependence rather than just using group constants?

MR. JORDAN: Yes. The code could actually, within each group, assume some form for the differential spectrum - linear, or exponential, or something else - and carry this along. A little more calculation goes into it but you would probably get better results.

TECHNIQUES USED IN THE GEM CODE FOR MONTE CARLO NEUTRONICS CALCULATIONS IN REACTORS AND OTHER SYSTEMS OF COMPLEX GEOMETRY

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1. Introduction

The Monte Carlo technique has become a practicable method for the solution of many neutronics problems through the development of fast computing machines, which are well suited for the large number of simple repetitive calculations that are required. The method has the attraction that it is, in principle, capable of treating any complexities in geometry and nuclear data without approximation. Such an ideal is not easily achieved. On the one hand, means of feeding in a large amount of geometrical and nuclear data need to be devised. On the other, this must be handled efficiently during the calculation, because a large number of neutron histories must be followed in order to obtain acceptable statistical accuracy.

Nevertheless, a number of codes have been and are being developed to exploit the advantages of the Monte Carlo technique. The GEM Code was designed initially to study criticality-safety problems in chemical plants, and a primary objective was to use nuclear data in as fine a detail as possible. Its geometrical capabilities were extended in 1962 to carry out a survey⁽¹⁾ on behalf of the International Atomic Energy Agency of the factors affecting the nuclear safety of arrays of transport containers carrying fissile materials. Developments since that time have enabled virtually all geometrical restrictions to be removed. The resulting program has proved versatile enough to make neutronic calculations for a complete reactor, incorporating all the significant structural features.

In the description which follows, it is assumed that the reader is familiar with the basic principles of Monte Carlo tracking, such as described, for example, by Parker and Woodcock.⁽²⁾

2. Basic Philosophy

The primary aim of the program is to calculate the overall reactivity of a system of any geometry. A number of possible parameters can be used as a measure of reactivity. Some of these have been discussed at length by Woodcock,⁽³⁾ who concluded that the most useful were the multiplication factor per fission generation, k_{eff} , and the quantity MR , where M is the surface multiplication of an inner portion of the system called the

"core" and R is the albedo of the remainder, which acts as a reflector. In GEM, the quantity MR has been chosen as fundamental and k_{eff} is treated as a derived parameter.

With minor exceptions neutron tracking is carried out by direct simulation. It was considered that the advantage to be gained in the type of problem to be tackled by GEM, from any currently suggested variance-reducing techniques did not merit the additional complexity of programming and the careful analysis required to ensure that no bias was introduced. Experience since making this decision has, so far, given no grounds for suggesting that it was an incorrect one.

A first essential in designing a Monte Carlo neutronics calculation is to ensure that the neutron tracking is as efficient as possible. Thus, the parameters to be calculated should achieve their eigenvalues quickly and should then have a small statistical variance. The time spent in tracking neutrons in any particular part of the system should be in proportion to the importance of that part in determining the values of the desired parameters. In GEM a deliberate attempt has been made to achieve this efficiency by adopting the following tracking cycle.

2.1 Tracking Cycle

As a first step in the specification, a "neutronically important boundary" B is chosen, and tracking proceeds by stages beginning and ending at this boundary. At the beginning of a stage a specified number of neutrons, N , enter the core across the boundary B . They and their descendants are followed through the system until they either escape, are captured, or reach the boundary B again, travelling in a direction to re-enter the core. This is the end of the stage. If during this tracking, N_0 neutrons crossed the boundary B travelling outwards and N' returned to the core, the ratios N_0/N and N'/N_0 are estimates of the surface multiplication of the core and the albedo of the reflector, respectively. The N neutrons required for the next stage are chosen at random from the N' re-enters.

When sufficient stages have been completed, the measure of reactivity MR is obtained as the mean ratio N'/N , being unity for a critical system and greater than unity for a supercritical system. If boundary B is well chosen, these parameters quickly settle to their equilibrium values provided a suitable distribution is used for the N neutrons starting the first stage. Such a distribution is usually obtained by running a preliminary stage started from fission neutrons at the centre of the core, on the argument that any neutron entering the core across boundary B must have originated from a fission in the core.

2.2 Choice of Boundary B

The specification of the boundary B is one of the vital features affecting the efficiency of the GEM technique. In designating this boundary, the three considerations of quick settling, small errors, and sampling importance must be borne in mind. In practice, it is difficult to plan or achieve the ideal precisely. Selection of boundary B can seldom be completely divorced from geometrical detail, although considerable ingenuity may be exercised. Moreover, compromise is necessary, since some of the desirable conditions conflict with each other. A mathematical analysis of optimum conditions has not yet been developed, and the following guidance as to choice of boundary B is based on experience. A poor choice usually reveals itself by creating difficulties in obtaining satisfactory answers.

One good choice, as it will achieve rapid settling, is to make boundary B surround the main bulk of fissile material as closely as possible. But large statistical errors will be encountered unless the core multiplication is small, generally less than 2. This is discussed more fully in Section 4.2 below. For a larger core multiplication it is advisable to choose some surface inside the fissile material. If an air gap exists between the core and reflecting material, the outer surface of the core is a better boundary B than the inside of the reflector, because then all initial neutrons for each stage will enter the core directly, satisfying the importance criteria.

Frequently, and particularly with symmetrical or near symmetrical systems, it is a good plan to include a central plane with mirror reflections as part of boundary B. The neutrons tracked across this plane will settle to an eigendistribution, exhibiting the proper relative importance, except for outer parts of the reflector, which may be oversampled.

Oversampling, such as may occur here or in other cases, in the outer parts of a thick reflector can be avoided by use of a filter. A filter surface is defined so that only a specified proportion of the neutrons reaching it in the outward direction are tracked beyond it and the sample size is restored when neutrons arrive back at the filter.

Careful choice of boundary B and the judicious use of filters enable the tracking to be so arranged that the importance criteria are adequately satisfied.

3. Criticality Parameters - Calculation of k_{eff}

For the usual case in which the boundary B divides the system into a core and reflector, the criticality parameter MR is determined from the neutron counts. To obtain k_{eff} , the direct method is to repeat the calculation with the mean number of neutrons per fission, $\bar{\nu}$, divided by k . In this

way M and R are obtained as functions of k and, by interpolation, both $1/M$ and R , being linear in k over a small range, the value of k for which $1/M = R$ can be obtained. This value of k is equal to the required k_{eff} .

Alternatively, a close estimate of k_{eff} can be obtained directly from one calculation in the following way.

Of the S neutrons which enter the core, assume that a fraction l_0 escape and a fraction f_0 cause a fission. Of the ν_0 neutrons which arise on average from each of these fissions, assume that a fraction l_1 escape and a fraction f_1 cause a further (second-generation) fission.

In general, of the ν_{i-1} neutrons arising from an i^{th} generation fission assume that a fraction l_i escape and a fraction f_i cause a further fission. Then the quantities F and M_B may be defined by the following relations:

$$\begin{aligned} F &= S\nu_0 f_0 + S\nu_0 \nu_1 f_0 f_1 + S\nu_0 \nu_1 \nu_2 f_0 f_1 f_2 + \dots; \\ M_B F &= S\nu_0 f_0 M_{B1} + S\nu_0 \nu_1 f_0 f_1 M_{B2} + \dots, \end{aligned} \quad (1)$$

where

$$M_{Bi} = l_i + \nu_i f_i l_{i+1} + \nu_i \nu_{i+1} f_i f_{i+1} l_{i+2} + \dots \quad (2)$$

Here F is the total number of fission children produced in the sample and M_{Bi} is the total number of neutrons leaving the core as the result of one fission neutron born in the i^{th} generation.

Also, the surface multiplication M can be expressed as

$$M = l_0 + \nu_0 f_0 l_1 + \nu_0 \nu_1 f_0 f_1 l_2 + \dots \quad (3)$$

Hence, by definition of k_{eff} ,

$$\frac{1}{R} = l_0 + \frac{\nu_0}{k_{eff}} f_0 l_1 + \frac{\nu_0 \nu_1}{k_{eff}^2} f_0 f_1 l_2 + \dots \quad (4)$$

Algebraic manipulation of Eqs. (1) to (4) leads to

$$\frac{S(M - l_0)[M - (1/R)]}{M_B F [(1/R) - l_0]} = (k_{eff} - 1)[1 + (k_{eff} - 1) \Phi(l_i, f_i \nu_i)], \quad (5)$$

where Φ is a function which is always finite and vanishes if $l_i = 1$, $f_i = f$, for all $i > 0$, and $\nu_i = \nu$ for all i .

Hence, it follows that the equation

$$k_{\text{eff}} = 1 + \frac{S(M - l_0)[M - (1/R)]}{M_{BF}[(1/R) - l_0]} \quad (6)$$

gives the true value when k_{eff} is unity or near unity and gives a good approximation elsewhere. Furthermore, this k_{eff} is a perfectly valid measure of reactivity and can for all practical applications be used in place of the more usually defined k_{eff} .

The quantities used in Eq. (6) are all readily derived from counts printed at the end of the calculation, and the k_{eff} given in the print out is obtained from the use of this formula. There is a point about the interpretation of Eq. (6). The fundamental definition of k_{eff} is the multiplication in a cycle that starts and ends in a fission. The k_{eff} from Eq. (6) refers to a cycle that starts and ends in a fission in the core. These represent slightly different definitions for systems which have fissions in the reflector.

4. Statistics

The purpose of the tracking technique used in a Monte Carlo code is to obtain neutron samples representative of the eigendistribution of the steady-state system, and then to estimate some numerical index of reactivity. Due to the probabilistic nature of the processes involved, some statistical error is associated with the reactivity. It is necessary to obtain an estimate of the size of this uncertainty. Furthermore, since the eigendistribution is unknown at the outset, a statistical analysis is needed to ensure that the desired steady-state distribution has been generated and is being sampled.

4.1 Tests for Settling

The GEM procedure for the tracking cycle, whereby the "enter" neutrons for one stage are obtained from the "re-enter" neutrons of the previous stage, has been designed as an efficient way of generating an eigendistribution. Two difficulties may arise. Firstly, the settling may be so slow that the early stages may not yield samples appropriate to the neutron eigendistribution on boundary B. Secondly, even if settling is rapid, successive stages may not lead to statistically independent estimates.

An analysis of variance has been applied to a number of GEM runs consisting of identical fissile cores in near-identical reflectors, so that the core surface multiplications were known to be the same. This indicated that any differences between the estimated core multiplications were due to chance variation; these runs had settled sufficiently to allow that parameter to be accurately and properly estimated.

Any interdependence from one stage to the next or following stages is likely to produce an oscillation or a gradual drift in the parameter to be estimated as the eigendistribution is reached. Under these circumstances the appropriate statistical test is the mean-square successive-difference test.⁽⁴⁾ Alternatively, an analysis of variance may be applied to subsets of a number of stages. No evidence of interdependence has yet been found.

The conclusions drawn from these studies are that neutrons settle rapidly to the eigendistribution and yield proper and independent random samples from this distribution. It follows that the best estimate of a criticality parameter is that obtained by totalling all the various neutron counts over all the stages completed in the particular run.

4.2 Calculation of Statistical Error

The parameter MR measures the return of neutrons to boundary B. The aim of GEM is to estimate its average value. It can be shown that the frequency distribution of the "re-enters" arising from a single "enter" neutron on boundary B will have finite mean and variance. Hence, it follows from the Central Limit Theorem that the mean MR from samples of N neutrons will have a statistical distribution which tends to Normal as N tends to infinity. In such cases the calculation of standard error is straightforward.

The size of sample required to achieve sufficient Normality has been investigated, but no clear answer has emerged. Some typical histograms of MR are shown in Fig. 1 for two cases, one with a core surface multiplication of 1.7 and the other of 3.9. For the former the distribution from 200 neutrons is clearly Normal, and that from 100 neutrons is adequately so. In the second case, samples of 500 neutrons are required before the skewness diminishes. These histograms reveal the expected and generally observed phenomenon that for a given number of neutrons in the sample, the distribution of MR becomes wider and more skew as the core surface multiplication increases.

Goodness of fit, skewness, and kurtosis tests have been applied to a number of such histograms. They indicate that samples of 100 neutrons per stage, which is a convenient number for the computer, are usually adequately normal provided that the core surface multiplication is below 2. Only slight error is introduced here, and this is an overestimate of the true standard error. A confidence interval for MR may be obtained from Normal-distribution theory.

Fig. 1. Frequency Histograms of Distributions of MR

It would appear that a similar argument could be developed for k_{eff} . However, experience has shown that the frequency diagrams of k_{eff} exhibit considerable more skewness than those of MR, making it difficult to calculate the statistical error directly. It is easier, therefore, to consider k_{eff} as a parameter derived from MR. Figure 2 illustrates the relationship

Fig. 2. Plot of k_{eff} against MR for Single Stages of 100 Neutrons

typically obtained between k_{eff} and MR from single stages of a GEM run. These results were taken from the example discussed in Section 10.4 below. Any curve drawn for this relationship must pass through the point (1,1) and also through the mean point obtained by totalling all the counts. It seems reasonable to approximate to the correct curve by the straight line joining these points. Consequently, the relationship between the standard error of k_{eff} and that of MR may be derived from Eq. (6) as

$$\text{standard error of } k_{\text{eff}} = \frac{S(M - \ell_0)}{RM_{BF}[(1/R) - \ell_0]} (\text{standard error on MR}). \quad (9)$$

5. Spectra and Flux Distribution

It can readily be deduced that when a steady-state neutron distribution has been achieved, whether in a critical system or in a subcritical system with an imposed neutron source, the flux of neutrons in any energy band in a given region is proportional to the total path length of neutrons in the region in that energy band divided by the volume of the region. In a critical system the factor of proportionality is immaterial, but if a source is present from which a total of N neutrons are started, the flux in neutrons per square centimetre per second will be equal to

$$\frac{\text{Total path length of neutrons in centimeters}}{\text{Volume of region in cubic centimeters}}$$

for a source of N neutrons per second.

Once the flux as a function of neutron energy is obtained, any desired reaction rate can be obtained as the sum over energy of the product of the flux with the macroscopic cross section for that reaction.

Fluxes and reaction rates are calculated in the GEM program in two ways. There is an option to calculate, during the tracking, the total path length in each region* in any specified energy groups. These path lengths are then multiplied by an arbitrary factor for each region, usually the inverse volume, and the results printed out.

Alternatively, the individual path lengths and corresponding neutron energies in specified regions can be read out on tape and subsequently analyzed by a subsidiary program, OPAL, which calculates both spectra and reaction rates. This latter method takes more machine time but will give

*The word "region" is here used in the special sense which is described below in Section 9.

the more accurate reaction rates, as it uses the precise energy of each neutron recorded and interpolates for the cross section at that energy.

6. External Source and Gamma-ray Problems

There is an option in GEM to specify an external source of neutrons which is usually, though not necessarily, specified as neutrons from a given spectrum and angular distribution emitted uniformly from a specified area of a certain surface. In this case the program will make a random choice of the variables to determine the coordinates of the start neutrons.

By use of the external-source option, with photon interaction data and scatter laws, calculations can be made for gamma-ray transmissions. However, since the tracking is basically by direct simulation, this method is suitable only for thin shields. For attenuations exceeding $\sim 10^{-3}$, it is better to use a program specifically designed for this type of calculation, such as UNC-SAM.⁽⁵⁾

7. Tracking Methods

The program is divided into two main parts: TRACK and CRASH. Of these, TRACK deals with the geometry of the system and the general organization, whereas CRASH deals with the nuclear data. In this section the flow pattern of the tracking is outlined. The following two sections give some detail of the manipulation of nuclear and geometrical data.

Each neutron is represented by a set of coordinates, defining position, direction of motion, energy, and history. These require eight 36-bit words to store.

At the start of each stage, the coordinates of a specified number of inward-moving neutrons, usually 100, on boundary B are available in the Birth Store. TRACK selects the first of these neutrons, and calls upon CRASH to calculate the mean free path and then, by a random selection, a path length, assuming the neutron remains in the same material. TRACK then compares this path length with the distance the neutron has to travel to reach the next interface. If the latter is the shorter, TRACK moves the neutron forward to that interface and starts the process again with the material on the other side. If the path length is the shorter, TRACK moves the neutron forward by this distance and calls upon CRASH to determine what happens at this collision point. CRASH will find, by a series of random selections, first the atomic nucleus involved, then the type of interaction and, finally, the directions and lethargies of the emergent neutrons. TRACK will then repeat the process with one of these neutrons, any others being stored at the top of the Birth Store to be picked up later. When, however, a neutron reaches boundary B again, moving inwards, it is placed in the Delay Store, and the next neutron taken from the Birth Store.

The stage ends when all the remaining neutrons are in the Delay Store. To start the next stage the specified number of neutrons are chosen at random from the Delay Store and transferred to the Birth Store. If there are insufficient neutrons in the Delay Store, some of them are chosen twice. During this whole process, counts are kept of all boundary crossings and of all neutron reactions and the various criticality parameters calculated.

8. Nuclear Data Routines - CRASH

The purpose of CRASH is to sample the Nuclear Data when requested by TRACK to provide a path length or to find the numbers, directions, and lethargies of neutrons emerging from a collision. The path length in a given material is derived from the total cross section and the parameters of emergent neutrons from the partial cross sections and collision laws.

8.1 The Total Cross Section

The total cross section of a composite material is obtained from the cross sections and atomic proportions of the constituent nuclides. In CRASH, the cross sections for each nuclide are obtained by interpolation from points given in the UKAEA Nuclear Data File.^(6,7) The energy points tabulated are chosen so that linear interpolation of log (cross section) against lethargy gives acceptably small errors. Each nuclide requires a different set of energy points, and CRASH can use either the complete set or a reduced set with a specified number of points, the reduction being such as to minimize the additional errors introduced.

8.2 The Type of Collision

When a collision has been found, the probability that this occurs with a particular nuclide N is given by the product of the macroscopic cross section for that nuclide with the mean free path in the material, and so random selection enables the nuclide to be identified. The next step is to determine the type of collision.

The probability that the collision is of a given type is just the ratio of partial to total cross section. These partial probabilities are approximated in CRASH by a step function of lethargy, typically with 64 or 80 steps, by a process designed to give a best fit to the original data. The position of the steps will vary from nuclide to nuclide.

Thus, by a random selection the type of collision can be determined. The numbers of collisions of each type with each nuclide are counted and recorded at the end of the print out as an action count.

8.3 The Emergent Neutrons

The final step is to determine the number, directions, and lethargies of all neutrons emerging from a collision. In the case of fission, the mean number of neutrons produced, $\bar{\nu}$, is obtained by interpolation and the actual number of emergent neutrons calculated by a random selection. If required, the value of $\bar{\nu}$ can be multiplied by a specified constant before making the random selection, a facility which is needed if it is desired to calculate k_{eff} by interpolation.

If the collision results in a fission or isotropic scatter, the determination of the emergent direction is straightforward. In the general case of anisotropic scatter it has been found that a cubic equation of the form

$$\mu = a + bZ + cZ^2 + dZ^3 \quad (10)$$

gives an adequate representation, where Z is a random number, and $\cos^{-1} \mu$ is the angle between the directions of the incident and emergent neutrons in centre-of-mass coordinates. The coefficients a , b , c , and d are functions of neutron energy, and can be tabulated at sufficient points to allow linear interpolation.

This method gives a better representation and requires less machine storage than would be needed for tables of equiprobable angles.

In general, the energy of the emergent neutron is dependent on the incident energy and the angle of scatter. When it can be uniquely determined, the appropriate equation is used. In other cases, it is necessary to sample from a probability distribution, which is dependent on the incident and possible emergent energies. A particular case of a probability distribution occurs after a fission, for which the emergent neutron energies are found by sampling from a standard fission spectrum.

8.4 Thermal Neutrons and Multigroup Data

It is necessary to treat thermal neutrons in a different way, since at low energies both the motion of the nuclides and the forces acting between them can have significant effects.

Because of these complications, a multigroup structure has been adopted for neutrons below a specified energy, the group constants depending on the molecules present, rather than the atoms, and on the temperature. The energies of neutrons upscattered out of the groups are estimated by random selection from an exponential distribution.

The multigroup constants have to be determined by a preliminary calculation, e.g., using the PIXSE program.⁽⁸⁾ However, for some applications, a single group of neutrons below 0.1 eV with no upscatter has proved adequate. By extending the multigroup structure to all energies, GEM can use any of the standard sets of constants.

9. Geometrical Specification

The problem in GEM, as in any other field for which a complicated geometrical specification is required, is to devise a method which can readily be applied, which uniquely defines the system, and which can be understood by a computer. In GEM this is achieved by combining a basic specification, by which a system is divided into regions, with a detailed specification which may be used inside any region. The former is built into the program and requires the reading in of certain dimensions and arrangements, whereas the latter calls on special subroutines, called HOLE routines, specifically written for the job.

9.1 Basic Specification

The system is divided into regions by boundaries that form closed nesting surfaces, which may touch or coincide, but may not intersect. The geometry is referred to rectangular Cartesian coordinates in which the boundaries can take the form of spheres, centred at the origin, cylinders with the z-axis as axis or cuboids with edges parallel to the axes. One of these region boundaries is designated as boundary B, dividing the system into core and reflector.

When the boundary B is cuboidal, the core can alternatively be divided into cells, called boxes, by planes parallel to the coordinate plates. These planes need not be equally spaced, but they must pass right through the core, so that boxes do not overlap. Each box has its own origin of coordinates, although no rotation of axes is permitted, and it can be divided into any number of regions by its own individual set of nested surfaces. Boxes with different geometrical or materials content are given different type numbers. The complete core is then specified by listing the type numbers to give the arrangement of boxes, the position of each box being defined by a set of three integral coordinates. If the outer boundary of the reflector is cuboidal, it can be surrounded by a close-fitting specular reflector by specifying an albedo for each face.

For regions which contain only one homogeneous material, this is specified merely by its atomic composition and density. Otherwise, the geometry of an inhomogeneous region is detailed using the stratagem of the HOLE routine.

9.2 HOLE Routines

It is possible to reduce the mean free path in a material to any desired value by adding to the total cross section obtained from those of the constituent nuclides, a cross section for a fictitious reaction in which the neutron experiences no change. Thus, the mean free path for each of the materials in the region can be reduced to the same value and the collision point obtained, using this value, independently of any internal boundaries. The material at the collision is then identified by a routine which tests a series of inequalities. A random test then decides whether this is a real or fictitious collision; in the former case the appropriate collision routine is called and in the latter a new path length is found, and the process proceeds to the next collision point.

In order to check a HOLE routine a program BABS has been written which both checks that the routine links correctly with the main program and gives, to scale, a pictorial cross section of the geometry in any plane perpendicular to the coordinate axes. A typical BABS picture is shown in Fig. 3.

10. Examples

To illustrate the use of GEM a few examples are given.

10.1 A Simple Array of Nesting Uranium Alloy Cups

This example is included to illustrate the basic specification and to show the typical print-out given in Fig. 4. The problem was to find the reactivity of a flooded array of 12 units of two different types placed alternately. Each unit consisted of two uranium alloy cups one inside the other.

Referring to Fig. 4, the core boundary (boundary B) is represented as region 11, which completely surrounds the array. In the reflector, which consists of water, about 15.7 in. thick, a filter has been placed to ensure that only one-third of the neutrons in the outer layers of water are followed. The nesting cylinders shown for each type build up the units, and the arrangement shows how they fit together to form a $2 \times 2 \times 3$ array. The z-direction is treated as the vertical one, and the sequence of numbers under "Arrangement" gives the order in which the types are arranged in each of the three layers, i.e., $^{12}_1$ in the lower, $^{21}_1$ in the middle, and $^{12}_2$ in the upper.

For each stage, the numbers of neutrons entering, leaving, and re-entering boundary B are printed together with the escapes from the system, core multiplication, reflector albedo, and k_{eff} . After each five stages a print is given of the neutron crossings of each boundary, and also a table

which shows the numbers of neutrons entering each face of the core and the faces from which their descendants leave the core. Finally, a print is given of the total cumulated counts together with the criticality parameters MR and k_{eff} .

```
X VARIES BETWEEN -1.0000 AND 1.0000 (LEFT TO RIGHT) AND
Y VARIES BETWEEN -1.0000 AND 1.0000 (BOTTOM TO TOP)
```

Fig. 3. BABS HOLE Picture

*PR261

FLOODED ARRAY OF NESTING URANIUM ALLOY CUPS

HS/6013

TIME SINCE BEGINNING OF JOB - 21.28 MINS.

TRACK5 VERSION 5MJ 30.10.64

REFLECTED-LATTICE

2 DIFFERENT TYPES OF ELEMENT

ARRAY DATA

	X	Y	Z
NUMBER OF ELEMENTS	2	2	3
PER CENT REFLECTION AT OUTER FACES, +	0	0	0
-	0	0	0

ARRANGEMENT

2 1 1 2 1 2 2 1 2 1 1 2

GEOMETRICAL DATA

	REGION NUMBER	GEOMETRY	MATERIAL NUMBER	RADIUS	X	Y	Z
TYPE 1	1	CYLINDER	1	1.44150			0 -4.18550
	2	CYLINDER	2	1.64800			0 -4.39200
	3	CYLINDER	1	1.83550			0 -4.39200
	4	CYLINDER	2	2.05100			0 -4.60750
	5	CUBOID	1		2.65120 -2.65120	2.65120 -2.65120	0.50000 -5.10900
TYPE 2	6	CYLINDER	1	1.63900			0 -4.17950
	7	CYLINDER	2	1.85050			0 -4.39100
	8	CYLINDER	1	2.03350			0 -4.39100
	9	CYLINDER	2	2.25150			0 -4.60900
	10	CUBOID	1		2.65120 -2.65120	2.65120 -2.65120	0.50000 -5.10900
CORE	11	CUBOID	0		5.30240 -5.30240	5.30240 -5.30240	1.50000 -15.32700
REFLECTOR	12	CUBOID	1		11.00000 -11.00000	11.00000 -11.00000	7.00000 -21.00000
	13	FILTER	POWER 3				
	14	CUBOID	1		21.00000 -21.00000	21.00000 -21.00000	17.00000 -31.00000

DIMENSIONS IN INCHES

Fig. 4. Typical GEM Print-Out

MONTE CARLO NEUTRONICS CALCULATIONS

DENSITIES ARE SCALED UP BY 2.5400

THE VERSION OF CRASH IS MASH7 THE UPPER LIMIT OF THE THERMAL GROUP IS 0.1000 EV.

NUCLEAR DATA

MATERIAL	DENSITY	NUCLIDE	PROPORTIONS	BY ATOMS		
		HDASH	ONAT	U238	U235	ALNAT
1	0.9980	2.0000	1.0000	0.	0.	0.
2	3.1700	0.	0.	0.0700	0.9300	34.8890

RANDOM NUMBER = 000000000001

STAGE 0 STARTS 64 FISSION NEUTRONS IN REGION 1, CO-ORDINATES (0. , 0., 0.) BOX (1, 1, 2)

FINISH AT STAGE 25. 100 NEUTRONS PER STAGE

STAGES

							<u>TOTALS</u>						
	ENTER	LEAVE	RE- ENTER	ESCAPE	MULT	REFL	ENTER	LEAVE	RE- ENTER	ESCAPE	MULT	REFL	
1 TO 1	100	125	85	0	1.2500	0.6800	100	125	85	0	1.2500	0.6800	
KEFF = 0.89934													
2 TO 2	100	175	110	0	1.7500	0.6286	200	300	195	0	1.5000	0.6500	
KEFF = 1.02703													
3 TO 3	100	188	106	0	1.8800	0.5638	300	488	301	0	1.6267	0.6168	
KEFF = 1.02165													
4 TO 4	100	96	64	0	0.9600	0.6667	400	584	365	0	1.4600	0.6250	
KEFF = 0.53846													
5 TO 5	100	114	78	0	1.1400	0.6842	500	698	443	0	1.3960	0.6347	
KEFF = 0.80198													

STAGES 1 TO 5

FROM	TO +X	+Y	+Z	-X	-Y	-Z	BOUNDARY	IN	TOTAL	OUT	TOTAL	OUT/IN	TOTAL		
+X	55	48	2	0	2	1	1	293	293	280	280	0.9556	0.9556		
+Y	70	16	74	8	9	6	2	314	314	360	360	1.1465	1.1465		
+Z	21	9	11	16	13	8	3	368	368	412	412	1.1196	1.1196		
-X	184	6	14	9	162	27	4	404	404	544	544	1.3465	1.3465		
-Y	147	19	12	9	37	131	5	982	982	1067	1067	1.0866	1.0866		
-Z	23	1	1	0	1	1	6	327	327	312	312	0.9541	0.9541		
							7	377	377	442	442	1.1724	1.1724		
TOTAL	500	99+	114+	42+	222+	175+	46 =	698	8	428	428	493	493	1.1519	1.1519
							9	451	451	619	619	1.3725	1.3725	1.1133	1.1133
							10	997	997	1110	1110	1.5756	1.5756	2.0000	2.0000
							11	443	443	698	698	2.0000	2.0000	2.0000	2.0000
							12	21	21	42	42	2.0000	2.0000	0	0
							13	7	7	14	14	0	0	0	0
							14	0	0	0	0	0	0	0	0

(ETC. TO STAGE 25)

REQUESTED NUMBER OF STAGES HAVE BEEN DONE

Fig. 4. (Contd.)

CUMULATED COUNTS		STAGES 1 to 25						
	TO	+X	+Y	+Z	-X	-Y	-Z	
FROM								
+X	479	469	40	23	22	51	22	
+Y	472	52	429	31	42	23	31	
+Z	204	28	24	178	31	20	3	
-X	681	37	77	37	630	83	47	
-Y	481	51	19	22	77	422	27	
-Z	183	31	46	8	39	33	148	
TOTAL 2500		668+	635+	299+	841+	632+	278 - 3353	
BOUNDARY NUMBER		(1) INS	(2) OUTS	(3) INS	(2)/(1)	(3)/(2)		
	1	1092	1046		0.95788			
	2	1227	1425		1.16137			
	3	1442	1634		1.13315			
	4	1594	2214		1.38896			
	5	4169	4558		1.09331			
	6	1295	1241		0.95830			
	7	1442	1686		1.16921			
	8	1681	1919		1.14158			
	9	1769	2438		1.37818			
	10	4054	4518		1.11445			
***	11 ***	2500	3353	2233	1.34120	0.66597	UNFISSIONED INS = 1393, OUTS = 1803,	
	12		215	120		0.55814		
	13		72	40		0.55556		
	14		0	0		0		
CORE. REFLECTOR.	MULTIPLICATION, REFLECTION TRANSMISSION	M = 1.3412 R = 0.6660 T = 0 M*R = 0.8932						
ACTION COUNT		STAGES 1 TO 25						
MATERIAL 1.	NUCLIDE	ABSORB	ELASTIC	(N,N*)	(N,2N)	(N,3N)	FISSION	FISSION CHILDREN
	HDASH	37	46261	---	---	---	---	---
	ONAT	0	6354	0	---	---	---	---
	THERMAL NEUTRON GAIN =	1568 -1605	45457				0	0
MATERIAL 2.	NUCLIDE	ABSORB	ELASTIC	(N,N*)	(N,2N)	(N,3N)	FISSION	FISSION CHILDREN
	U238	2	13	2	0	0	0	0
	U235	65	159	10	0	0	136	334
	ALNAT	6	1618	47	---	---	---	---
	THERMAL NEUTRON GAIN =	175 1401	121				1000	2451
SUM OF FISSIONS FOR ALL NEUTRONS LEAVING CORE = 5588								
LIMIT OF 128 FISSIONS PER NEUTRON PER STAGE EXCEEDED 0 TIMES								
KEFF = 0.94300								
TIME SINCE BEGINNING OF JOB = 35.98 MINS								
TIME TAKEN FOR THIS CASE = 14.70 MINS								

Fig. 4. (Contd.)

10.2 A Lattice of Rods in Water

The second example is a calculation made, as a check on the nuclear data, to reproduce an experimental measurement of critical size of a lattice of $\text{PuO}_2\text{-UO}_2$ rods in light water reported from Hanford.⁽⁹⁾ The rods, of 0.372-in. diameter and 48.5 in. long, were loaded at a spacing of 0.80 in. in a hexagonal lattice and completely reflected by water.

For this calculation the core was taken as a single cylindrical region and the hexagonal lattice geometry incorporated by means of a HOLE routine. In the HOLE routine for a hexagonal lattice it is convenient to make the transformation

$$X = N + \frac{2x}{\phi\sqrt{3}};$$

$$Y = N - \frac{x}{\phi\sqrt{3}} + \frac{y}{\phi};$$

$$Z = N - \frac{x}{\phi\sqrt{3}} - \frac{y}{\phi},$$

where ϕ is the lattice pitch and N is an integer large enough to ensure that X , Y , and Z remain positive. All values of X , Y , and Z such that $X + Y + Z = 3N$ then represent points in the x , y plane, and the lattice points are given by integral values of these coordinates.

By making use of this latter property the nearest lattice point to X , Y , Z can readily be found, and a test can then be applied to ascertain whether or not the point is inside the rod centred at that position.

A BABS picture from this HOLE routine is given as Fig. 3, in which 1 represents water, 2 fuel, and 3 cladding.

A time of 87 min was taken on the IBM-7090 for this problem, during which 44 stages were completed and the k_{eff} was calculated to be 1.011, with a standard error of 0.01.

10.3 An Experimental Graphite Moderated Reactor

The Dragon reactor, as described at the third Geneva Conference,⁽¹⁰⁾ has a core built up of hexagonal elements,* each containing 7 fuel rods embedded in graphite, and the reflector is of graphite.

For the purpose of calculation, the complete core was broken into elements of the shape shown in Fig. 5. For convenience the shape of the coolant channels was altered slightly, but, apart from this, these elements fit together to make a core identical with the Dragon core.

*See Fig. 5 of Ref. 10.

Fig. 5. Fuel Element (See 10.3)

Each element was divided into boxes by the dashed lines shown in the figure. In each box a simple HOLE routine was needed to allow for the fueled region, but the rest of the geometry could be built up of the basic shapes. The boundary B was chosen to be cuboidal, with one face bisecting the reactor horizontally, one lying along the top of the core, and the other four enclosing the core as closely as possible. Outside was a reflector, being 100% specular on the bisecting plane and the correct thickness of graphite elsewhere. Thus the core for calculations was a lattice of size $37 \times 21 \times 1$.

For one particular loading calculated, 50 stages were run in 38 min and a k_{eff} of 1.115 obtained, with standard error 0.01.

10.4 A Thermal Power Reactor

A calculation, for which the statistical analysis of the results is discussed in Section 4.2 above, was for a gas-cooled graphite-moderated power reactor. The core of this reactor consisted of cylindrical fuel elements, control rods, experimental channels, etc., arranged on a hexagonal lattice. Each element consisted of a number of fuel pins. The elements, except for a few treated separately, were spaced widely enough for the core to be built up of cuboidal boxes, alternate ones containing fuel elements and the others graphite moderators. A HOLE routine was required to describe the geometry of the elements. Again, boundary B was chosen to include a horizontally bisecting plane, and the core consisted of a lattice of $41 \times 23 \times 4$ boxes. A typical calculation of this series took 120 min for 100 stages and gave a k_{eff} of 0.948, with a standard error of 0.01.

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Discussion of Paper
Presented by Mr. Woodcock

MR. MILLER (Argonne National Laboratory): I understand this code represents the cross sections quite accurately. You have the energy of the resonance cross sections and, in some regions, very high cross sections.

Then you make the cross section in other regions equal to this, introducing a large number of interactions for a neutron crossing a region which has, physically, a small cross section. Can you give me some idea of the effect this has on increasing computing time?

MR. WOODCOCK: There are two cases. If one material has a high cross section over an extended range of energy, such as in the case of a control rod, it is better to separate that material into a separate region. But in the case of a resonance--a comparatively narrow area of very large cross section--the chance that a neutron is actually of the right energy for that resonance to need a large number of small steps is comparatively small. In fact, I think the best thing to say about this is that we have done quite a number of calculations with U^{238} and other materials, and there has been no indication that the time of computation has been increased unduly because of this effect.

MR. IRVING (Oak Ridge National Laboratory): How do you handle the angular distributions and the inelastic scattering in the program?

MR. WOODCOCK: I doubt whether I can say very much in a few words. We take the AWRE data file which contains tabulated values, giving an angular distribution. We have, up to the present, tended to take the value from this tabulated list by interpolation. We are now in the process of changing these tabulated values back into some formula which gives the angular scatter as a function of a random number. This sort of formula takes up less space in the machine and also has the advantage that one can interpolate over energy more easily. For inelastic scatter energy loss we apply a standard formula.

MR. WADE (AERE, Harwell): Can you tell me what treatment of thermal-neutron scattering you use?

MR. WOODCOCK: In the current system neutrons below a certain energy, which we specify, are treated in multigroup fashion. The multigroups are obtained from calculations at Harwell. We are planning to extend this by dividing the energy range into three regions.

We will treat the higher-energy region, in which there is a negligible probability of an upscatter, as in our present general treatment. In the low-energy region a multigroup representation will be used. In an intermediate region we can use a simple formula for a distribution of neutrons from an inelastic scatter. We are looking into the possibility of incorporating that type of scheme.

MR. CHURCH (Savannah River Laboratory): I missed your justification for replacing the actual cross section of a region by the cross section of the surrounding medium.

MR. WOODCOCK: In a Monte Carlo calculation if one gets a neutron passing through regions, one has to calculate each boundary crossing point before he can find a collision point. This calculation takes quite a lot of machine time. By doing this trick with cross sections we ensure that a mean free path in each of these regions is the same, so we can find the collision point without having to find the point at which the boundaries have been crossed. Having found a point in this system, the arithmetic to find out which material that point is in is a much simpler and quicker problem. It also has the advantage that these HOLE routines for this different geometry can be written as separate subroutines which can be plugged in. We are gradually building a library of those.

MR. BRICKSTOCK (AWRE, Aldermaston): What are your criteria for determining when k has settled down to an equilibrium value, bearing in mind the statistical deviations for the k values you determine?

MR. WOODCOCK: First of all, we use MR as the fundamental parameter. We first want to find when MR has settled down to its correct value and then deduce the k from it. This is the standard type of statistical test. One can compare the value coming out of successive samples and compare these with the mean values.

MR. BRICKSTOCK: Suppose you have an MR value that is varying slowly; you must relate the rate of change of this to the statistical deviation. At what stage do you say that it is not changing?

MR. WOODCOCK: This doesn't happen. We don't get a monotonic change in MR.

A MONTE CARLO APPROACH TO THE CALCULATION OF CHARACTERISTIC REACTOR PARAMETERS IN THREE-DIMENSIONAL ASSEMBLIES

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Introduction

In this paper the calculation of stationary and time-dependent reactor parameters by the use of the Monte Carlo method will be discussed. The first question is: What justifies the large amount of time spent on the development of an elaborate Monte Carlo program when a number of powerful analytic-numerical methods already exist? One answer to this question is that the Monte Carlo method is able to take into account a greater number of basic nuclear cross sections and spatial dimensions than the existing methods. This holds also for the TIMOC code which will be described here.

But there is another equally important reason. The TIMOC code has been designed so that the physical process in a multiplying system can be simulated very exactly by following the lifecycles, while the sampling procedure employed allows the calculated results to be analyzed and interpreted with a view to testing mathematical and physical models based on a transport or diffusion-theory approach.

Almost all analytical methods used for the calculation of multiplying systems are based on the assumption that the equilibrium distribution is already established. Therefore, one calculates the characteristic quantities like reactivity, generation time, and flux spectra only for this case. This is suitable for the assessment of stationary reactor operation but not for the study of strongly time-dependent situations, such as one finds, for example, in a pulsed reactor or in certain pulsed neutron experiments. Calculations in connection with the latter have shown that in many cases the measurements were performed at a time before the equilibrium condition was established. In the study of such transient phenomena the TIMOC code has proved to be particularly powerful.

In the literature there are described a number of Monte Carlo programs for the assessment of critical assemblies.⁽¹⁻⁵⁾ It appears that most of these codes are designed for somewhat specialized problems. Also, the description of the nuclear processes does not use more accurate models than the analytic-numerical methods. They are also unduly influenced by these classical methods and do not make full use of new possibilities offered by the Monte Carlo method.

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Description of the Mathematical Methods Used in TIMOC

a) Stationary Problems

For the mathematical description of the neutron transport in multiplying media, the stationary Boltzmann equation can be written in the following integral form:

$$\phi(x) = \int_R D(y \rightarrow x) \phi(y) dy + \int_R P(y \rightarrow x) \phi(y) dy + S(x), \quad (1)$$

where $\phi(x)$ describes the neutron density and "x" the six-dimensional space vector (r,E). The kernel $D(y \rightarrow x)$ stands for the nonmultiplying neutron transport and $P(y \rightarrow x)$ for the (x,E)-dependent multiplication process. $S(x)$ describes the external source.

The method of solving Eq. (1) follows closely the picture of subsequent generations. A certain initial source distribution $S(x)$ decays and builds up the source distribution for the next cycle, and so on. This generalized source-iteration procedure can be described by splitting Eq. (1) into a system of coupled integral equations of the form

$$\phi_i(x) = \int_R D(y \rightarrow x) \phi_i(y) dy + S_i(x), \quad (2)$$

where

$$S_1 = S(x) \quad (3)$$

and

$$S_i = \int_R P(y \rightarrow x) \phi_{i-1}(y) dy; \quad i = 2, 3, \dots \quad (4)$$

In each equation the following conditions are satisfied:

$$S_i(x) > 0$$

and

$$0 < \int_R D(y \rightarrow x) dx < 1$$

for all x of R, since this term contains only elastic and inelastic scattering. The problem is now reduced to the well-known Monte Carlo calculation of nonmultiplying media. The summation of all $\phi_i(x)$ leads to

$$\sum_{i=1}^N \phi_i(x) = \int_R D(y \rightarrow x) \sum_{i=1}^N \phi_i(y) dy + \int_R F(y \rightarrow x) \sum_{i=1}^N \phi_i(y) dy + S(x) - \int_R F(y \rightarrow x) \phi_N(y) dy. \quad (5)$$

The sum

$$\sum_{i=1}^{\infty} \phi_i(x) = \phi(x)$$

becomes a solution of (1) if

$$\int_R P(y \rightarrow x) \phi_N(y) dy \rightarrow 0$$

for $\lim N \rightarrow \infty$. This means in physical terms that the reactor is subcritical. If, however, for $\lim N \rightarrow \infty$, the quantity $\phi_{N-1}(x)$ converges to $\phi_N(x)$, i.e., the value of $\phi_N(x)$ does not change for higher iterations, then $\phi_N(x)$ becomes a solution of the homogeneous integral equation

$$\phi(x) = \int_R D(y \rightarrow x) \phi(y) dy + \int_R P(y \rightarrow x) \phi(y) dy. \quad (6)$$

The ratio

$$k_i = \int_R P(y) \phi_i(y) dy / \int_R P(y) \phi_{i-1}(y) dy \quad (7)$$

is the multiplication factor from generation "i-1" to "i." It can easily be obtained in this form as a Monte Carlo sample value.

If, furthermore, $k_{i-1} = k_i$ and $\phi_{i-1}(x) = k_i \phi_i(x)$, i.e., the fundamental mode or the equilibrium distribution has been established, then $k_i = k_{\text{eff}}$ becomes the parameter for the stationary criticality. In this case the well-known solution

$$\phi(x) = \frac{1}{1 - k_{\text{eff}}} \phi_i(x) \quad (8)$$

for $i > N(i)$ applies.

In the case that $k_N > 1$ for the $\lim N \rightarrow \infty$, this procedure diverges, i.e., the calculated assembly is supercritical. Such systems require the introduction of an artificial reduction parameter to obtain convergency.

In addition to the stationary criticality factor, defined by Eq. (7), the dynamical criticality factor can also be obtained easily as a sample value. It is the average multiplication factor of all neutron generations and is defined from the equation

$$k_{\text{eff}}(\text{dyn}) = \int_R P(y) \sum_{i=1}^{\infty} \phi_{i+1}(y) dy / \int_R P(y) \sum_{i=1}^{\infty} \phi_i(y) dy. \quad (9)$$

b) Time-dependent Problems

Other important reactor parameters include the mean neutron lifetime and generation time. For their calculation the time variable has to be introduced explicitly into the Monte Carlo calculations as it was done in the TIMOC code. The code offers two possibilities for their determination.

One follows directly the experimental measuring technique, using the relation between $(k_{\text{eff}} - 1)$ and the corresponding decay constant. This corresponds to the "census taking" procedure described in Ref. 4.

The second method follows the pictures of the generation cycles. One assumes that at $t = 0$ a neutron population of the energy and space distribution of the fundamental mode is inserted into the assembly. The decay of this population is studied and the estimates of the time-dependent parameters are therefore carried out for this one neutron generation only; no use is made of perturbation theory. The corresponding transport equation reads like this:

$$\begin{aligned} \phi_i(x, t) = & \int_R dy \int_{t_0}^t \delta\left(t - t' - \frac{|y_r - x_r|}{\sqrt{y_E}}\right) D(y \rightarrow x) \phi_i(y, t') dt' \\ & + S_i(x) \delta(t_0). \end{aligned} \quad (10)$$

The code now calculates for these neutrons of one generation the time-dependent destruction rate composed of absorption and leakage. If $D^*(x)$ is the corresponding absorption and leakage kernel,

$$N_D(t) = \int_R D^*(x) \phi_i(x, t) dx \quad (11)$$

or

$$N_D(t) = \int_{E_{\min}}^{E_{\max}} dE \int_B d\vec{r} \Sigma_a(E, \vec{r}) \phi(\vec{E}, \vec{r}, t) + \oint_B \frac{\partial \phi_i(\vec{E}, \vec{r}, t)}{\partial n} d\vec{r}. \quad (12)$$

In the same way one can calculate the time-dependent buildup of the next neutron generation. With $P^*(x)$ the corresponding production kernel,

$$N_p(t) = \int_R P^*(x) \phi_i(x, t) dx \quad (13)$$

or

$$N_p(t) = \int_{E_{\min}}^{E_{\max}} dE \int_B d\vec{r} \nu(E, \vec{r}) \Sigma_f(E, \vec{r}) \phi(\vec{E}, \vec{r}, t). \quad (14)$$

By the usual procedure the mean values in time for the above-quoted quantities are then calculated. The mean time a neutron stays in the reactor is

$$\tau_1 = \int_R dx \int_0^\infty t dt D^*(x) \phi_i(x, t) / \int_R S_i(x) dx, \quad (15)$$

where, for physical reasons,

$$\int_R S_i(x) dx = \int_R dx \int_0^\infty dt D^*(x) \phi_i(x, t). \quad (16)$$

The mean time necessary to produce a neutron in the next following neutron generation can be expressed by

$$\tau_g = \int_R dx \int_0^\infty t dt P^*(x) \phi_i(x, t), \quad (17)$$

where

$$\int_R dx \int_0^\infty dt P^*(x) \phi_i(x, t) = k_i \int_R S_i(x) dx, \quad (18)$$

if one makes use of the relations (4) and (7). The product $\tau_g k_i = \Lambda$ could be interpreted as the mean time necessary to build up the next neutron generation.

Furthermore, it can be seen that there is generally no relation between τ_1 [Eq. (14), the mean time necessary a neutron lives in the reactor] and τ_g [Eq. (16), the mean time necessary to generate a new neutron] except if

$$\int_R dx [P^*(x) - k_1 D^*(x)] \phi_i(x, t) = 0 \quad \text{for } \phi_i(x, t) \neq 0. \quad (19)$$

In this case $\tau_1 = \tau_g = \Lambda$. This condition is only satisfied for certain calculational models or material compositions. In the classical terminology τ_g corresponds to the neutron lifetime and Λ to the generation time.

Description of the Physical Models and the Variance-reducing Methods Used in TIMOC

In the TIMOC code the phase space (x) is subdivided into geometrical regions filled with mixtures of isotopes and into energy groups with group-averaged nuclear parameters. The scattering kernel $D(y \rightarrow x)$ allows for each isotope the description of the following scattering processes:

- a) isotropic scattering in the CM system;
- b) anisotropic scattering in the CM system if either a table of measured angular distributions or six Legendre coefficients are specified (see Ref. 7). Also a P_1 -approximation is possible if the averaged value of the angular distribution of the laboratory system is entered; the energy loss is calculated by the use of the classical scattering law after determining the scattering angle;
- c) inelastic scattering by level excitation;
- d) inelastic scattering by the evaporation model;
- e) inelastic or elastic scattering by transfer matrices, in which case a factor for the average angular distribution can be specified.

The production or fission kernel $P(y \rightarrow x)$ calculates for each isotope the number and energy of the secondary neutrons as a function of incident neutron energy by a third-order polynomial for $\nu(E)$ and a Watt-type fission spectrum.

The neutron transport is described by the choice of random walks taken from an exponential distribution.

By use of the source term $S(x)$, it is possible to start with mono-energetic neutrons or with neutrons with the energy distribution of the fission spectrum. These neutrons can originate from a point source or be equally distributed in a geometrical region. If the primary neutrons start

with a fission spectrum energy distribution, "systematic sampling" is applied. The direction vector of the primary neutrons can be chosen to be isotropic or into a fixed direction.

During the course of a neutron history, space and time coordinates are calculated for each boundary crossing and collision. For the latter also the energy vector and the weight are determined. The weight "w" decreases at each collision point "c" by the amount of the absorption probability:

$$w_c = w_{c-1} \frac{\Sigma_s}{\Sigma_t}, \quad (20)$$

where w_{c-1} is the weight before, and w_c the weight after the collision.

Fission: During the decay of the neutrons of one generation, new neutrons of the next generation are born. In the TIMOC code they are calculated by the method of fractional generated neutrons. Fractional neutrons are generated at each collision point and for each fissionable isotope. The fractional generated neutrons are then accumulated separately for each isotope until their sum reaches the magnitude of the initial weight factor " w_0 ." Thus,

$$\psi_{k,c} = \psi_{k,c-1} + w_c \frac{[\nu(E) \Sigma_f(E,r)]_k}{\Sigma_t} \quad (21)$$

For further information, see Ref. 7.

When $\psi_{k,c}$ becomes equal to or greater than w_0 , the location at which this happened and other characteristic parameters like the time, etc., are stored in a buffer storage, and $w_{k,c}$ is reduced by w_0 . The current history is continued normally. The next history (or histories) is, however, a secondary neutron which starts according to the previously-stored information.

History Termination

Neutron histories are finished by leakage, by slowing down below a specified energy limit, or by a Russian roulette procedure which can be used as an optional feature.

The Calculation Schemes and the Sampling Procedures of TIMOC:

Generally one has to distinguish between two types of calculations: one where transient phenomena are studied, and the other where the final fundamental mode distribution is of interest. Depending on the specified option the code can treat:

Transient studies, neutron burst experiments, and assemblies with constant external sources require that the primary neutrons be taken into account in the sampling procedure. On the other hand, it is possible to exclude a certain number of neutron generations at the beginning in order to calculate reactor parameters which are characterized by the fundamental mode distribution. Calculations have shown that in many cases the neutron population died away before the equilibrium distribution was obtained. For this reason the code is equipped with a mechanism which allows a continuous iteration of neutron generations. This is done by filling up the buffer storage to its total capacity with additional starting parameters for secondary neutrons. These parameters are taken by a random choice from the last set stored in the memory.

The sampling procedures of TIMOC calculate the following reactor parameters:

- a) reactivity, dynamical or statical, as defined in Eqs. (7) and (9);
- b) geometrical escape probability (or leakage factor);
- c) slowing-down density below the specified energy limit;
- d) number of secondary neutrons per inserted primary neutron for each fissionable isotope;
- e) the neutron flux as a function of energy group and region. It is calculated by using the sum of the product of track lengths (per specified energy group and region) and the corresponding weight factor;
- f) the transmission coefficient between geometrical boundaries in both directions. This is particularly useful, for example, for the calculation of leakage spectra.

The following parameters include time estimates. Depending on the aim of the calculations, the time is set to zero for each fission neutron starting in the system or only for the primary or source neutrons. If it is set to zero for each fission neutron and if the transient generations are neglected, this procedure is equivalent to the insertion of neutrons with the equilibrium distribution at $t = 0$, as was requested for Eq. (10).

If, however, the time behavior of neutron chains or of transient phenomena is studied, the time is set to zero only for the start of primary neutrons.

- g) the time-dependent production rate as defined by Eq. (13) and (14) for certain time intervals specified in the input:

$$N_p(t_i^*) = \frac{\sum_h \sum_c \sum_k \psi_{h,c,k} t_{h,c}^*}{(t_{i+1} - t_i) \sum_h \sum_c \sum_k \psi_{h,c,k}}, \quad (22)$$

where $t_i \leq t_{h,c}^* < t_{i+1}$ and $t_i^* = (t_{i+1} - t_i)/2$. The summation index h is taken over all histories; the summation index c is over all collisions, and k is over all fissionable isotopes.

h) the average time for generating a new fission neutron [see Eq. (15)]:

$$\tau_g = \frac{\sum_h \sum_c \sum_k \psi_{h,c,k} t_{h,c}}{\sum_h \sum_c \sum_k \psi_{h,c,k}} \quad (23)$$

i) the time-dependent destruction rate as defined by Eq. (12) for certain time intervals:

$$N_D(t_i^*) = \frac{\sum_h \left(\sum_c w_{h,c}^{ab} t_{h,c}^* + w_h^{\text{leak}} t_h^* + w_h^{\text{slow}} t_h^* \right)}{(t_{i+1} - t_i) h w_0} \quad (24)$$

where $w_{h,c}^{ab}$ is the absorbed weight at collision c in history h :

$$w_c^{ab} = w_{c-1} - w_c,$$

w_h^{leak} is the weight factor at the time of leakage in history h , w_h^{slow} the weight factor at the time the neutron slows down below the lowest energy limit, and

$$t_i \leq t_{h,c}^* < t_{i+1}.$$

j) the mean time the neutron lives in the reactor defined by Eq. (15):

$$\tau_l = \frac{\sum_h \left[\left(\sum_c w_{h,c}^{ab} t_{h,c} + w_h^{\text{leak}} t_h + w_h^{\text{slow}} t_h \right) \right]}{h w_0} \quad (25)$$

Details about TIMOC

The TIMOC code was developed out of the MOCA-II code.^(6,8) It is written for the IBM 7090. The code is split into three parts. Part I (FORTRAN II) is used to write the nuclear-data library on the library or systems tape. Part II (FORTRAN II) selects from the library tape the nuclear parameters which are used for a particular calculation. This part of the program prepares these parameters, sets up the isotope mixtures, and calculates probability tables for use by the main program. The intermediate information is written on a "scratch" tape and read by Part III (FAP), which carries out the Monte Carlo calculations. All the scattering and sampling calculations are done in the main program. The geometry routines in the main program can be easily exchanged.

At the present time TIMOC includes routines for multilayered spherical shells, multilayered finite cylinders, and a three-dimensional mockup of the pulsed reactor SORA.⁽⁹⁾ The present system allows the use of up to 50 energy groups, 15 geometrical regions, 15 isotope mixtures, 15 isotopes per mixture, and 50 time intervals.

Comparisons with equivalent two-dimensional TDC calculations showed that the consumption of computer time was considerably below that of the S_N code, if a 0.5% standard deviation in k_{eff} was specified. In three-dimensional assemblies the gain in time is even more significant.

Recent Development of the Code

In a further development of the code, a subprogram has been added to write the characteristic parameters (weight, time, energy vector, etc.) at each boundary crossing and collision process into a buffer storage and simultaneously during the calculation on a tape. Later on this tape can be scanned under different points of view by another program, which provides a greater flexibility for the study of time-dependent effects.

Application and Experience

Because of the calculational procedure used in TIMOC, the code is mainly applicable to small systems in which the geometrical dimensions of the fission zone are of the same order of magnitude as the mean free path.

In a first set of test calculations, a number of fast assemblies was calculated by TIMOC, and compared with experimental measurements and equivalent S_N -calculations. In these calculations the 16-group set of YOM,⁽¹⁰⁾ and, below 500 keV, the parameters of the 18-group set of LASL⁽¹¹⁾ were used. At energies above 2 MeV the group structure was more refined, so that there existed altogether 33 groups in the range from 0.1 eV to 10 MeV.

The calculated values of k_{eff} for more than 20 different fast assemblies⁽⁷⁾ showed a good agreement with measured values. In almost all calculations the reactivity worth was slightly overestimated by 0.5 to 1.5%. Good test cases were the beryllium-reflected spheres with a 1-, 2-, and 4-in. reflector. In these assemblies one gets a significant spectral shift for different reflector thicknesses. In a second series of test calculations, the 26-group constants published by a Russian team⁽¹²⁾ were applied with equally good success. The second aim of the TIMOC program was the calculation of lifetimes.

Contrary to the results with S_N -calculations, good agreement with measured Rossi-lifetimes was observed. The deviation was less than 5% from the measured values.

Another wide field of application is studies of neutron burst experiments in multiplying and nonmultiplying assemblies. In particular, the time-dependent growth and decay of neutron populations has been studied for different assemblies as a function of energy and position of the source.

The calculation of neutron yields in accelerator boosters as a function of the neutron-source parameters is foreseen as a future application in this field.

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SUMMARY AND PANEL DISCUSSION

MR. KOWARSKI (European Nuclear Energy Agency): Let's start the summary. Each chairman has about five minutes in which to give his impression of the session he has chaired.

MR. AVERY (Argonne National Laboratory): The first session consisted of the invited talk on some of the trends in computers and their implications. This was followed by a series of papers on calculations in reactor physics and shielding. The most interesting aspects were when, either in the papers or in the discussions, we touched on what seems to me a very important problem, that of the proper role of the computer. One can treat it both in its very general aspect of the proper role, and also in the specific aspects of which codes or methods are best for specific problems. Worlton, in talking about the trends gave impressive statistics about the growth of computers. In a matter of a few years we will have computers of the order of twenty times the speed of STRETCH. He also pointed out that the needs for this growth of computers are there, in terms of our needs in reactor calculations.

Schaefer, perhaps, took a somewhat opposite point of questioning whether in fact in all cases some of these very large calculations are required. The particular example he gave was that of thermal-neutron distributions in space and energy in a lattice form, certainly not a simple case. His evidence seemed to be quite good that in this particular case some of the simpler methods are in fact right. None of us involved in reactor calculations can really deny that many times computers are misused and that far greater detail is sought than is actually required.

Brissenden followed with a discussion involving somewhat detailed calculations of neutron spectra in the Doppler region. Here, perhaps, the most interesting questions relate to treatments in the unresolved region and statistical aspects. One uses the straightforward treatment, as did Brissenden, or one can, perhaps, do something in a more mathematical way by dealing with the statistical aspect of the problem.

Lathrop, and also Penkuhn, discussed some of the photon-diffusion problems. Lathrop showed that the discrete-ordinates method, considering not too great a number of terms in the scattering angular distribution, seemed to give good results and apparently is much better than, at least, the Monte Carlo methods that he quoted in comparison in terms of time. The moments method has also been used for these problems. His conclusion seemed to hold for the simple geometries discussed.

Pull also made comparisons with Monte Carlo (generally, it seemed to be a bad morning for Monte Carlo). I don't know if anyone intended it so, but, again, the point was made that even in complex geometries the use of collision probabilities may be the way to handle many cases.

MR. EHRLICH (Knolls Atomic Power Laboratory): Session II dealt with numerical analysis in reactor mathematics. The invited paper, Margaret Butler, Johnny Rosen, and Betty Maskewitz' discussion of the three library and information centers, was somewhat apart from the mathematics and analysis. The paper dealt with the history of the past decade, during which the users began to need some means of communicating with one another as to what kinds of codes they had, what they could do, and, in general, to the extent that the machines and the languages allowed, making their codes available to each other. Under this stimulus, we now have the Argonne and the ENEA library centers and specialized centers, such as RSIC at Oak Ridge. For the future these are tools, which if we are cooperative and use them intelligently, I suspect can aid in solving the problem that Avery has just mentioned. Are our computers monsters, or are they useful to us, and can we use them economically? I would hope that by intelligent and cooperative use of the Centers' efforts we could keep the computer situation in a fruitful path. I would hope that these centers would encourage people to move, as the last speaker of that paper indicated, towards universal languages, adequate documentation, and adequate communications to make their efforts effective.

In the contributed papers on numerical analysis and mathematics, all made use of the variational principle. All depended on developing an appropriate functional and deriving the useful properties. The papers dealt with the stationarity of this functional.

Galligani showed how such an approach could be used in handling the time-dependent kinetics problem and solving the resulting equations either by the Kantorovich or the Euler methods. In some practical problems where he was able to try these two approaches, I had the impression that the conclusion was somewhat inconclusive, namely, you get comparable times and comparable results from either of these approaches to the solution.

In Kellogg's paper on the Ritz-difference equations on the triangulation, we obtained some rigorous mathematical discussion of the accuracy, the truncation error, and what have you, involved in setting up this variable-spaced triangular mesh. Mr. Kellogg was able to indicate rigorously the behavior of this difference-equation approach. This is probably a fruitful sort of tool to help us advance to meshes where the geometry and the space points tend not to be synonymous. That seemed to be one of the strong features of this definition.

Finally, there were two papers on multidimensional diffusion with new techniques for iterating. After ten years people still are coming up with new ideas which seem to offer big improvements, and there would seem to be a field here for continued effort. We seem to be making interesting progress.

MR. MOUNT (Bettis Atomic Power Laboratory): In the session on linked calculations I have chosen to look at only three of the papers. By way of explanation, I am a machine man with a vast ignorance of physics.

Mr. Stevens indicated that the system about which he was talking should be big, fast, flexible, and simple. Mr. Breen indicated the importance of balancing generality and cost. Stevens allowed a variety of models and options. Breen allowed user specification of the depletion chains. Stevens fitted tables to simple expressions. Breen supplied tables for interpolation purposes. In both cases, the input data are saved, in one case on tape and in the other on cards. Mr. Stevens emphasized several time-saving gimmicks in the program--minimal use of exponentials, for example. Mr. Breen indicated the importance of saving space, using dynamic storage allocation for this purpose. Both indicated the saving of output on tape; both provided edit options. I think a most significant thing was the graphical output and the absence of digital output which Mr. Stevens has managed to stuff down the throats of the engineers. That is, I think, a very significant success.

It appeared to me that the goal of Mr. Turner was the saving of programmer time, providing flexibility through the use of modules and the use of input-output files from the DATAPOOL. It disturbed me a little that, in the written paper at least, all of the storage except the main core was to be included in the DATAPOOL. There was a reference, also, to a routine called the Director--actually the control program itself--which controlled all the modules. I think there are a few serious questions in the application of this technique. One will be the necessity to modify the Director as different pluggable modules are added to the system. Using the DATAPOOL concept for the scratch storage, particularly in an iterative process, looks like it could be very inefficient. Finally, the concept of the generalized matrix in the representation of the diffusion equation also indicates a great possibility for inefficiency.

MR. SYRETT (General Electricity Generating Board, London): In Session IV the papers fell into two halves. The first three papers were on fuel-cycle and reactor-lifetime studies, and to some extent were an extension of those in the previous session. What I propose to concentrate on, in the short time available, is the latter three papers which were on reactor kinetics as such. I think there was a rather interesting feature, at least interesting to one coming from Europe.

On the static side, in calculation of reactivity and static power distributions the tendency has been, all through this conference, for American methods to be very much more elaborate than those used in England. The converse seems to be true in the kinetic field. On the reactor static side the European views were typified by the papers of Schaefer and Griggs in the earlier sessions, in which simple methods of computation were suggested; not too simple, but just sufficiently sophisticated to be quite adequate to give good agreement with experiment, and sufficient for competent

reactor design. In contrast to this was the American approach of making the model as complicated as one could in the hope it would then be as accurate as it could be.

On the kinetic side, though, the picture seems entirely reversed. Here the U. S. work was, I think, typified by the paper we heard on the AIROS code, a point-kinetic code, and, I would say, by European standards, a fairly simple kinetics code. In the United Kingdom and in France, on the other hand, quite a lot of computing effort has gone into writing much more elaborate kinetic programs. I think this is largely historical, and it is based on the way reactor design has gone in the two countries. In the United Kingdom and France most reactor design work, until now, has been on large graphite reactors with positive temperature coefficients, and core diameters of, perhaps, fifty migration lengths. This, of course, is the ideal system to produce spatial instabilities in flux. This, combined with the fact that these large systems have no containment, means that one has to adopt a very stringent safety philosophy to ensure that there is no possibility of any significant fission product release. In fact, a very, large amount of effort in the United Kingdom and France has gone into these complicated safety calculations, in which one carries out very many three-dimensional kinetic calculations. So far, this has been unnecessary in the United States. I wonder, now that people over here are considering big water reactors--1000-MW light water reactors--where the core size is increasing relative to migration lengths, whether, in fact, we will find that over here, too, spatial kinetics will become more and more important.

MR. OKRENT (Argonne National Laboratory): My first comment is going to be that I expect an increasing amount of computational work on reactor safety in the United States. Only a part of this will be related to the stability questions in the larger reactors. I think Mr. Ergen's paper and some of the comments made during the discussion indicated many problems in reactor safety that will have to be calculated in a more sophisticated fashion, for one reason or another. The other papers were all very good, each on a different subject. The paper on neutron resonance phenomena indicates graphically that computers tend to make us less and less approximate in our calculations, and give us a good chance to see what errors have been introduced in the past by various approximations in the treatment of resonances. Hopefully, this does not mean that all calculations will be done in the most sophisticated way, hereafter; I feel still a little in sympathy with Mr. Schaefer's plea for doing what you need to do and not much more.

The paper by Mr. Hutchinson gave a very good example of how one has a chance of improving both accuracy and running time by looking at past history to see if there is a departure in method which really represents a considerable improvement. He further stated that this should even make things easier for the engineers' use. I would say that this combination is remarkable, indeed.

Mr. Crowther dealt with a very important reactor-design technique which I think is slightly related to the dynamic questions mentioned by the previous chairman, and I would like to come back to that in a moment in another sense.

The paper on energy yield in a fast reactor accident suggested some ideas for improvement in what is still a beginning field so far as reactor calculations go. I expect more work will be done in this area in the coming years; the discussion pointed out that there is a lot to be done in the equation-of-state field here, and one has to be cautious and learn more about applying this method when one has, let's say, a thermalizing reflector around a fast core or the equivalent. One thing that occurred to me during this session and some of the earlier sessions was whether, in addition to a computer god, there wasn't, perhaps, a computer demon, or a computer devil, in this sense.

We saw in Mr. Crowther's paper a great reliance placed on the computer in designing the system, computing burnout ratios, and so forth. People are now thinking of schemes of controlling the positions of control rods during operation by the use of computers and, in part, this is related to safety.

I have enough experience myself with errors coming out of computing machines; sometimes, long chains of apparently consistent results were wrong. I wonder if there isn't going to be a fruitful field of research to see whether you can find computer-caused accidents.

MR. UNDERHILL (AERE, Winfrith): Notwithstanding the last speaker, I would like to say, quite unashamedly, that my view of a computer is that it should be used in such a way as to save people thinking. If I may go back ten or fifteen years, before computers really started, to calculate the critical size of a bare sphere of enriched uranium was something to occupy the top physicists' brains of the country for quite some time. Once computers started, that kind of problem was reduced to triviality; in a little while, the top physicists' brains were being used on more complicated problems. I would like to see this situation continue and continue, until the kind of problems we are worrying about now are themselves reduced to trivialities which one can put on a computer, get an answer, and forget all about, except for the answer. In this sense, of all the methods which are currently available to us, I feel Monte Carlo is the one most likely to meet this kind of objective.

Although Mr. Honeck had some doubts as to whether his paper, connected with the processing of nuclear data, was relevant to this session, I think it really was relevant. Nuclear data are, of course, the start of the chain for Monte Carlo calculation. We really need exact data and it is essential to have an automated procedure. He described the various attempts

which are currently being made along this line. Great progress has already been made though there is room for a great deal more progress in the future.

The second paper dealt with a fairly specialized technique for dealing with the main fault, or main annoyance, of Monte Carlo--the great amount of computer time it takes and the rather annoying statistical error one gets from the results. One can say that there are many such techniques; the one described seemed very interesting. I wonder, though, in the light of my general objective of a black box which I needn't worry about, whether in ten or twenty years, when computers are ten or a hundred times more powerful than they are now, such techniques will still exist or we will be back to the real "brute force and ignorance" type of Monte Carlo tracking.

As to the last paper, with no disrespect to the author, I think it can be categorized as the "brute force and ignorance" technique, and because of that, it is a valuable example of a Monte Carlo program. This really is an attempt to create a program in which you put in the geometry and let the computer do the rest. With present computers you cannot go all the way; nevertheless, this is the type of program of which, I am sure, we shall see a lot more in the future.

Finally, one more remark about nuclear data. No matter how good the method of calculation, it must rely on the accuracy of the nuclear data; therefore, this type of development will create a greater and greater demand for more and more really, physically-accurate nuclear data.

MR. KOWARSKI: We still have something like twelve minutes left and I certainly do not propose to talk for twelve minutes. I always like to see a good fight; is there enough in these briefly expressed opinions to start one? Does anyone feel that something outrageous has been said by one of his colleagues?

MR. SYRETT: Could I open the discussion by making a rather contemptuous remark? In the very first paper there was a discussion on the new-generation computers with which we are being threatened, any day now. It was strongly pointed out there that these would make computing very cheap because the cost per mathematical operation would be reduced by an order of magnitude. Is this really important? The ultimate thing of importance is surely the cost per useful piece of output. I think experience in the past has shown that a sort of Parkinson's law applies to computing and that the computing requirements always expand to fill the machine available. With the faster computers it is probable that computing costs per organization will rise, not fall, because people will do many more things; whether these will be worth doing is another question. Along this line I think one has to be wary of the danger of erecting a complex edifice of highly sophisticated numerical methods for, say, solving the homogeneous diffusion

equation, on shaky foundations. For example, Griggs suggested that the process of refining calculations of this sort by taking more mesh points in fact did not improve accuracy, although it increased machine time by a large factor. In fact, the accuracy decreased because of the errors in the diffusion theory he was starting with.

MR. OKRENT: This brings us back to the black-box desire mentioned by my colleague. I am concerned that this box may get too black. After a certain time it would be believed that it can do no wrong, and then none of these top brains that were mentioned would any longer be there to notice an obvious error, perhaps one fatal to the reactor, of a kind that doesn't turn up until the reactor is turned on.

MR. KOWARSKI: In this domain, as in every other, there should be a combination of sufficient and competent computations together with some amount of good common sense to see that the black box hasn't led us astray. If a computer is properly checked in its black-box role, there is not much more danger that it will create an accident than for the computation made at my bank to present me with an unexpected one-thousand dollar surplus at the end of the month. It just doesn't happen!

MR. OKRENT: It has happened.

MR. EHRLICH: Aren't you apt to make computer mistakes or interpretation mistakes as readily in a simple computer program, so-called, as in a complicated one? Just because the computer completes more operations, and so on, are you necessarily going to make a bad mistake that you might not make in a simple calculation? As long as you look at what you are doing and see that it bears some relation to things you can observe and use as checks, and as long as you have the power to calculate some of these complicated phenomena that go on in reactors, then, maybe, you really can design and build a better reactor. If you are careful, your chances of being wrong are probably no worse than by use of a slide rule.

MR. OKRENT: At this stage I should say that some of my best friends are computers. My concern is that if you omit all intermediate understanding from the beginning of the problem to the final output, there is a greater chance that errors will come in that are not caught.

MR. ERLICH: I agree. We should not try to omit the understanding.

MR. UNDERHILL: My black-box philosophy does not necessarily lead to the omission of this understanding. It just means that one is not wasting one's time thinking about problems which can be trivially done on some future computer. A comment on the question of computer speeds and costs: it seems to be fairly general that, as computers have got

faster, they haven't cost substantially more per hour to run. A few hundred dollars per hour is now the cost of a modern computer, and it was the cost of a modern computer any numbers of years back. In practice, a convenient program runs for an hour or a couple of hours. This gives us the chance, as computers get faster, to do much more complicated things in this given time at this given cost. One can spend an awful lot of hours on a computer before one matches the cost of doing the same thing by an experiment.

MR. AVERY: As we go, and we probably will, to these far more complex calculations, we should perhaps try to define rather carefully what the objectives are. One might well be the reduction of critical experiments, etc., which could then be translated to economic evaluation relative to the computer costs involved. There may be also other objectives: to trace the time history of a reactor and its control rods, or the programming of fuel management. We are almost able to do such things now.

MR. KOWARSKI: We have heard a warning that computers should not be used too blindly and that there will still remain a role for intervening humans to use their common sense for checking purposes, if they have any common sense. We also hear an optimistic note that, therefore, computers, at least in this particular branch of human endeavor, will not create too much unemployment, but then we hear another warning--that the availability of very fast computers which do not cost very much, and the concern for job security may lead people to create work consisting of unnecessarily complicated computational problems. It is an interesting balance of optimism and warnings, as usual.

I have the pleasant duty to congratulate the organizers of this conference for an excellent job. Since one of the sponsors is the European Nuclear Energy Agency with which I am connected myself, the moderator has to exert some moderation in that particular direction. This leaves me more free to lavish my praise on the Argonne part of the organization. Its numerous committees have all contributed to the success of this conference; all their members ought to be mentioned, but there are only two minutes left. So let us concentrate on the general chairman, Mrs. Butler, whom I would like to single out for these last words of thanks and praise. The conference is adjourned.