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Mathematics Division

*Annual
Progress Report*

Period Ending December 31, 1972

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MATHEMATICS DIVISION
ANNUAL PROGRESS REPORT
for Period Ending December 31, 1972

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Mathematical Research

EXISTENCE OF NONOSCILLATORY SOLUTIONS

J. M. Dolan

For the differential equation

$$y''' + py = 0, \quad p \in C[a, \infty),$$

the question of whether or not there is a solution with at most a finite number of zeros is an unsolved problem. Significant contributions to this problem have been made by (1) giving equivalent formulations of this problem and (2) stating sufficient conditions for a nonoscillatory solution in terms of upper and lower solutions of the above differential equation.

Dominant Sets of Solutions

For the linear third-order differential equation

$$(H) \quad y''' + py' + qy = 0, \quad p, q \in C[a, \infty), a \text{ real},$$

let $\mathcal{S}$ denote the three-dimensional solution space. For a decomposition

$$\mathcal{S} = \mathcal{S}_1 \cup \mathcal{S}_2, \quad \mathcal{S}_1 \cap \mathcal{S}_2 = \{0\},$$

the set $\mathcal{S}_1$ is said to dominate the set $\mathcal{S}_2$ at the number c ($|c| \leq \infty$) if for each $y_i \in \mathcal{S}_i$, $i = 1, 2$, there is a number interval (a, b) containing c such that

$$y_1 + \lambda y_2 \in \mathcal{S}_1, \quad \lambda \in (a, b).$$

For the case in which sets in the decomposition are $\mathbb{R}$ and $\mathbb{C}$, respectively, the set of nonoscillatory and oscillatory solutions of (H), the above definition is shown to have particular relevance when $c = 0$ or $c = \infty$ and to give a useful way of classifying the asymptotic properties of solutions of (H).

ENERGY RELEASE INTEGRAL

S. J. Chang

The energy release integral is a useful expression to measure the energy flow due to the mobile inhomogeneities in a continuum medium such as the moving dislocations or defects. Its integrand can be

identified as the energy-momentum tensor, which is well known in classical field theory. To make it applicable more appropriately in continuum mechanics, we generalized it to finite elasticity and finite viscoelasticity^{1,2}. We shall continue to investigate along this line so as to develop a fundamental field theory in continuum mechanics.

VISCOELASTIC WAVES

S. J. Chang

The propagation of stress waves as generated by an unsteady crack in a viscoelastic medium has been investigated. A solution is derived from a system of recursive Abel's integral equations which are obtained from an integral representation similar to Poisson's formula for the wave equation. The present solution contains an additive branch which can be identified as the exponential decay of the corresponding elastic solution, a phenomenon first discovered by Lee and Kanter.

STOCHASTIC PARTICLE TRANSPORT PROCESSES

R. R. Coveyou

The aim of this effort is to produce a consistent and coherent theory of particle transport processes as stochastic processes. This is, on the technical level, a difficult but approachable problem. However, there are great conceptual difficulties. These difficulties may be traced back through the foundations of particle transport theory, through those of statistical mechanics (to which particle transport theory owes, historically, its conceptual basis), to the way in which stochastic concepts have been introduced into physics. There has always been a certain conceptual fog over this process. This is probably due, historically, to the fact that, when statistical mechanics originated, probability theory itself lacked a sound mathematical basis.

The theory of probability now possesses such a sound basis, but modern treatments of stochastic physics do not reflect this fact. Hence, as preliminary to the examination of the particle transport processes which are the major theme of this study, an analysis is being made of the more fundamental problem of the application of stochastic concepts in physical theory.

ERGODIC ACTIONS OF GROUPS

G. K. Haeuslein

We consider the problem of constructing new ergodic actions from known ergodic actions. Let G_1 be a locally compact group acting ergodically on the space S , and let G_2 be another locally compact group. Mackey described a construction which turns the product space $S \times G_2$ into an ergodic $G_1 \times G_2$ space.³ We have studied ergodic flows on the torus obtained by application of this construction.⁴

1. S. J. Chang, "Path-Independent Integral for Rupture of Perfectly Elastic Materials," *Z. Angew. Math. Phys. (ZAMP)* **23**, 149 (1972).

2. S. J. Chang and Barry Bernstein, "Energy Release Integral for Finite Elastic and Viscoelastic Materials," Proc. Sixth Intern. Congress on Rheology, Lyon, France, Sept. 4-8, 1972.

3. G. W. Mackey, "Ergodic Theory and Virtual Groups," *Math. Ann.* **166**, 187-207 (1966).

4. G. K. Haeuslein, "Skew Product Ergodic Flows on the Torus," submitted to *Math. Ann.*

KWIC INDEX

A. S. Householder⁵

A KWIC Index of publications in linear algebra had previously appeared in two parts, and one on the numerical treatment of nonlinear equations, algebraic and transcendental, in one. A new volume⁶ combines all these items with a number of others, some previously overlooked, but mostly new publications, for a total of 5436 titles. Included with the listings are references to reviews in the four standard review journals: *Computing Reviews*, *Mathematical Reviews*, *Referativny Zhurnal*, and *Zentralblatt*.

A supplementary volume is now being prepared and will be issued shortly, to contain, again, mostly new publications, but also some that had been omitted, and, in addition, new review references to items already listed.

APPLICATIONS OF THE METHOD OF INVARIANT IMBEDDING

P. Nelson D. E. Amurios W. Robert Boland⁷

This item is a continuation from the 1971 annual report.⁸ The computer program embodying the application to a large boundary-value problem of structural mechanics has been developed to a point which has permitted extensive trial computations for more or less realistic systems. Its performance has been generally satisfactory, although there is an occasional computational difficulty whose source is not fully understood, but which is currently under investigation. In general support of this work, mechanical interpretations have been developed⁹ for the auxiliary functions which appear in the Scott¹⁰⁻¹² version of invariant imbedding, and this method has been compared,¹³ as regards computational efficiency and effectiveness for a somewhat limited class of problems, with a commonly used version of the method of superposition.

A preliminary study has been made of the feasibility of applying product-type quadrature¹⁴⁻¹⁶ formulas within the discrete-ordinates method of neutron transport. An application to one-dimensional criticality problems was successful but did not appear to offer significant advantages over the usual quadrature formulas. There does appear to be a possibility that product-type formulas will be advantageous for deep-penetration problems such as are of interest in shielding, although this remains to be investigated in detail. The one-dimensional criticality studies did lead to development of an efficient and accurate computer code for determining critical size by integrating the R equation of invariant imbedding to

5. Consultant.

6. A. S. Householder, *KWIC Index for Numerical Algebra*, ORNL-4778 (June 1972).

7. ORAU Summer Faculty Fellow from Clemson University.

8. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 6.

9. P. Nelson, "Mechanical Interpretations for Invariant Imbedding," submitted to *J. Eng. Mech. Div., Amer. Soc. Civil Eng.*

10. M. R. Scott, "Invariant Imbedding and the Calculation of Internal Values," *J. Math. Anal. Appl.* 28, 112-19 (1969).

11. P. Nelson and M. R. Scott, "Internal Values in Particle Transport by the Method of Invariant Imbedding," *J. Math. Anal. Appl.* 34, 628-43 (1971).

12. P. Nelson and M. R. Scott, "The Relationship between Two Variants of Invariant Imbedding," *J. Math. Anal. Appl.* 37, 501-5 (1972).

13. P. Nelson, "A Comparative Study of Invariant Imbedding and Superposition," to appear in *Int. J. Comput. Math.*

14. W. R. Boland and C. S. Duris, "Product Type Quadrature Formulas," *BIT* 11, 139-58 (1971).

15. W. R. Boland, "The Numerical Solution of Fredholm Integral Equations Using Product Type Quadrature Formulas," *BIT* 12, 5-16 (1972).

16. W. R. Boland, "The Convergence of Product-Type Quadrature Formulas," *SIAM J. Numer. Anal.* 9, 6-13 (1972).

machine overflow. A supporting theoretical analysis has been made, and it is anticipated that these results will be reported in the literature in the near future.

VARIATIONAL SYNTHESIS IN NEUTRON TRANSPORT

P. Nelson

Variational synthesis with discontinuous trial functions has recently been the subject of considerable controversy in the literature.¹⁷⁻²⁰ One aspect of this subject which has been somewhat disturbing is the "overdetermination problem," whose existence was first observed by Buslik.²¹ Several schemes have been proposed for avoiding this difficulty, but with regard to many of these Stacey²² makes the following comment. "Thus all of these stratagems for removing the overdetermination of interface conditions have certain unsatisfactory features. Moreover, there is a sense something is fundamentally wrong when the variational derivation yields overdetermined interface conditions for trial functions which are theoretically admissible."

Work has been initiated on a series of articles (a total of three is currently projected) in which the basic viewpoint is that indeed "something is fundamentally wrong" with discontinuous variational synthesis as usually presented in reactor physics, namely, a general failure to adhere to basic physical and mathematical principles. In the first article²³ of this series there is presented a new variational functional which admits discontinuous trial functions but is not subject to the overdetermination problem. The basic idea, as suggested by physical considerations, is to consider the flux and current *at* the interface as independent quantities, in particular being *independent of the limiting values from either side*. The mathematical details are developed by first suitably generalizing the Roussopolos²⁴ variational principle and then applying this generalization to the transport equation considered in appropriate function spaces.

A STUDY OF THE PHASE TRANSITION FUNCTION OF R. L. DOBRUSHIN

W. Robert Boland⁷

In two related papers,^{25,26} R. L. Dobrushin introduced the phase transition function

$$Q(T) = \frac{S_\nu e[1 - \exp(-1/2T)]}{3[1 + \exp(-\nu/T)]} \sum_{k=2\nu}^{\infty} [3 \exp(-1/2T)]^{k\nu/(\nu-1)}$$

17. P. Nelson, "Variational Synthesis with Discontinuous Trial Functions: Comments on a Paper by Lambropoulos and Luco," *J. Nucl. Energy* **26**, 43-44 (1972).

18. P. Lambropoulos and V. Luco, "A Reply to Nelson's Letter 'Variational Synthesis with Discontinuous Trial Functions,'" *J. Nucl. Energy* **26**, 211-12 (1972).

19. A. J. Buslik, "Comments on Variation Flux Synthesis Methods for Multigroup Diffusion Theory," *Nucl. Sci. Eng.* **49**, 112-14 (1972).

20. W. M. Stacey, Jr., "Reply to 'Comments on Variation Flux Synthesis Methods for Multigroup Diffusion Theory,'" *Nucl. Sci. Eng.* **49**, 114-15 (1972).

21. A. J. Buslik, "A Variational Principle for the Neutron-Diffusion Equation Using Discontinuous Trial Functions," *Trans. Amer. Nucl. Soc.* **9**, 199 (1966).

22. W. M. Stacey, Jr., "Variational Flux Synthesis Methods for Multigroup Neutron Diffusion Theory," *Nucl. Sci. Eng.* **47**, 449-69 (1972).

23. P. Nelson, "Variational Principles Which Admit Discontinuous Trial Functions - Part I: The Overdetermination Problem," submitted to *Nucl. Sci. Eng.*

24. P. Roussopolos, "Méthodes Variationnelles en Théorie des Collisions," *Compt. Rend.* **236**, 1858-60 (1953).

25. R. L. Dobrushin, "Existence of a Phase Transition in the Two-Dimensional and Three-Dimensional Ising Models," *Dokl. Akad. Nauk SSSR* **160**, 1046-48 (1965), translated as *Sov. Phys. Dokl.* **10**, 111-13 (1965).

26. R. L. Dobrushin, "Existence of a Phase Transition in the Two-Dimensional and Three-Dimensional Ising Models," *Theor. Probab. Appl.* **10**, 193-213 (1965).

for qualitatively proving the existence of phase transitions in the Ising model. Here S_v is the volume of a v -dimensional sphere of unit surface area [$S_2 = (4\pi)^{-1}$ and $S_3 = (6\sqrt{\pi})^{-1}$]. Dobrushin's main result is that if $v > 1$ and

$$Q(T) < \frac{1}{v} < 1 - Q(T),$$

then a phase transition takes place at the point (v, T) . Using analytical properties of Q , regions of the volume-temperature plane where phase transitions occur were determined. A table of values of $Q(T)$ for a range of values of T was generated.²⁷

GENERALIZED PRODUCT-TYPE QUADRATURE

W. Robert Boland⁷

A study of product-type quadrature, a concept introduced by Boland and Duris,¹⁴ was extended. Some of the results were generalized and reported elsewhere.²⁸ Other effort in this area was the application of the generalized product-type rules to linear Fredholm integral equations of the second kind with rapidly varying kernels. This is an extension of work previously published.¹⁵

TIME-DEPENDENT LINEAR TRANSPORT

D. G. Wilson

Two papers on this topic have been submitted for publication. These concern existence, uniqueness and continuous dependence of weak solutions, and approximation of such solutions by finite differences. Projected papers concern continuity properties of weak solutions and convergence of the discrete-ordinates approximation. These papers include and extend results from my dissertation.²⁹

PIECEWISE LINEAR APPROXIMATIONS

D. G. Wilson

We have modified a previously published algorithm³⁰ to approximate tabulated data within specified tolerances. A computer program implementing the new algorithm has been placed in the subroutine library.

MATRICES PERMUTATIONALLY SIMILAR TO DIRECT SUMS

J. A. Carpenter

Let $A = (\alpha_{ij})_{n \times n}$, where the α_{ij} are arbitrary, but not all zero, for specified values of $k = i - j$, $-(n-1) < k < n-1$, and otherwise the elements of A are all zeros. The parallels to the principal diagonal of A specified by k are termed stripes if they are separated by parallels (nulls) consisting of only zeros. If $k > 1$

27. W. R. Boland, "A Study of the Phase Transition Function of R. L. Dobrushin," Technical Report No. 119, Clemson University, 7 pp.

28. W. R. Boland, "Generalized Product-Interpolatory Quadrature Formulas," Technical Report No. 120, Clemson University, 15 pp; also submitted for publication to *Mathematics of Computation*.

29. D. G. Wilson, "The Time Dependent Linear Transport Equation in a Multidimensional Parallelepiped with Partially Reflecting Walls," Ph.D. thesis, Mathematics, University of Maryland (1971).

30. D. G. Wilson, "Piecewise Linear Approximations of Fewest Line Segments," *AFIPS Conf. Proceedings*, vol. 40, Spring Joint Computer Conference, 1972, pp. 187-98.

contiguous parallels consist of arbitrary elements, these k parallels are said to be a stripe of width k . Mention was made³¹ of the principal result employed in the investigation of matrices with equispaced stripes of unit width symmetrically placed with respect to the diagonals. The general problem is to determine for what stripings of the matrix A there exists a permutation P for which $P^{-1}AP = B$, where B is a direct sum, and to characterize P in terms of the striping of A as was done before³¹ but for more general stripings. Consideration is given to other permutations Q for which the submatrices of B may be reduced in bandwidth. The search continues for the unifying thread in the characterizations of P for the more general stripings of A .

31. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 1.

Computing Applications

INTRODUCTION

A. A. Brooks

The 1972 calendar year in the Computing Applications Department has been characterized by an increase in the work areas of plasma physics, environmental modeling, and information processing. Two new projects for other federal agencies have been started: (1) a combined atmospheric and hydrologic model for the environmental transport of pollutants for NSF/RANN and (2) an information processing project dealing among other activities with access of literature through chemical names, formulas, and structures.

The current staff has increased to and stabilized at 88 technical and 8 support personnel. The percentage utilization of available time has been about 90%. A small contingent of staff is now assigned to the Y-12 site to provide service to the divisions located there. The staff has been expanded into the areas of chemistry, soils physics, computer science, and business management.

ANALYTICAL CHEMISTRY DIVISION

ANALYTICAL CHEMISTRY MANAGEMENT INFORMATION PROGRAMS

J. D. Amburgey

There are five programs in the analytical chemistry management information procedure. The programs perform an analysis on financial data supplied monthly on fiscal and calendar year periods. Two of the programs produce plots showing three-year trends in different financial areas. The programs were modified to handle the new fiscal year management information procedures.

Sponsor: Analytical Chemistry Division

Ray Beatty

BIOLOGY DIVISION

TABULAR ANALYSIS OF ENVIRONMENTAL MUTAGEN INFORMATION

V. A. Singletary

A tabular report generator was developed for the Environmental Mutagen Information Center (EMIC). The tabular report aids the analysis of literature on mutagenicity and teratogenicity of food additives on the Food and Drug Administration's (FDA) Generally Regarded as Safe (GRAS) list No. 3 (see Fig. 1). The table generation program is flexible in that any data base file stored in the generalized ADSEP format may be so formatted. Program control is simple and free form, structured to be compatible with the ORLOOK program, to which it may be eventually integrated.

Sponsor: Biology Division

Diogenylbutane (Dibutylse dioposides) (DBD)

ENTRY	ORGANISM	ASSAY SYSTEM	TREATMENT CONDITIONS	CONCENTRATION	TIME	TEMP	BIOLOGICAL EFFECT	AUTHOR'S REMARKS	REMARKS
005507	STREPTOCOCCUS C1152	Adenine reverse mutations	Candida treated at density of 1×10^7 per ml. At end of treatment, DBD decanted and candida washed twice in H ₂ O. Candida either plated immediately or held in H ₂ O with samples removed at intervals. Samples either allowed to stand or are shaken; or have 02 or H ₂ bubbled through. Mutation and survival scored after 5-7 days.	0.1% DBD	60 min	25C	Metabolic action of DBD continued when candida allowed to stand at room temperature. No after-effect when plated immediately, stored at 0C-4C, or kept stirred by shaking or continuous bubbling. After-effect increased with incubation density. Filtrate from washed candida did not cause mutations in fresh candida preparations.	After-effect caused by traces of DBD, or metabolic action products, which are not readily removed by washing, but may be removed by diffusion from cells when kept in suspension for long period.	

Diogenylbutane (DBD)

ENTRY	ORGANISM	ASSAY SYSTEM	TREATMENT CONDITIONS	CONCENTRATION	TIME	TEMP	BIOLOGICAL EFFECT	AUTHOR'S REMARKS	REMARKS
005508	STREPTOCOCCUS C1152	Adenine and isonitro reverse mutations	Candida of adenine revertant strain were exposed to DBD, twice washed, then either plated at once or resuspended. Suspensions made in medium either with or without isonitro. Suspensions agitated and sampled at intervals for plating.	0.2% ; 0.1% DBD	33 min; 30 min	Room temp- ature	There was high level of adenine reversions, but very low isonitro reversions either with or without isonitro in the medium. Ratio of ad to isonitro reversions ranged from low of 50 in adenine-less medium to high of over 200.	Clear that differential response to DBD is not due to isonitro-less death	
005509	Vicia faba	Cytological alterations in root tip cells e.g. chromosome aberrations, abnormal mitosis	Circulating cells exposed to a solution of colchicine (5 mg/100 ml) for 60 min after which they were exposed to a solution of agent.	0.1 mg (0.6 mg/liter)	1 hr		Chromosome aberrations were analyzed in the 2n and 4n metaphase after 17 and 32 hr post-treatment; abnormal percentages of metaphases observed during the 2n cell population which increased and decreased until 32 hr post-treatment		
005510	STREPTOCOCCUS C1152	Adenine and isonitro reverse mutations	Ad-ison-rev strains grown on slants of medium containing small quantity of DBD. After colonization candida plated as slants and grown at 35C for colony formation. Suspected revertants picked and tested. Other experiments done to determine dose/rate effect.	0.05% DBD	10 days	25C	Ad-ison ratio was 3.6. There were fewer adenine reversions and proportionally more isonitro reversions. There did not appear to be a dose-rate effect.	Low ratio in growing cultures may reflect lack of selectivity at 50% level while high ratio in candida may be due to some secondary effect of treatment which specifically promotes pathway leading to adenine reversions.	

Fig. 1. Tabular format for ADSEP files.

CHEMICAL TECHNOLOGY DIVISION

NUMERICAL TECHNIQUES FOR THE HEAT TRANSFER ANALYSIS OF THE PROPOSED NATIONAL RADIOACTIVE WASTE REPOSITORY

W. D. Turner R. D. Cheverton¹ J. Smith² W. R. Wade²

During the past year we continued the analyses of the thermal effects on the proposed National Radioactive Waste Repository and its geological environment.^{3,4} Calculations were performed to help answer questions which arose in the design of the facility and to evaluate the effects of new data. The heat transfer code HEATING3⁵ and the three-dimensional code using the alternating direction implicit (ADI) procedure mentioned in last year's annual report³ were used in the analysis.

Since the nature of most of the parametric studies requires running many cases involving a large number of grid points, there is a strong incentive to utilize the most efficient code possible. Therefore, a general three-dimensional heat transfer code has been written which uses either the Crank-Nicolson or the fully implicit finite difference approximation or any combination of the two. The resulting system of equations is solved by Stone's three-dimensional strongly implicit procedure (SIP).⁶ This code is currently being evaluated and refined. Preliminary results indicate that for a typical problem involving temperature-independent thermal properties, the SIP code runs about twice as fast as the ADI code for comparable accuracy.

Sponsor: Chemical Technology Division

R. D. Cheverton

THERMAL ANALYSIS OF NL INDUSTRIES' RAIL CASK DESIGN

R. D. Cheverton¹ W. D. Turner

We conducted a partial thermal analysis of NL Industries' proposed rail cask design to serve as an independent check on their analysis. Temperatures which would exist at selected points during normal operation as well as transient temperatures at several points of interest due to exposure to a 30-min fire were determined. The heat transfer code HEATING3⁵ was used to perform the calculations.

Sponsor: Chemical Technology Division

L. B. Shappert

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1. Chemical Technology Division.
 2. Consultant, University of Tennessee.
 3. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, pp. 8, 9.
 4. R. D. Cheverton and W. D. Turner, *Thermal Analysis of the National Radioactive Waste Repository: Progress through March 1972*, ORNL-4789 (September 1972).
 5. W. D. Turner and M. Siman-Tov, *HEATING3 - an IBM 360 Heat Conduction Program*, ORNL-TM-3208 (February 1971).
 6. H. G. Weinstein, H. L. Stone, and T. V. Kwan, "Simultaneous Solution of Multiphase Reservoir Flow Equations," *Soc. Petrol. Eng. J.*, June 1970, pp. 99-110.

CHEMISTRY DIVISION

A PERMUTATION MODEL FOR CHEMICAL REARRANGEMENTS

P. R. Coleman

Chemically, some molecules undergo various rearrangements through successive reactions. These reactions can be considered mathematically as permutations. It is sometimes desirable to know all possible

products which can be generated from a given starting position as well as the path from one product to another. A program¹ has been written to generate these permutations and enumerate the resulting products.

Sponsor: Chemistry Division

C. K. Johnson

COMPUTER "EXPERIMENTS" ON LIQUID SODIUM

R. H. Fowler

We have used the Monte Carlo method to study the structure and equilibrium properties of liquid sodium at a temperature of 397.6°K. The calculation treats a system of 512 particles enclosed in a cubic box of length $L = 27.6 \text{ \AA}$, thus providing a density of 0.928 g/cm^3 . Periodic boundary conditions were employed in order to improve on the inaccuracies due to the small sample volume and to avoid surface effects. The particles are assumed to interact through an effective two-body potential.

An "experiment" involved the generation of a Markov chain of 330,000 configurations. The quantities calculated were the radial distribution function $g(r)$, the liquid structure factor $S(K)$, the excess internal energy U , the specific heat C_v , and the compressibility factor PV/NKT . The radial distribution function obtained is in excellent agreement with the molecular dynamics work of A. Rahman.² The agreement between the calculated $S(K)$ and recent experimental measurements is good.

The favorable agreement between the calculated and experimental values of $S(K)$ indicates that the potential used is a realistic representation of the effective interaction. We are currently developing a molecular dynamics code to calculate transport coefficients of interest.

Sponsor: Chemistry Division

A. H. Narten

PREDICTION OF THE CHEMICAL PROPERTIES OF ELEMENTS 111 AND 112

C. W. Nestor, Jr. O. L. Keller²

We have used the relativistic Hartree-Fock-Slater program⁴ to compute electronic wave functions and binding energies for the neutral atoms and the first few ions of elements with atomic number 111 and 112, assuming that they lie under gold and mercury in the periodic table, and for the elements in the same columns of the periodic table. We have also estimated the electron affinities of negative ions of the sequence Cu^- , Ag^- , Au^- , and 111^- , using the procedure of Glocker,⁵ and an extension of this procedure based on the possibility of using fractional values of the atomic number⁶ as a computational artifice in the relativistic Hartree-Fock-Slater program. In general, the calculated ionization potentials agree fairly well with available experimental values. The electron affinities calculated with Glocker's procedure and experimental ionization potentials agree rather poorly with the experimental values for Cu, Ag, and Au.

1. *Chem. Div. Annu. Progr. Rep. Mar 20, 1972*, ORNL-4791.

2. A. Rahman, in *Battelle Colloquium, Interatomic Potentials and Simulation of Lattice Defects*, eds. P. C. Gehlen and J. R. Beeler, Jr., p. 233, Plenum Press, New York, 1972.

3. Chemistry Division.

4. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 73.

5. G. Glocker, *Phys. Rev.* **46**, 111 (1934).

6. *Math. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4514, p. 39.

Extrapolations of approximate ionization potentials for fractional Z values also do not agree with experimental electron affinities.

Sponsor: Chemistry Division

O. L. Keller

INTERPRETATION OF THE L X-RAY EMISSION SPECTRUM OF ZIRCONIUM

C. W. Nestor, Jr. M. O. Krause³ F. Willeumier⁷

We have used the relativistic Hartree-Fock-Slater program⁴ to compute the energies of the diagram and satellite x rays arising from transitions between various states of singly and multiply ionized zirconium. We have obtained the x-ray energies by subtraction of the computed total energies, and the energy shifts of the satellite lines from the parents by subtraction of the computed x-ray energies. The calculated and experimental shifts of the satellites from the $L\alpha_{1,2}$ and $L\beta_1$ x rays are about 8 eV and 7.5 eV respectively.

Sponsor: Chemistry Division

M. O. Krause

CHARACTERISTIC X-RAY ENERGIES OF THE LANTHANIDE AND ACTINIDE ELEMENTS

C. W. Nestor, Jr. M. O. Krause³

We have used the "doubly modified Moseley diagram" of Hagstrom⁸ to fit the energies of the $K\alpha_1$ and $L\alpha_1$ x rays of the lanthanide and actinide elements. We write the square root of the x-ray energy E_x in the form

$$E_x^{1/2} = \alpha_2 Z^2 + \alpha_1 Z + \alpha_0, \quad (1)$$

where Z is the atomic number and the constants α_2 , α_1 , and α_0 are determined by a least-squares fit, using the x-ray energies compiled by Bearden⁹ for the lanthanides and the lower- Z actinides and recent data from two other sources^{10,11} for the higher- Z actinides.

In Figs. 2 and 3 we have plotted the residuals

$$r = E_x^{1/2} - P(Z) \quad (2)$$

computed by subtracting the least-squares fitted values from the observed values of $E_x^{1/2}$, using both second- and third-degree polynomials $P(Z)$. The improvement in the fit for the lanthanides is obvious; there is some improvement in the actinides, but there are fewer data points, and the standard errors are generally much larger.

We used the polynomial fits to produce estimates of the parameters for a nonlinear, weighted least-squares fit to a function of the form:

$$E_B = A(Z - \bar{Z})^3 + B(Z - \bar{Z})^2 + C(Z - \bar{Z}) + D^2,$$

where $\bar{Z}$ is the arithmetic mean of the Z values included in the fit. In Figs. 4 and 5 we have plotted the residuals obtained from the nonlinear fit with the experimental standard deviations; the solid lines

7. Laboratoire de Chimie Physique de l'Université, Paris, France.

8. S. Hagstrom, *Z. Phys.* **178**, 82 (1964).

9. J. A. Bearden, National Bureau of Standards report NSRDS-NBS-14 (1967).

10. G. C. Nelson, B. G. Saunders, and S. I. Salem, *Z. Phys.* **235**, 308 (1970).

11. P. F. Dittner and C. E. Bemis, Jr., *Phys. Rev. A* **5**, 481 (1972); Y. Y. Chu, M. L. Perlman, P. F. Dittner, and C. E. Bemis, Jr., *Phys. Rev. A* **5**, 67 (1972).

LANTHANIDE K-ALPHA 1 X-RAY ENERGIES (BEARDEN, NSRDS-NBS-14, 1967)

Fig. 2. Differences between square root of observed x-ray energies and values calculated from quadratic (O) and cubic (+) polynomial fit for lanthanide elements.

ACTINIDE K-ALPHA 1 X-RAY ENERGIES

Fig. 3. Differences between square root of observed x-ray energies and values calculated from quadratic (O) and cubic (+) polynomial fit for actinide elements.

LANTHANIDE K-ALPHA 1 X-RAY ENERGIES (BERDEN, NSRDS-NBS-14, 1967)

Fig. 4. Differences between observe. and calculated $K\alpha_1$ x-ray energies for the lanthanide elements.

ACTINIDE K-ALPHA 1 X-RAY ENERGIES

Fig. 5. Differences between observed and calculated $K\alpha_1$ x-ray energies for the actinide elements.

Table 1. X-ray energies for the actinide elements

Z	Energy (eV)			
	$K\alpha_1$		$L\alpha_1$	
	Experimental	Calculated	Experimental	Calculated
89		90,880 $\pm$ 10		12,652 $\pm$ 2
90	93,352 $\pm$ 2	93,352 $\pm$ 4	12,968.9 $\pm$ 0.6	12,970.0 $\pm$ 0.7
91		95,871 $\pm$ 4	13,291 $\pm$ 1	13,289.9 $\pm$ 0.3
92	98,441 $\pm$ 3	98,442 $\pm$ 5	13,614.9 $\pm$ 2	13,614.9 $\pm$ 0.2
93	101,685 $\pm$ 6	101,067 $\pm$ 5	13,944.3 $\pm$ 2	13,944.3 $\pm$ 0.2
94	103,750 $\pm$ 6	103,747 $\pm$ 5	14,278.8 $\pm$ 5	14,278.4 $\pm$ 0.3
95	106,488 $\pm$ 7	106,481 $\pm$ 5	14,617.4 $\pm$ 2	14,617.4 $\pm$ 0.2
96	109,273 $\pm$ 5	109,273 $\pm$ 6	14,959 $\pm$ 2	14,962 $\pm$ 1
97	112,112 $\pm$ 5	112,122 $\pm$ 6		15,311 $\pm$ 3
98	115,031 $\pm$ 5	115,031 $\pm$ 7		15,667 $\pm$ 6
99	118,020 $\pm$ 10	118,000 $\pm$ 14		16,030 $\pm$ 10
100		121,030 $\pm$ 30		16,400 $\pm$ 20
101		124,120 $\pm$ 50		16,770 $\pm$ 30
102		127,280 $\pm$ 80		17,150 $\pm$ 40

indicate the estimated standard deviations of the energies computed from the fit. In Table 1 we list the energy values computed for atomic numbers 89 through 102, with the estimates of the standard deviations.

Sponsor: Chemistry Division

M. O. Krause

DIRECTOR'S DIVISION

GENERIC STUDIES OF HEATED DISCHARGE PLUMES IN IRREGULAR COOLING LAKES

R. E. Textor M. N. Ozisik¹

As hot water moves down a main channel with cooler side arms, the negative temperature gradient in the direction of a side arm induces motion of hot water down the side arm. A model, which consists in part of a system of nonlinear first-order differential equations, has been developed to calculate the initial velocity, motion, and temperature loss in the hot water as it flows down the side arm, and the effectiveness of the side arm in cooling the water in the main channel. The system of differential equations has been treated with Hamming's predictor-corrector method.

The basic equations governing the surface discharge of hot water from a narrow channel into a cooling lake are the Navier-Stokes equations, the heat equation, and an equation for the concentration of some substance (e.g., salt) of interest. The model presently being considered for this problem consists of a nonlinear, autonomous, singular first-order system of differential equations. The singularity occurs at the initial point, and methods for treating the system numerically are being investigated.

Sponsor: Environmental Impact Reports Project

M. M. Yarosh

¹ Consultant, North Carolina State University.

ANALYSIS OF BUOYANT JETS

R. E. Textor

The development of a momentum jet discharged to an infinite ambient through a submerged diffuser was analyzed by Hirst.^{2,3} In order to obtain a model consisting of ordinary differential equations, he assumed the jet to be axisymmetric and introduced assumed velocity profiles and an entrainment function. In an effort to determine the radial distribution of velocity and temperature within the jet, the feasibility of treating the partial differential equations that precede these assumptions is being investigated.

Sponsor: Environmental Impact Reports Project

V. R. Cain

COMPUTER PROGRAM FOR THE COMPUTATION OF DIFFUSION COEFFICIENTS IN COMPLEX SYSTEMS

R. E. Funderlic

The estimation of ionic self-diffusion coefficients from experimental data taken on systems made up of small composite spheres with an inner core initially containing radioactive tracer and an outer shell for which the diffusion coefficient differs from that for the core depends on fitting the data to the solution of the appropriate radial diffusion equation with the appropriate boundary conditions. The diffusional process in the core is given by Fick's second law, and there is an equation which describes the amount of transfer between the core and shell.

Under these assumptions, a solution may be obtained for the concentration profile of tracer in the core at any time. Experimentally, however, it is more convenient to determine the redistribution of tracer by measurements on the external stirred liquid to give the fractional attainment of the final or equilibrium distribution $F(t)$ as a function of time. G. W. Westley's nonlinear least squares program,⁴ NONLS2, was very effective in fitting the series form of F to the experimental data and thereby giving diffusion coefficients. Each term of the appropriate truncated infinite series required the numerical solution of a transcendental equation.

Sponsor: Director's Division

G. E. Boyd

DIFFUSION OF HYDROGEN FROM A POINT SOURCE

R. B. Hofstra

We are doing computation and plotting for the determination of the concentration profile of a gas leaking from a point source, as a function of leak rate and time. This project is undertaken in order to optimize the placement of hydrogen sensors in a laboratory building. The current investigations have been using a geometry of infinite extent, and we plan to alter the approach to include the effects of physical boundaries.

Sponsor: Director's Division

A. P. Malinauskas and R. Affel

2. E. A. Hirst, *Analysis of Round, Turbulent, Bouyant Jets Discharged to Flowing Stratified Ambients*, ORNL-4685 (June 1971).

3. Eric Hirst, *Analysis of Bouyant Jets within the Zone of Flow Establishment*, ORNL-TM-3470 (August 1971).

4. G. W. Westley and J. A. Watts, eds., *Computing Technology Center Numerical Analysis Library*, CTC-39 (October 1970).

COMPUTER PROGRAM FOR ESTIMATING THE CONCENTRATION DEPENDENCE OF OSMOTIC COEFFICIENTS OF POLYELECTROLYTE SOLUTIONS CONTAINING FULLY STRETCHED MACROMOLECULES

R. E. Funderlic F. D. Hammerling

The cylindrical symmetry of a fully stretched charged macromolecule allows an exact solution to be obtained for the Poisson-Boltzmann equation for its electrostatic potential. The free energy of aqueous salt-free solutions of rodlike ionized polyelectrolytes may be deduced from this potential, and the colligative and other properties of the solution may be obtained. For example, the osmotic coefficient ϕ , as a function of the polyelectrolyte concentration, is found by solving a transcendental equation.

Sponsor: Director's Division

G. E. Boyd

EXECUTION TIME TRANSLATE SUBROUTINES

A. F. Joseph

A set of FORTRAN callable routines⁵ was developed to generate any number of translation tables and to facilitate their use. Any number of translation tables may be created. This is only limited by the region allocated to the job. The tables do not have to be used in the order generated, and the area allocated to the tables can be released and used for other tables or purposes.⁶ The routines have been used to make special character translation in FORTRAN programs. There is an additional option which can be used to translate any hex byte into an integer.

Sponsor: Director's Division

PROFESSIONAL WORK EXPERIENCE QUESTIONNAIRE

A. F. Joseph C. H. Gard

Several computer programs were written to analyze the results of the Professional Work Experience Questionnaire of June 28, 1971, to obtain relationships among age, years of Laboratory service, job function, division membership, negative attitudes, general background, and degree of participation in interdisciplinary work.

Sponsor: Director's Division

M. Roberts

THE BIORAD PROGRAM

V. A. Singletary

The BIORAD program is a multi-user code that computes dose to the biota for inclusion in environmental impact statements for nuclear power stations. Output of the BIORAD program has been used in every impact statement produced for the AEC to date by ORNL. It is coded in the BASIC language for the ORNL DEC-10 system. It is an interactive system that allows data file maintenance, computation, and output control.

Sponsor: Director's Division

5. A. F. Joseph, *Execution Time Translate Subroutine*, ORNL-TM-3810 (July 1972).

6. R. C. Durfee, *FORTTRAN Dynamic Storage Allocation*, ORNL-CF-70-8-59 (Aug. 18, 1970).

ENVIRONMENTAL INFORMATION SYSTEMS OFFICE

THE ORLOOK PROGRAM

V. A. Singletary A. F. Joseph

The ORLOOK program¹ (Phase I), an interactive information retrieval program, was modified in several ways: (1) to allow inverted file search, (2) to have improved initial data file loading and searching, (3) to search and output document fields having hierarchical structures, (4) to perform set operations on the file and file subsets, (5) to automatically account for data base usage, (6) to optimally save retrieval results for off-line processing, and (7) to reflect more natural teleprocessing of user requests. Also, the on-line interactive version has been modified to provide identical on-line or off-line data retrieval for larger files. This version is necessarily run without the teleprocessing capability, but with identical commands in card image form. Some preparation of ORLOOK for time sharing on the IBM 360/75 was made.

Sponsor: Environmental Information Systems Office

INVERTED FILES FOR ORLOOK

C. H. Gard A. F. Joseph
D. W. Altom²

Programs have been written to generate inverted pointer files for any field of an ADSEP³ data base so that the ORLOOK program can retrieve information by getting the ADSEP numbers of the records containing the desired information from the pointer files rather than sequentially searching the whole data base. The ORLOOK program¹ was modified to search inverted files associated with some of the indexed data bases accessible to ORLOOK. This entailed providing the user with two new commands:

1. a search and retrieval command that restricts the search to the inverted file instead of the entire data base,
2. a search only command that displays all entries in the inverted file that are first n character identical with the n -character request (e.g., a request of "DON" might display "DONALD," "DONNER," and "DONNOR").

Sponsor: Environmental Information Systems Office

DUPLICATE CHECKING

D. W. Altom²

We extracted the duplicate checking portion of the book ordering code⁴ and made it a stand-alone program.

The duplicate checking program allows the user to select a variable number of data fields (title, author, etc.) to be used for comparison. For each entry in the user's data set, the information in the selected data

1. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, pp. 16-17.

2. Now with the Technical Information Center, USAEC, Oak Ridge.

3. A. A. Brooks, *ADSEP, an Automated Data Set Editing Program*, CTC-34 (May 12, 1970).

4. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 18.

fields is concatenated into a character string. All characters in the string except alphabetic and numeric are removed, thus producing a reduced string. A hashing technique is then applied to the reduced string to produce a hash number. Next, the entire data set is sorted by hash number. When two entries are found to have the same hash number, their reduced strings are compared character by character. If the reduced strings are identical, the two entries are considered identical.

Sponsor: Environmental Information Systems Office

G. U. Ulrikson

ADSORT: A PROGRAM TO SORT ADSEP DATA BASES

F. D. Hammerling A. A. Brooks

A program was written to sort an ADSEP³ data base on any number of fields. The user must specify the data type (numeric or character) and the fields in the order they are to be sorted. Since the ADSEP fields are variable in length, the user must also specify the number of characters he wishes to sort from each field. The program consists of three steps:

1. Retrieve the given fields, and concatenate the specified number of characters from each field into a fixed-length sort field. Form a new record by adding this field to the front of the existing record. All characters in the sort field are converted to upper case.
2. Sort the new records using the IBM sort-merge program.
3. Remove the sort field, and renumber the sorted records if desired.

Documentation is in progress.

Sponsor: Environmental Information Systems Office

G. U. Ulrikson

ADBASE: A PL/I VERSION

F. D. Hammerling A. A. Brooks

A PL/I version of ADBASE⁵ was written so that PL/I programs could access ADSEP³ data bases. The PL/I version is similar in function to the FORTRAN version except that it is intended only for fetching fields and not for forming records. The philosophy is one of based variables and pointers.

Sponsor: Environmental Information Systems Office

G. U. Ulrikson

PUBLISH: A PROGRAM FOR PAGE COMPOSITION FROM ADSEP DATA BASES

F. D. Hammerling A. A. Brooks Ruth Slusher

The PUBLISH program⁶ has been improved and generalized. The user now has more control over the page format by way of input parameters. There is now a choice of one-column or two-column pages. Documentation of the program is now in progress. Several reports have been published using the output from the program.

Sponsor: Environmental Information Systems Office

G. U. Ulrikson

5. A. A. Brooks and D. L. Wilson, *ADBASE -- a Subprogram to Access ADSEP Data Sets*, ORNL-CF-71-9-21 (Sept. 20, 1971).

6. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 16.

ENVIRONMENTAL SCIENCES DIVISION

WALKER BRANCH WATERSHED

L. J. Campbell M. T. Heath

The Walker Branch Watershed project has been collecting hydrologic data since 1968 in a paper-tape—punched-card format. The tabulation and analysis of these data have been documented.¹ In the near future, the old system will be replaced by a remote data-logging system featuring a PDP-8 computer with magnetic tape drives. To accommodate changes necessitated by the new system and to correct known errors in the old computer programs, we have taken this opportunity to completely reorganize and rewrite the data processing codes for this project. This should also eliminate some of the redundancy and need for human intervention in the old system and more fully utilize the greater flexibility and capacity of the new system. In order to make the existing data compatible with the new programs, the punched cards are being put on magnetic tape in a format simulating the tapes produced by the PDP-8. A program has been written to summarize both the rain gage and streamflow data over arbitrary periods of time in a format convenient for direct photographic reproduction and publication. This program also tabulates weekly chemical concentration data taken at rain gage and stream sites for various ions. Yet to be adapted are the storm definition and hydrographic analysis programs.

Sponsor: Environmental Sciences Division

G. S. Henderson

J. D. Sheppard

APPLICATION OF THE METHOD OF WEIGHTED RESIDUALS TO WETTING AND DRYING IN SOILS

M. Reeves J. Smith²

A study is being made of weighted-residual techniques for solving the moisture-flow equation in unsaturated soils. The motivation is to improve the soil-water transport in the hydrological transport model and to provide the framework from which the dispersion and mass transport of a pollutant may be studied. Five Galerkin algorithms — linear, logarithmic, quadratic chapeau, smooth cubics, and spline — along with a spline collocation method, are being considered as possible alternatives to the traditional finite-difference spatial discretization. In addition, three different time-integration algorithms are being examined, namely, Crank-Nicolson, completely implicit, and a technique which is 60% implicit and 40% explicit.

Sponsor: Environmental Sciences Division

STAND WATER MODEL

J. B. Mankin R. A. Goldstein³

A phenomenological model was developed that simulates atmosphere-plant-soil moisture relations on a day-to-day basis. A combined energy-balance—aerodynamic approach is used to derive the equation for

1. W. M. Snyder and J. W. Curlin, *Walker Branch Watershed Project: Hydrologic Analysis and Data Processing*, ORNL-4392 (April 1969).

2. Department of Mathematics, University of Tennessee, Knoxville.

3. Environmental Sciences Division.

evapotranspiration from a conceptualized surface including both ground and canopy surfaces. The soil is divided into several layers having different physical properties and containing different quantities of roots. By applying a mass balance to the evapotranspiration surface, surface water potential, evapotranspiration, the volumetric water content of the different soil layers, and runoff can be calculated. This model has been applied, with reasonable results, to simulate evapotranspiration on the Walker Branch Watershed.⁴

Sponsor: Environmental Sciences Division

R. A. Goldstein

PROPORTIONAL MODEL OF HYSTERESIS IN SOILS

M. Reeves E. E. Miller⁵

Since moisture retention may be strongly influenced by hysteresis, this characteristic of soils was included in our analysis⁶ of an approximation for infiltration. The model used assumed that all scanning loops were identical to primary loops, an assumption which was found to be inconsistent with experimental data in the wetter regions of the moisture-retention curve. One of the authors⁷ has developed variations of the independent domain theory which allow one to determine the higher-ordered loops from the primary curves. The purpose of our work is to examine higher-ordered loops obtained from the parameterization of primary loops presented in ref. 6.

Sponsor: Environmental Sciences Division

HYDROLOGICAL MODELING

J. B. Mankin S. G. Bozeman
R. J. Luxmoore⁸ R. A. Goldstein³
D. D. Huff⁸

The hydrological transport model (HTM) is being developed by the Lake Wingra Site, Eastern Deciduous Forest Biome, International Biological Program. HTM is designed to estimate the time response of water flows and the transport of associated trace elements within a watershed. Among the many possible pathways for water are evapotranspiration, runoff, drainage, and storage within the soil. Since these phenomena are computed in a highly empirical manner in HTM, work is proceeding to place certain portions of HTM with the algorithm PROSPER. In conjunction with this, PROSPER is being modified to account for an arbitrary number of soil layers, and techniques necessary to calculate lateral flow within the soil are being considered.

Sponsor: Environmental Sciences Division

4. R. A. Goldstein and J. B. Mankin, "PROSPER: A Model of Atmosphere-Soil-Plant Water Flow," *Proceedings of 1972 Summer Computer Simulation Conference, June 14-16, 1972, San Diego, Calif.*, pp. 1176-81.

5. Department of Soils and Physics, University of Wisconsin, Madison.

6. M. Reeves and E. E. Miller, to be published in *Water Resource Research*.

7. E. E. Miller, to be published in *Soil Science Society of America Proceedings*.

8. Lake Wingra Site, University of Wisconsin.

NUTRIENT CONTENTS IN FOUR FOREST STANDS ON WALKER BRANCH WATERSHED

C. H. Gard

In order to characterize nutrient cycles of the forest floor, it is imperative that estimates of seasonal nutrient pools in organic and soil horizons are quantified. For throughfall⁹ it is of interest to compare this method of input to the forest floor with other cycling methods. Computer programs have been written to do the above for litterfall¹⁰ and throughfall data.

Sponsor: Environmental Sciences Division

G. S. Henderson

PRODUCTIVITY MAPPING

R. L. Stephenson

Several expressions are available for estimating the primary biomass production from climatic data, for example, precipitation, potential or actual evapotranspiration, and temperature. Climatic data are measured at about 500 weather stations in the continental United States whose latitude and longitude are known. We have written a program which converts latitude and longitude to rectangular coordinates and computes the primary production by several expressions. SYMAP¹¹ is then used to produce maps which display production as computed by various expressions or the difference between the values predicted by different expressions. Figure 6 shows a map of primary production as predicted by the Rosenzweig equation.¹²

Sponsor: Environmental Sciences Division

STRIPED BASS POPULATION IN THE HUDSON RIVER ESTUARY

P. R. Coleman

A program was written to implement a compartmental model developed by C. P. Goodyear. This model attempts to determine the fate of the striped bass population in the Hudson River estuary over a period of several years. An important input variable to the program is the condenser flow of nuclear power plants at various points along the river. Thus the program is used to project the population effect from the addition of new power plants.

Sponsor: Environmental Sciences Division

C. P. Goodyear

A PROGRAM TO MONITOR FISH ACTIVITIES

J. D. Amburgey

Fish in Melton Hill Lake had water-temperature sensors attached to their scales. Temperature data were recorded on a paper tape punch, converted to cards, and used as input to the program FISH. FISH

9. G. S. Henderson and D. E. Todd, *Nutrient Return in Throughfall for Four Forest Stand Types and Its Importance in Annual Nutrient Cycles*, EDFB Memo Report No. 72-154.

10. G. S. Henderson, *Litter Biomass and Nutrient Contents in Four Forest Stands on Walker Branch Watershed*, EDFB Memo Report No. 71-91.

11. *User's Reference Manual for Synographic Computer Mapping (SYMAP) Version V*, Laboratory for Computer Graphics, Harvard University, June 1968.

12. M. L. Rosenzweig, "Net Primary Productivity of Terrestrial Communities: Prediction from Climatological Data," *Amer. Natur.* 102, 67-74 (1968).

ORNL-DWG 72-12579

Fig. 6. Primary production as predicted by Rosenzweig's equations.

produced plots showing the temperatures that fish preferred during eating, sleeping, and other daily routines. With these results an analysis can be made on the change in water temperature in a fish's environment.

Sponsor: Environmental Sciences Division

C. Coutant

ACQUISITION, STORAGE, RETRIEVAL, AND DISPLAY OF GEOGRAPHICALLY ORIENTED DATA BASES FOR THE BIOME AND REGIONAL SYNTHESIS GROUP

R. L. Stephenson T. C. Tucker

We are continuing¹³ to develop techniques and computer programs for the various data bases required for Biome and Regional Synthesis. As before,¹⁴ problems and results are common to this group and the ORNL-NSF Environmental Program and are reported in the latter section of this report.

Sponsor: Environmental Sciences Division

F. G. Goff

AIR DIFFUSION MODELING

R. L. Stephenson

We have written a program which computes the distribution of airborne pollutants. The program accepts data describing a latitude and longitude grid over a section of the earth's surface. Sources of pollutants are allocated to cells of the grid (each source is assumed to be at the center of the cell). The program computes the great-circle distance from the center of the source cell to the center of a receiving cell and the compass bearing of the great circle at the source cell. The contribution of the source at the center of the receiving cell is calculated from the source strength, source elevation (stack height), distance, average wind velocity, and the probability that the wind will blow in the appropriate direction using a published expression.¹⁵ The foregoing is repeated for each cell in the grid.

In this way the contribution of each source to the pollutant concentration at the center of each cell is computed, and the results are accumulated in a matrix which, at the end of execution, reflects the total concentration due to all sources. The matrix is displayed in the form of a rudimentary map.

The program has been implemented in two forms. One version operates on the IBM 360 machines and is intended for use with large numbers of sources in large matrices. The other has been converted to run on the PDP-10 and model air diffusion over the East Tennessee Development District (ETDD). It will be used to simulate the effect of small numbers of proposed sources on the ETDD.

Sponsor: Environmental Sciences Division

DATA ANALYSIS OF ATMOSPHERIC INPUT OF TRACE ELEMENTS TO THE CESIUM FOREST FLOOR

C. H. Gard

In order to analyze the amounts of calcium, sodium, magnesium, phosphorus, potassium, and nitrogen that hit the forest floor, three types of data were collected bimonthly on a 500-m² plot in the tagged area

13. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 19.

14. *Ibid.*, p. 68.

15. D. Slade, ed., *Meteorology and Atomic Energy*, USAEC report TID-24190, p. 113 (1968).

of the cesium forest. Dryfall and throughfall were collected at three stations on the ground and at one control station in the treetops, while stemflow was collected from around the trunks of five trees.

A computer program was written to calculate the amounts (in kilograms per hectare) of the trace elements present from the analytical results, taking into account any blanks used in the chemical analysis. For each type of data, each collection period, and each element, the means and standard errors were given for the noncontrol stations as well as corrected for the control station. Cumulative totals and means of each element are given and updated for each station within each data type.

Sponsor: Environmental Sciences Division

N. T. Edwards

M. H. Shanks

AN INTERACTIVE PROGRAM FOR SOLVING INITIAL-VALUE PROBLEMS

B. W. Rust J. B. Mankin

We have written a package of programs for interactively solving initial-value problems on the COMSHARE system. An early prototype of the program was written by Phillip Sollins of the Environmental Sciences Division. The present program is a much more flexible, sophisticated, and faster version of the earlier one. Although it was designed for solving problems in ecological modeling, it can be used for other applications as well. It contains many prompters so that it can be easily used by people with no knowledge of computer programming. It was thoroughly tested in this respect during the August 1972 IBP Woodlands Workshop, when it was used quite satisfactorily by ecologists from all over the world, many of whom had never used a computer before.

The integration method used by the program is a variable-step-size Runge-Kutta routine which was written by F. D. Hammerling.¹⁶ This subroutine automatically adjusts the step size to the maximum possible value which will give the desired accuracy. This method has the usual stability properties of the more conventional Runge-Kutta method but is considerably faster. The program also has the ability to handle large discontinuities in the derivative functions. This is a very useful property in ecological modeling because such discontinuities often occur in nature, for example, leaf fall.

The program has a number of very useful convenience features. One of these is the ability to address variables by name during execution. This allows the user to change the values of his parameters during execution and to refer to those parameters by name from the console. Another useful feature is a plotting package which allows the user to plot his solutions on the output paper at the console.

Although this program was written for the COMSHARE system, it would easily be transferred to any other on-line system, for example, the PDP-10 system.

Sponsor: Environmental Sciences Division

WOODLANDS WORKSHOP OF THE INTERNATIONAL BIOLOGICAL PROGRAM

J. B. Mankin D. E. Fields B. W. Rust

A Woodlands Workshop was hosted by the Environmental Sciences Division as part of its commitment under the International Biological Program. Participants were biologists with little or no mathematics background from a number of foreign countries. The purposes of this workshop were to familiarize the

16. G. W. Westley and J. A. Watts, eds., *Computing Technology Center Numerical Analysis Library*, CTC-29, pp. 114-20 (October 1970).

participants with modeling techniques and to synthesize data which the participants were to have brought with them. The workshop was extremely successful in introducing the potential of mathematical modeling to the participants, but the success of the latter purpose was severely limited because, in many cases, the data were preliminary and/or incomplete. Some preliminary models for forested ecosystems were developed, and efforts on these are still continuing.

Sponsor: Environmental Sciences Division

MODIFICATIONS TO THE RADIATION DOSE PROGRAMS EXREM AND INREM

J. D. Amburgey

EXREM and INREM,¹⁷ computer codes for estimating radiation doses to populations from various sources, have been modified to accept free-form input. This was done so users could use a CRBE terminal to submit their input and run a problem without using card decks. This greatly speeds turnaround time, since the option of having the printout at the CRBE terminal is now available. In addition, all Beta, Gamma, Nuclide, and Nuclide Pathway data cards are now on disk and need not be entered as input.

Sponsor: Environmental Sciences Division

S. V. Kaye

THE ENERGY COST OF GOODS AND SERVICES

J. A. Carpenter

FORTTRAN IV codes were prepared to convert the U.S. Department of Commerce (Office of Business Economics) 1963 input-output tables to energy terms. Three hundred sixty-two sectors of these tables were used. In addition, considerable manipulation of raw data was required to produce inputs to this dollar-energy conversion program. Attention was given to the breakdown and tabulation of output variables to facilitate the use of the results by varied groups of energy researchers.

The main purpose of the study was to determine, for a wide range of goods and services, the energy required for their production including all steps of manufacture. The resulting energy input-output matrix is an important consideration in problems such as the following: (1) obtaining energy requirements resulting from various buying and consumption patterns, (2) comparison of energy units of production costs vs operation and maintenance costs of various products, and (3) estimation of energy requirements entailed by energy-saving projects such as mass transit.

Sponsor: Environmental Sciences Division

Robert A. Herendeen¹⁸

THE MODELING OF ENERGY TRANSFER IN A FOREST CANOPY

J. B. Mankin C. E. Murphy, Jr.¹⁹ K. R. Knoerr¹⁹

A model was developed to study the dynamics of the atmosphere-soil-plant energy system. This model consists of two coupled nonlinear partial differential equations describing the transfer of latent and sensible

17. W. D. Turner, S. V. Kaye, and P. S. Rohwer, *EXREM and INREM Computer Codes for Estimating Radiation Doses to Populations from Construction of a Sea-Level Canal with Nuclear Explosives*, ORGDP report K-1752 (1968).

18. The Center for Advanced Computation, University of Illinois, Urbana, Ill.

19. School of Forestry, Duke University.

heat through a forest canopy and an ordinary differential equation describing the energy balance on the canopy leaves. Simulation runs with both step and sinusoidal changes in the radiation input suggest that this system is reasonably well described by a steady-state model. Since computer runs with this program are relatively expensive, it has been decided to use the steady-state model until more efficient techniques are developed.

Sponsor: Environmental Sciences Division

A TERRESTRIAL ECOSYSTEM ENERGY MODEL

J. E. Mankin³ H. H. Shugart³ R. A. Goldstein³ R. V. O'Neill³

A model for the energy dynamics in a forest ecosystem has been developed. This model consists of a system of nonlinear ordinary differential equations describing vegetation and terrestrial consumer and decomposer growth. The model has been tailored to accommodate the types of data which are likely to be available. For instance, the data for terrestrial consumers are likely to be estimates of biomass, while the terrestrial decomposer data are likely to be population dynamics.

The vegetation, consumer, and decomposer growth models have been developed as separate modules. This phase is largely complete except for a rather extensive revision of the decomposer module. Work is now proceeding in combining the three modules in a total energy model.

Sponsor: Environmental Sciences Division

R. V. O'Neill

PREEDIT

P. G. Fowler A. A. Brooks C. H. Gard

A FORTRAN program, PREEDIT,²⁰ has been written for the purposes of editing ADSEP text input^{21,22} to locate errors in input sequence and input format and for the absence of essential fields.

The program has more extensive checking than ADSEP and produces copy which is convenient for further proofreading and editing for content. Errors in input are flagged with a brief diagnosis. Several options exist for checking alternate formats of input, and the user must select the correct option if other than the default options stated in the CRBE file which contains the standard control cards.

Sponsor: Environmental Sciences Division

20. P. G. Fowler, A. A. Brooks, and C. H. Gard, *PREEDIT - a Preedit Program for ADSEP Text Input*, ORNL-TM-3897 (August 1972).

21. A. A. Brooks, *ADSEP - an Automated Data Set Editing Program*, CTC-34 (May 12, 1970).

22. A. A. Brooks, *ADSEP Text Impact*, ORNL-CF-71-9-3 (Sept. 6, 1971).

GENERAL ENGINEERING AND CONSTRUCTION DIVISION

PLCEST: PLANT COST ESTIMATE

C. C. Webster

This program has been developed to take input data normally used in making engineering cost analyses and determining the cost of a fuel reprocessing plant. The costs are broken down into the different

categories, and the output displays the several pieces of input data and the costs of different components of the plant along with unit costs of output products, expected plant life, and plant capacity for different sized plants. The program has provisions for adding a plotting subroutine to make graphs of the results.

Sponsor: General Engineering and Construction Division

T. W. Pickel

HEALTH PHYSICS DIVISION

DOSE FROM GAMMA-RAY SOURCES

G. G. Warner W. S. Snyder¹

The man phantom previously described²⁻⁴ having been developed initially for internal photon sources has been extensively revised for use with external photon sources by correcting some defects in the legs and head. In earlier versions, the testes have been imbedded in a single truncated elliptical cone which represented both the legs. To get closer to reality the legs were separated into two truncated circular cones defined by

$$(100 + z \pm 10x)^2 + 100y^2 = (100 + z)^2,$$

where $-80 \leq z \leq 0$. This provided approximately the same total volume for the legs as formerly. The testes remain the same size and have been moved forward into a region in front of the confluence of the two legs bounded by the lateral surfaces of the legs, the planes $z = 0$ and $z = -4.8$, and the plane $z + 10y + 100 = 0$. The testes are given by

$$\left(\frac{x \pm 1.3}{1.3}\right)^2 + \left(\frac{y + 8}{1.5}\right)^2 + \left(\frac{z + 2.3}{2.3}\right)^2 = 1.$$

The head was an elliptical cylinder, and thus some parts of the skull were surrounded by a mass of soft tissue. The top half of the head is now described by

$$\left(\frac{x}{7}\right)^2 + \left(\frac{y}{10}\right)^2 + \left(\frac{z - 85.5}{8.5}\right)^2 = 1.$$

The lower portion remains the same:

$$\left(\frac{x}{7}\right)^2 + \left(\frac{y}{10}\right)^2 = 1, 70 \leq z < 85.5.$$

1. Health Physics Division.

2. G. G. Warner and A. M. Craig, Jr., *ALGAM, a Computer Program for Estimating Internal Dose from Gamma-Ray Sources in a Man Phantom*, ORNL-TM-2250 (June 1968).

3. W. S. Snyder et al., *Estimates of Absorbed Fractions for Monoenergetic Photon Sources Uniformly Distributed in Various Organs of a Heterogeneous Phantom*, MIRD Pamphlet No. 5, Supplement No. 3, *J. Nucl. Med.* (August 1969).

4. G. G. Warner, M. J. Cook, and W. S. Snyder, *Health Phys. Div. Annu. Progr. Rep. July 31, 1970*, ORNL-4584, pp. 200-203.

To use the new surfaces generated by these revisions as source areas for the impingement of photons from a cloud source, we developed sampling techniques which would select points uniformly distributed on these surfaces. For the top of the head, when x and y are chosen uniformly in the ellipse

$$\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 = 1$$

and

$$z = \sqrt{1 - \left(\frac{x}{a}\right)^2 - \left(\frac{y}{b}\right)^2},$$

then

$$F(x, y, z) = \left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 + \left(\frac{z}{c}\right)^2 - 1 = 0,$$

$$\mathbf{N} = \text{grad } F = -i \frac{\partial z}{\partial x} - j \frac{\partial z}{\partial y} + \mathbf{k},$$

and

$$\cos \alpha = \frac{\mathbf{N} \cdot \mathbf{k}}{|\mathbf{N}| |\mathbf{k}|} = \frac{1}{\sqrt{(\partial z / \partial x)^2 + (\partial z / \partial y)^2 + 1}}$$

is the probability of acceptance. For the legs, when x and y are chosen uniformly in the circle

$$(x \pm 10)^2 + y^2 = R^2,$$

the point (x, y) is projected downward vertically until it intersects with the surface of the leg. This gives the value of z and is acceptable unless it lies behind the planes which bound the region containing the testes. In this case (x, y) is chosen again. For the bounding planes, points are chosen uniformly in them.

Other surfaces of the phantom remained the same. They are the side of the head, the shoulders, the trunk, and the bottom of the legs (feet). Methods for choosing on these surfaces are straightforward. For instance, to pick uniformly on the perimeter of an ellipse.

$$dS/d\theta_{\text{ellipse}} = \frac{x^2 + y^2}{a^2 b^2} (a^4 y^2 + b^4 x^2)^{1/2}$$

and

$$dS/d\theta_{\text{circle}} = a = \text{radius}.$$

The probability for success of (x, y) on the ellipse is

$$\frac{dS/d\theta_{\text{ellipse}}}{dS/d\theta_{\text{circle}}}$$

A surface is picked according to its own relative area randomly. Areas such as the side of the head, the shoulders, the trunk, and the bottom of the legs are easily determined – some with the evaluation of an elliptical integral. The area of the top of the head is calculated by evaluating the double integral

$$4 \int_0^{\pi/2} d\theta \int_0^{\pi/2} \frac{(\sin^2 \phi \cos^2 \theta/a^4 + \sin^2 \phi \sin^2 \theta/b^4 + \cos^2 \phi/c^4)^{1/2} \sin \phi}{(\sin^2 \phi \cos^2 \theta/a^2 + \sin^2 \phi \sin^2 \theta/b^2 + \cos^2 \phi/c^2)^2} d\phi.$$

The total area of both legs (truncated circular cones) is determined by evaluating the integral

$$(R^2 - r^2) \int_0^{2\pi} \sqrt{102 - 2 \cos \theta} d\theta$$

and then subtracting the area covered by the testical region and adding on the areas of its bounding planes.

So what we have is a revised man phantom more suitable for external sources with the capabilities of choosing points uniformly distributed in his surface area. New computer runs were made with the spectra of attenuated energies and with the angles of incidence from a cosine distribution for 12 monenergetic sources in infinite clouds.

Sponsor: Health Physics Division

MEDICAL X-RAY DOSE ESTIMATION

G. G. Warner J. W. Poston¹

We have described⁵ an approach to the calculation of average absorbed dose in several internal organs of a man phantom per unit of incident radiation exposure for external x-ray beams in the medical diagnostic photon energy range 20 keV to 150 keV. We propose to obtain a complete set of basic dosimetry data for selected photon energies on a spatial grid from which one can construct certain organ doses from typical diagnostic x-ray exposures of specified average energy or energy spectrum and varying field size and location. The doses will be estimated by Monte Carlo computer techniques described elsewhere using the anthropomorphic and heterogeneous phantom also previously described.²⁻⁴ The phantom has been modified to include approximations of lenses of the eyes, a diagnostic x-ray table, and the presence of iodine in the thyroid. The primary organs of interest in the study are the thyroid, lenses of the eyes, red bone marrow, and gonads. Preliminary work consisted of about 50 hr of computer runs on the IBM 360/91 to obtain data for 4 X 4 cm beams impinging on the trunk of the phantom for photon energies of 30 keV, 55 keV, and 80 keV.

Sponsor: Health Physics Division

ABSORBED FRACTION OF PHOTON ENERGY

G. G. Warner

Buildup factors, B , to 40 mean free paths from a point source of photons in an infinite homogeneous medium of water have been tabulated.^{6,7} These have been used⁸ to estimate the specific absorbed fraction

5. J. W. Poston and G. G. Warner, *Medical X-Ray Dose Estimation Program Progress Report for Period Ending August 31, 1972*, ORNL-TM-3986 (October 1972).

6. Martin J. Berger, *Energy Deposition in Water by Photons from Point Isotropic Sources*, MIRD Pamphlet No. 2, Supplement No. 1, *J. Nucl. Med.* (February 1965).

7. Martin J. Berger, National Bureau of Standards, private communication.

8. W. S. Snyder et al., *Health Phys. Div. Annu. Progr. Rep. July 31, 1971*, ORNL-4720, pp. 121-24.

$\Phi(T \leftarrow S)$ for extended source and target organs in a man phantom as a six-dimensional integral over the source organ and the target organ T :

$$\Phi(T \leftarrow S) = \frac{1}{|S| |T|} \int_S dX \int_T dY \frac{\mu_{ab} e^{-\mu|X-Y|}}{4\pi|X-Y|^2} B(\mu|X-Y|).$$

A density of 1 is assumed. It has been suggested that values of $\Phi(T \leftarrow S)$ obtained using B as defined for the infinite space are reasonable approximations to the values of $\Phi(T \leftarrow S)$ in the human body.⁸ The integral is evaluated by a Monte Carlo procedure and used in cases where another Monte Carlo technique³ does not provide statistically reliable estimates — principally for small organs such as gonads. In evaluating the integral, two difficulties arise: (1) buildup factors have been tabulated only to 40 mean free paths, and this is not adequate for some organ pairs ($T \leftarrow S$); (2) the integrand becomes infinite as X and Y tend to coincide, which is troublesome when S is T . The first difficulty has been met by substituting the buildup factor for 40 mean free paths even when the distance is greater. These substitutions have not affected the first four significant digits of Φ , and thus this difficulty is dismissed. We studied the second difficulty by replacing the estimator

$$\frac{e^{-\mu|X-Y|}}{|X-Y|^2} B(\mu|X-Y|)$$

by its average over a small sphere of radius k whenever $|X-Y| < k$. The value $k = 0.1$ has been found suitable for this purpose.

Sponsor: Health Physics Division

TOTAL ABSORBED RADIATION ENERGY FOR CALCULATION OF DOSE

G. G. Warner W. S. Snyder¹ L. T. Dillman⁹

We completed the coding of SPEFEN,¹⁰ and some amendments were made. The number of source organs was increased to 24 by the addition of skin and the semi-infinite source of attenuated photons in a cloud. The source in the skin now makes it possible to calculate internal bremsstrahlung dose from photons produced by betas striking the skin. For this purpose, photons per day spectra normalized to 1 μ Ci of a radionuclide per gram of air are provided by Dillman. The input table of specific absorbed fractions of photon energy is continually being updated by the application of improved methods of estimating these fractions.^{11,12}

Sponsor: Health Physics Division

URBAN RESEARCH

N. A. Buhl W. B. Malthouse N. B. Gove

We maintain the DUAL LABS retrieval software for extracting information from the 1960 and 1970 Census Summary tapes. We added a median option to the statistics options already available. We helped

9. Consultant, Ohio Wesleyan University

10. G. G. Warner et al., *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 29.

11. G. G. Warner, "Absorbed Fraction of Photon Energy," this report.

12. G. G. Warner and W. S. Snyder, "Dose from Gamma-Ray Sources," this report.

Urban Research Project personnel in the development of a generalized system for searching DUAL LABS compressed Census Summary tapes. The user can write his own FORTRAN for special-purpose aggregations or call on statistics or plotting packages.

We are developing programs to edit and use the DIME (Dual Independent Map Encoding) file. This file will be combined with other files to yield population density distributions within metropolitan areas.

We wrote programs to compress, decompress, and search the 1960 and 1970 Census Public Use Sample tapes. The compression scheme involved packing integers two per byte instead of one per byte as on the original tapes, which number about 200. Some further reduction in tapes was obtained by reblocking.

Sponsor: Urban Research Project, Health Physics Division

MIGRATION STUDIES

C. H. Gard P. G. Fowler

Analysis programs were written for the SADS program¹³ for studies on the migration of people into and out of the following cities: Boston, Detroit, Minneapolis, Wilmington, and Dallas.

Sponsor: Civil Defense Research Section, Health Physics Division

K. P. Nelson

LEED ADSEP DATA BASE

F. D. Hammerling

A numeric ADSEP¹⁴ data base was created from the LEED (Longitudinal Employee Employer Data) Atlanta subfile. The file is designed primarily for studies dealing with socioeconomic relationships, over time, such as

1. estimated total wages paid to a worker by his employer,
2. personal characteristics (age, sex, race) of the individual receiving the wages, and
3. characteristics of the employer (geographic location, industrial activity, coverage group) paying the wages

Sponsor: Civil Defense Research Section, Health Physics Division

Ruth Kemper

GRAPHIC DISPLAY OF CRIME STATISTICS

M. T. Heath

A methodology has been developed for graphically displaying crime statistics and other economic and sociological statistics related to crime. Using data supplied by the U.S. Census Bureau, the Saint Louis Police Department, and similar sources, a data base containing these statistics has been generated in the form of square grids for the Saint Louis area. A shading algorithm has been devised for the cathode ray tube plotter such that variations in optical density give a quantitative as well as qualitative visual indication of

13. A. A. Brooks and A. Hume, *The SADS Program - Statistical Analysis of Data Subsets*, CTC-19 (October 1969).

14. A. A. Brooks, *ADSEP - an Automated Data Set Editing Program*, CTC-34 (May 12, 1970).

the numerical value of a given statistic in a given region. This allows the social scientist to make geographic correlations between the various factors relating to crime.

Sponsor: Urban Research Project, Health Physics Division

M. M. Williams

CIVIL DEFENSE RESEARCH

M. T. Heath

The principal effort in Civil Defense Research for the past year has been the study of risk reduction for the civilian population by emergency evacuation of dense urban areas to sparse rural areas. To facilitate this study a number of population data bases have been created, including a 0.01° coordinate grid for the entire United States based on the 1970 census. A similar grid for 1960 is planned so that population projections into the future will be possible. To aid in locating feasible evacuation routes, a graphical display system has been developed so that areas of high and low population density can be identified visually on computer-generated maps of the United States. The next phase of this project is the development and programming of algorithms to simulate the movement of the population in an actual evacuation.

Sponsor: Civil Defense Research Section, Health Physics Division

C. M. Haaland

SIMULATION OF ELECTRON-SWARM TRANSPORT EXPERIMENT

V. E. Anderson

A mathematical model to simulate an electron-swarm transport experiment has been developed and will be used to determine the transport parameters (drift velocity and diffusion coefficients), especially for very low energy electrons. Data to be analyzed include oxygen, argon, and water.

Sponsor: Health Physics Division

DeVaughn Nelson

NEW UNFOLDING TECHNIQUE

V. E. Anderson

Cross sections for many types of reactions were unfolded from data gathered by different groups in the division. This unfolding technique was developed last year¹⁵ and used on a routine basis this year.

Sponsor: Health Physics Division

MONTE CARLO CALCULATIONS FOR MOLECULAR DISSOCIATION

V. E. Anderson

Metastable negative ions of the form $C_xH_yCO_2^-$ are produced in the source of a time-of-flight mass spectrometer. The ions decay into the products $C_xH_y + CO_2 + e$, and the spreading in time of the pulse of neutral products is observed. A Monte Carlo procedure was used to describe the time-of-flight distribution

15. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 31.

of these products and, using the kinetic energy of dissociation as an undetermined parameter, to fit experiment with theory.

Sponsor: Health Physics Division

R. M. Compton

MONTE CARLO ANALYSIS OF AN NE213 DETECTOR

S. N. Cramer

A Monte Carlo analysis of a nominal 2 X 2 in. cylindrical NE213 detector has been performed using the ESP code.¹⁶ The investigation involved calculation of the alpha-particle spectrum due to the $(n,n')3\alpha$ and the (n,α) reactions with carbon and the proton spectrum due to neutron collisions with hydrogen. These spectra were volume integrated over the detector. The source consisted of monoenergetic beams of neutrons incident on one end of the cylinder. The spectra were calculated from an energy balance following each type of collision, and it was assumed that each neutron could produce only one alpha particle and one proton, with each particle having the combined energy of all like particles actually produced. The energy of each particle is the energy loss of the neutron less the reaction Q value.

Sponsor: Health Physics Division

16. S. N. Cramer, R. S. Carlsmith, G. W. Morrison, G. W. Perry, and J. L. Lucius, "ESP: A General Monte Carlo Reactor Analysis Code," this report.

INFORMATION DIVISION

FORMAT CONVERSION PROGRAMS

C. A. Giles

Several programs have been written which facilitate the translation of data in magnetic tape form from one format to another. Two programs convert data published by outside sources to the format used in the Text Search System. These two data bases are the *Chemical-Biological Activities* and the *NTIS Bibliographic Data File*. In addition, a program has been written which translates ADSEP data bases into a format suitable for the Text Search System. The reverse procedure has also been implemented. Data retrieved by the Text Search process can be converted to the generalized external format for further processing by ADSEP and ORLOOK.

Sponsor: Information Division

CURRENT AWARENESS SERVICE FOR LARGE-SCALE BIBLIOGRAPHIC DATA BASES

C. A. Giles J. S. Gillen

The Mathematics Division operates a computerized current awareness or SDI (selective dissemination of information) service for the Information Division. Profiles of researchers' interests are provided to the Mathematics Division by the Information Division or by individuals. These profiles are entered into the system via computer terminal. The profiles are then matched with the data bases available. The current files include *Nuclear Science Abstracts*, *Biological Abstracts*, *Bio-research Index*, *Chemical-Biological Activities*,

Searchable Physics Information Notices, and *NTIS Bibliographic Data File*. During the past year, 165 searches were made for 76 people, resulting in 188,347 references to the published literature.

Sponsor: Information Division

INSTRUMENTATION AND CONTROLS DIVISION

THERMOCOUPLE AND RESISTANCE THERMOMETER CALIBRATION DATA REDUCTION

T. C. Tucker R. L. Simpson¹

We have begun a major revision of an existing program² for reducing and reporting thermocouple and resistance thermometer calibration data. This revision incorporates the International Practical Temperature Scale (IPTS) of 1968.³ It features an input section that interprets most instructions from English words or abbreviations. Further, a number of input error detectors enable the program to skip a case with bad data, list the data cards which form an invalid set, and proceed to the next set of data.

To decrease job turnaround time and computer costs, this program is designed to use computer memory and system scratch disks only.

Sponsor: Instrumentation and Controls Division

R. K. Adams

PCAP: PRINCETON CIRCUIT ANALYSIS PROGRAM

C. C. Webster

PCAP is designed to analyze electrical and electronic circuits, both linear and nonlinear. The problem-oriented input language is similar to that of the ECAP program. It provides a more flexible output format than ECAP, including a printer-plot type of graphic output. It can handle transmission line models, idealized delay elements, and sample-and-hold elements. This program is available in the Mathematics Division on tape or on computer cards.

Sponsor: Instrumentation and Controls Division

J. T. DeLorenzo

ECAP: ELECTRONIC CIRCUIT ANALYSIS PROGRAM

C. C. Webster

This code, as it existed at the time of the last annual report,⁴ has had further modifications. The addition of subroutines that use the ORNL plotting program ORGRAPH and a Calcomp plotter provides the option of making graphs of the results. Improvements have been made in the program so that the output is displayed in a more convenient and usable form.

Sponsor: Instrumentation and Controls Division

J. T. DeLorenzo

1. Instrumentation and Controls Division.

2. R. L. Simpson and R. K. Adams, *Instrumentation and Controls Div. Annu. Progr. Rep. Sect. I*, 1965, ORNL-3875, p. 85.

3. "The International Practical Temperature Scale of 1968," *Metrologia* 5(2), 35-44 (April 1969).

4. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 32.

EDITING AND REPORTING PROPERTY RECORDS FOR THE INSTRUMENTATION AND CONTROLS DIVISION STANDARDS LABORATORY

R. B. Hofstra

So that the availability and location of equipment which is seldom used can be more readily known, the Standards Laboratory is instituting a new filing system. As a part of this system, a punched card is generated for each item. We have coded a collection of programs to edit, reformat, and repunch the cards and to prepare reports listing the equipment in various logical sequences.

Sponsor: Instrumentation and Controls Division

R. K. Adams

ISOTOPES DIVISION

CALCULATION OF THE ELECTRON-DIATOMIC-MOLECULE OPTICAL POTENTIAL

L. W. Owen G. D. Alton¹

The electron-diatomic-molecule optical potential² is being calculated with the projection operator formalism of Feshbach.³ Coupling to rotational and vibrational intermediate states is approximated by a free-particle Green's function and yields a complex nonlocal potential. Computer codes⁴ developed at Oak Ridge will be used to solve the resulting integrodifferential Schroedinger equations for the elastic scattering of low-energy electrons by CO and other diatomic molecules.

Sponsor: Isotopes Division

ELECTRON SCATTERING FROM HYDROGEN

M. Reeves G. D. Alton¹

Low-energy ($E \lesssim 15$ rydbergs) elastic scattering of electrons from hydrogen has been examined and found to be in satisfactory agreement with previously published studies.⁵ Using the Feshbach formalism,³ intermediate-state couplings to all excitation and ionization states have been included. Exchange has not been included. Bound states are assumed to have the usual hydrogenic wave functions, and ionization states are taken to have Coulomb wave functions. The incident electron, however, has been modeled with plane waves in the intermediate state. At present, the computer codes are being modified so that these wave functions may be distorted by the presence of the initially bound electron.

Sponsor: Isotopes Division

1. Isotopes Division.

2. G. D. Alton, doctoral dissertation, University of Tennessee (unpublished).

3. H. Feshbach, *Ann. Phys.* 19, 287 (1967).

4. M. Reeves III and L. W. Owen, *J. Comput. Phys.* 4, 572 (1969).

5. G. D. Alton, W. R. Garrett, M. Reeves, and J. E. Turner, *Physical Review* (to be published).

MATHEMATICS DIVISION

NUMERICAL METHODS NEWSLETTER

R. E. Funderlic

In order to improve communications in the area of numerical methods and their related computer programs, the Mathematics Division is periodically issuing pertinent newsletters. The first one appeared in November 1972.

The content of the newsletters will include announcements and critiques of computer programs, ideas related to numerical algorithms, modifications of methods or programs, and a question section.

Sponsor: Mathematics Division

EISPACK: SUBROUTINES FOR EIGENSYSTEMS

J. D. Amburgey R. E. Funderlic

The package of FORTRAN subroutines for eigensystem computations that were recently certified at Argonne has been implemented at OKNL. These subroutines were adapted from ALGOL routines.¹ The problem areas covered include real symmetric, nonsymmetric, complex Hermitian, and non-Hermitian matrices. A user's manual and card decks are available in the computer librarian's office. The routines may also be obtained from disk storage by use of the appropriate control cards.

All the programs have been checked with the driver programs provided by Argonne. The routines performed quite well and probably should be used in preference to any other eigensystem routines presently in use.

Sponsor: Mathematics Division

MODULAR FOURIER ANALYSIS ROUTINE

E. C. Long M. R. Patterson

This routine is an outgrowth of combining the best features of a number of Fourier analysis codes into an efficient, easily modified modular routine. Subroutine FFT² (Fast Fourier Transform) is used for computing the Fourier transform and inverse transform. Solution of the convolution integral by FFT is used in subprograms for computing autocorrelation, cross correlation, power spectral density, cross spectral density, and digital filtering. Also included are routines for reflecting data points at each end of the complex data array used in FFT; generating a filter (low, band, or high pass); and plotting.

Sponsor: Mathematics Division

1. J. H. Wilkinson and C. Reinsch, *Handbook for Automatic Computation*. Vol. II. *Linear Algebra*, Springer Verlag, 1971.

2. G. W. Westley and J. A. Watts, eds., *Computing Technology Center Numerical Analysis Library*, CTC-39 (October 1970).

MODIFICATION TO FORTDOC

R. C. Durfee C. C. Webster

A modified version of the computer programming package FORTDOC has been prepared and tested. The modified version numbers the cards sequentially in columns 73–80 without altering the statement numbers. The program then proceeds with step 2 and step 3 of the original FORTDOC program.

Sponsor: Mathematics Division

REGULAR CLUSTERS IN TWO DIMENSIONS

J. A. Carpenter

Given an n -by- n lattice A of points on a square grid, a subarray of A taken from s contiguous rows and s contiguous columns of its lattice points is called a regular cluster of size $S = s \times s$. There are $N = (n - s + 1)^2$ such regular clusters of A . Given any k ($1 \leq k \leq N$) regular clusters of size S , the number of points p ($S \leq p \leq n^2$) of the lattice A that belong to the set union of the k regular clusters is determined. There are $\binom{N}{k}$ possible combinations of k distinct clusters, and for each such combination a value of p is determined for given n , s , and k . Define $F(k, p)$ as the number of set unions of k clusters of size S that include p points of the lattice A . A FORTRAN IV program has been constructed to evaluate and tabulate the function $F(k, p)$ and to evaluate the means and variances of $F(k, p)$ for $k = 1, \dots, N$. We note as computational checks

$$\sum_{p=S}^{n^2} F(k, p) = \binom{N}{k} \sum_{r=1}^N \sum_{p=S}^{n^2} F(k, p) = 2^N - 1.$$

Since there are $2^{(n-s+1)^2} - 1$ evaluations of p for given n and s , the time requirements for the evaluation of $F(k, p)$ for $n - s$ large quickly become dominant, and further refinements are necessary to evaluate the function for such arguments.

Sponsor: Mathematics Division

COMPUTER OUTPUT FOR REPRODUCTION PURPOSES³

F. D. Hammerling A. A. Brooks

A FORTRAN subroutine, a PL/I procedure, and a new PL/I DECPRNT (prints PDP-10 runoff files on the 360 with the extended print chain) were written to facilitate producing computer output suitable for reproduction purposes. These subroutines enable the user to conveniently reproduce the fiduciary marks and margins of the UCN-2477C reproduction form. The subroutines have entries for both $8\frac{1}{2} \times 11$ in. and $11 \times 8\frac{1}{2}$ in. pages.

Sponsor: Mathematics Division

3. ORCID Memo, June 13, 1972.

CONVERSION OF CDC-160A PROGRAMS TO PDP-10

P. R. Coleman

Work is being completed on the project of converting all paper tape work from the CDC-160A to the PDP-10.⁴ Several new, more general paper tape programs are being written and documented with the hope that any new paper tape work will be greatly simplified. These programs will copy paper tapes, written in ASCII or other codes, onto cards, magnetic tape, or disk files.

Sponsor: Mathematics Division

4. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 36.

METALS AND CERAMICS DIVISION

LITHIUM HYDRIDE THERMAL EXPANSION DATA

D. E. Fields O. S. Robinson M. R. Patterson

A linear least squares analysis was performed and plots were made for thermal expansion data obtained from the material lithium hydride in the temperature range 32° to 1112°F. The data were measured by H. E. McCoy of the Metals and Ceramics Division. The following quadratic form was assumed for the length of a specimen as a function of temperature:

$$l = l_0 [1 + a(T - T_0) + b(T - T_0)^2] .$$

The thermal expansion coefficient α was calculated from

$$\alpha = \frac{\partial}{\partial T} \left(\frac{l - l_0}{l} \right)$$

$$\approx a + 2b(T - T_0) ,$$

where l = length, T = temperature, the starting values are indicated by the subscript zero, and the parameters a and b were extracted from the data. Our results were in agreement with prior analyses of high-temperature data on this compound.

Sponsor: Metals and Ceramics Division

H. E. McCoy

IMPEDANCE OF COILS ENCIRCLED BY OR ENCIRCLING MULTIPLE COAXIAL CYLINDRICAL CONDUCTORS

R. B. Hofstra C. W. Nestor, Jr. C. V. Dodd¹

We have adapted computer programs² written in BASIC to FORTRAN for use on the IBM 360 computers and have made several changes in the programs to improve the accuracy of the calculations. We

1. Metals and Ceramics Division.

2. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, pp. 37-39.

have used the rational approximations given by Blair and Russon³ for the modified Bessel functions of real argument $I_0(x)$, $I_1(x)$, $K_0(x)$, and $K_1(x)$ in a subroutine to compute these functions to 15-figure precision. We have used the backward recurrence scheme of Miller⁴ in a subroutine for the computation of the modified Bessel functions $I_0(z)$ and $I_1(z)$ of complex argument z . We have also used the Padé approximations given by Luke⁵ for the computation of the modified Bessel functions $K_0(z)$ and $K_1(z)$ of complex argument z . We have also developed a special procedure for the treatment of thin conducting regions to avoid the loss of significant figures in the subtraction of quantities that become equal in the limit of zero region thickness.

To aid the remote user of these programs, we have written a FORTRAN program for the PDP-10 computer to allow the user to construct a data file for submission to the IBM 360 computer. The 360 program places selected portions of the output in a data file for later retrieval at the user's remote Teletype.

Sponsor: Metals and Ceramics Division

C. V. Dodd

ANALYSIS AND PROCESSING OF CREEP-RUPTURE DATA

R. B. Hofstra

We have modified the data management system CADCAPS⁶ to allow for a new application, and we have included a new graphics program⁷ in the system.

Sponsor: Metals and Ceramics Division

H. E. McCoy

R. T. King

3. J. M. Blair and A. E. Russon, *Rational Minimax Approximations for the Bessel Functions $K_0(x)$ and $K_1(x)$* , Chalk River Nuclear Laboratories report AECL-3461 (October 1969).

4. J. C. P. Miller, *Bessel Functions, Part II, Functions of Positive Integer Order*, British Association for the Advancement of Science Mathematical Tables, Cambridge, 1952, p. 16.

5. Y. L. Luke, *The Special Functions and Their Approximations*, vol. 2, Academic, New York, 1969.

6. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 39.

7. R. T. King, personal communication.

NEUTRON PHYSICS DIVISION

COMPLETION OF VERSION I OF TASK, A TRANSPORT AND DIFFUSION CODE FOR REACTOR KINETICS ANALYSES

O. W. Hermann R. J. Hinton

A. R. Buhl¹

Major modifications to the TASK code,²⁻⁴ including the work to incorporate several significant features,⁵ have been completed. The user's manual⁶ was published, and several decks of this version have been distributed to installations interested in using the code.

1. Neutron Physics Division.

2. Acronym for Transfer and Scattering Matrix Method in Reactor Kinetics.

3. H. L. Dodds, Jr., J. C. Robinson, and A. R. Buhl, "The Formulation and Application of the Transfer-Scattering Matrix Method to Space-, Energy-, and Angular-Dependent Fast Reactor Kinetics," *Nucl. Sci. Eng.* **47**, 262-74 (1972).

4. H. L. Dodds, Jr., *A New Calculational Method for Space-Energy-Angular-Dependent Reactor Kinetics*, ORNL-TM-3136 (1971).

5. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 33.

6. A. R. Buhl, H. L. Dodds, Jr., J. C. Robinson, R. A. Lillie, O. W. Hermann, and R. J. Hinton, *A User's Manual for TASK - a Generalized One-Dimensional Transport and Diffusion Kinetics Code*, ORNL-TM-3811 (1972).

The TASK code was developed to solve the one-dimensional multigroup form of the reactor kinetics equations using either transport, diffusion, or telegrapher's theory and allowing any number of delayed neutron groups. It can also be used to solve standard statics problems, for example, distributed source, boundary source, and eigenvalue problems. The code has been verified, for example, in computing generation times in subcritical fast reactor systems.⁷ TASK applies a combined scattering and transfer matrix technique in order to eliminate certain difficulties which arise in finite difference approximations. Within-group (inner) iterations are not used, allowing convergence independent of spatial mesh size. Thus, problems resulting from sources in highly multiplicative media are circumvented. A basic innovation was implemented in TASK in removing the time variable by Laplace transformation of the initial equations. The outer iteration⁸ mode is also an available option which may be more expeditious in solving larger-type problems.

Several features were added to facilitate the use of TASK. Flexible dimensioning permits the number of groups or mesh points or other data to be somewhat arbitrarily chosen. The data input utilizes "free-form FIDO." A definite attempt was made to list all input data in the form of meaningful-type tables. Intermediate-type results are printed only upon option. Output of final results was given better organization. Legendre polynomial computations⁹ are done internally if desired. The core storage requirement has been reduced to 154K bytes plus the size of data block in execution on the IBM 360.

Sponsor: Neutron Physics Division

A. R. Buhl

SPECTRAL UNFOLDING AND ILL-CONDITIONED LINEAR SYSTEMS

M. T. Heath B. W. Rust

This work is the result of a synthesis of two independent approaches to the spectral unfolding problem. One approach was discussed in last year's annual report¹⁰ and has its culmination in the following theorem about iterative solutions to ill-conditioned linear systems.

Theorem. For any $m \times n$ matrix A ($m \geq n$), m -vector b , initial n -vector x_0 , and real scalar τ , the sequence of n -vectors defined by

$$x_{i+1} = (A^T A + \tau^2 I)^{-1} (A^T b + \tau^2 x_i)$$

converges to the least squares solution of the system: $Ax \approx b$.

The significance of this theorem is that the scalar τ acts as a stabilizing influence to make the problem better conditioned than the original formulation. The τ should be chosen small enough for rapid convergence but large enough for numerical stability. The iteration should be halted, however, before any oscillations of the true solution appear. This method produces no error bounds for the solution, a defect alleviated by the subsequent method.

7. A. R. Buhl and J. C. Robinson, "Verification of a New Method for Calculating and Measuring Generation Time in a Subcritical Fast Reactor," presented at New Developments in Reactor Physics and Shielding Meeting, Kiamesha Lake, N.Y., Sept. 12-15, 1972.

8. R. A. Lillie, "Incorporation of Outer Iteration Techniques into the TASK Algorithm," M.S. thesis, Univ. of Tenn. (1972).

9. Utilized subroutine POLY, written by J. R. Knight, Mathematics Division, ORNL.

10. M. T. Heath, "Ill-Conditioned Linear System," *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 36.

The other approach is the constrained interval estimation approach which was pioneered by W. R. Burrus and his co-workers.¹¹⁻¹⁵ So far, the main emphasis has been on FERDOR-type, suboptimal methods, and the chief result has been an iterated FERDOR technique which for many of the test cases tried produces better error bounds than FERDOR. This method is called FERDIT. It uses a FERDOR calculation as the initial estimate for the iteration. Thus, FERDIT always does at least as well as FERDOR, and for many problems, it gives sharper results.

Some effort has gone into development of an OPTIMO linear programming code, but for the most part, this task has been left for future development. Future plans also include an efficient quadratic programming code designed for solving unfolding problems.

All of the techniques that have been and are being developed are currently being applied to a very difficult unfolding problem originated by C. E. Clifford of the Neutron Physics Division. This problem involves the combination of Blosser spectrometer measurements with Bonner ball measurements in order to obtain better resolution of the low-energy portion of a neutron spectrum.

Sponsor: Neutron Physics Division

C. E. Clifford

**INTRIGUE-II-C: AN IBM 360 SUBROUTINE PACKAGE
FOR MAKING LINEAR, LOGARITHMIC, AND SEMILOGARITHMIC GRAPHS
USING EITHER THE CALCOMP PEN-AND-INK OR CATHODE-RAY-TUBE PLOTTER¹⁶**

M. B. Emmett

The previously reported INTRIGUE-II¹⁷ has been modified in order to allow use of the cathode-ray-tube plotter. The modifications also include use of scale factors for labeling linear graphs and addition of a subroutine for inserting numerical values in a subtitle. This package may be used in place of INTRIGUE-II but does not provide large-size lettering, as INTRIGUE-II-L does.

Sponsor: Neutron Physics Division

**SWANLAKE: A COMPUTER CODE UTILIZING ANISN TRANSPORT CALCULATIONS
FOR SENSITIVITY ANALYSIS**

D. E. Bartine F. R. Mynatt¹
E. Oblow¹

A code has been written to determine the relative importance of a specific cross section in a given calculation. Required input includes forward and adjoint angular flux tapes of the form produced by

11. W. R. Burrus, *Utilization of A Priori Information by Means of Mathematical Programming in the Statistical Interpretation of Measured Distributions*, ORNL-3743 (June 1965).

12. J. Repogle, B. D. Holcomb, and W. R. Burrus, "The Use of Mathematical Programming for Solving Singular and Poorly Conditioned Systems of Equations," *J. Mathe. Anal. Appl.* **20**, 310-23 (November 1967).

13. W. R. Burrus and V. V. Verbinski, "Fast-Neutron Spectroscopy with Thick Organic Scintillators," *Nucl. Instrum. Methods* **67**, 181-96 (1969).

14. B. W. Rust and W. R. Burrus, *Mathematical Programming and the Numerical Solution of Linear Equations*, American Elsevier Publishing Co., Inc., New York, 1972.

15. B. W. Rust and W. R. Burrus, *Suboptimal Methods for Solving Constrained Estimation Problems*, DASA-2604 (January 1971).

16. Abstract of ORNL-TM-3947 (October 1972).

17. M. B. Emmett, *INTRIGUE II, an IBM 360 Subroutine Package for Making Linear, Logarithmic, and Semilogarithmic Graphs Using the CALCOMP Plotter*, ORNL-4664 (1971).

ANISN¹⁸ and an ANISN-type description of the problem. Output includes the sensitivity as a function of position in the cross-section matrix, where the sensitivity is a measure of the importance of a given cross section in the calculation being investigated. The sensitivity is summed and presented as a function of energy group and spatial zone. In addition, a plot of sensitivity per unit lethargy vs energy is an option. The plots are created by INTRIGUE-II¹⁷ and can display sensitivity for the entire physical system or as a function of spatial zone. The cross sections studied can be total collision cross sections or partials such as elastic or inelastic.

Sponsor: Neutron Physics Division

NEUTRON CROSS-SECTION SENSITIVITY ANALYSIS: A GENERAL APPROACH ILLUSTRATED FOR A SODIUM-IRON SYSTEM¹⁹

D. E. Bartine E. Oblow¹
F. R. Mynatt¹

A general approach to sensitivity studies is introduced using a quantitative definition of cross-section sensitivity. The definition offered is intended to be both practical and physically meaningful. Its advantages in comparison with other approaches are discussed, and its use in analysis is illustrated for a sodium-iron transport problem. Results of the analysis include a discussion of the role of important total cross-section minima in deep penetration in sodium and iron and the importance of certain energy ranges and partial cross sections for the sodium-iron system. The predictive aspect of the approach is demonstrated in comparisons of rigorous and predicted results for small cross-section perturbations and in conclusions about the order of Legendre expansion of the scattering kernel.

Sponsor: Neutron Physics Division

A SENSITIVITY ANALYSIS OF NEUTRON AND GAMMA TRANSPORT IN AIR²⁰

D. E. Bartine F. R. Mynatt¹
E. Oblow¹

Sensitivity profiles, which show the relative importance of specific cross sections for a given calculation, were obtained for problems involving determination of the tissue dose in air at 2000 m resulting from 14-MeV, thermonuclear, and fission neutron sources. Calculated sensitivities to neutron total collision cross sections were obtained for neutron and gamma dose responses.

For the thermonuclear source, sensitivity profiles were also determined for individual reaction cross sections – elastic, inelastic, $(n,2n)$, (n,α) , etc. In general, the sensitivity was high for nonelastic cross sections above ~ 2 MeV, while the sensitivity to the elastic cross section dominated at lower energies.

In addition to the sensitivity profiles, a first attempt was made to utilize the sensitivity results to estimate the effect of cross-section uncertainties on the calculated tissue dose. A preliminary nitrogen error file provided by the evaluator, Phil Young of Los Alamos Scientific Laboratory, was used for the estimation, which pointed up the relative importance of the nitrogen (n,α) cross section.

Sponsor: Neutron Physics Division

18. W. W. Engle, Jr., *A Users Manual for ANISN, a One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1693 (1967).

19. Abstract of OKNL-TM-3944 by D. E. Bartine, E. Oblow, and F. R. Mynatt.

20. Summary of a paper presented at the American Nuclear Society Meeting, Washington, D.C., Nov. 12–17, 1972.

SENSITIVITY STUDIES FOR AIR-CONCRETE CALCULATIONS

D. E. Bartine J. V. Pace R. Q. Wright
E. M. Oblow¹ F. R. Mynatt¹

Sensitivity studies were initiated on an air-concrete system using the unclassified thermonuclear source and neutron displacement and gamma-ray ionization response functions. Preliminary calculations utilized the 22-18 coupled neutron-gamma cross-section sets for air and concrete which were used in the FY 1971 and 1972 silo calculations. Concurrently, an effort was commenced to determine an energy group structure for air-concrete calculations. A 129-neutron-group structure was selected to fit the major valleys in the nitrogen and oxygen total cross sections, and a 42-gamma-ray-group structure was selected to represent the major gamma-ray production lines. The resultant 129-42 coupled neutron-gamma group structure will be the basis for further sensitivity studies, for comparison with nonmultigroup calculations, and for comparisons with few-group calculations.

Sponsor: Neutron Physics Division

A SENSITIVITY ANALYSIS OF THE CTR STANDARD BLANKET

D. E. Bartine R. G. Alsmiller¹ J. Barish
E. Oblow¹ F. R. Mynatt¹

A sensitivity analysis has been performed for tritium breeding by ${}^6\text{Li}$ and ${}^7\text{Li}$ in the CTR standard blanket.²¹ The calculation used a 14-MeV source and cylindrical geometry. Sensitivities were obtained for Nb, ${}^6\text{Li}$, ${}^7\text{Li}$, and C cross sections.

Sponsor: Neutron Physics Division

CROSS-SECTION SENSITIVITY STUDIES FOR THE LLL PULSED-SPHERE EXPERIMENTS

S. N. Cramer R. W. Roussin¹ F. G. Perey¹ E. Oblow¹

The calculations of the LLL pulsed-sphere experiments²² have been extended to include sensitivity studies of the cross-section data in an effort to determine which specific areas of the data have an important effect on the final results. Primary attention has been given to the iron data, where the calculations show the poorest agreement with experiment. Other experiments investigated included the nitrogen, oxygen, and water spheres.

The O6R Monte Carlo code²³ is being used in these studies owing to its applicability in isolating specific aspects of the transport and collision processes. In this manner the results at various times can be analyzed with respect to (1) reaction type, (2) secondary energy distribution, (3) reaction energy, and (4) number of collisions. The MORSE Monte Carlo code²⁴ has been used to a lesser degree in order to verify the results from O6R. Although the two codes process basic cross sections by entirely different methods, the calculated time-dependent count rates compare favorably in all cases.

21. D. Steiner, ORNL, private communication (1972).

22. R. W. Roussin et al., "O6R Calculations of Nitrogen and Iron LLL Pulsed Sphere Experiments," *Trans. Amer. Nucl. Soc.* 14(2), 925-26 (1971).

23. C. L. Thompson and E. A. Straker, *O6R-ACT'FK, Monte Carlo Neutron Transport Code*, ORNL-CF-69-8-36 (1969).

24. E. A. Straker et al., *The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585 (1970).

Calculations for the iron spheres indicate that the fast spectrum above 2 MeV is highly sensitive to uncollided neutrons from the source and the partial cross sections and secondary energy distribution of nonelastic reactions at source energies. An analysis of the data for these reaction processes has provided useful information to the evaluation effort on iron at ORNL.

Sponsor: Neutron Physics Division

**INVESTIGATION OF THE ADEQUACY OF NITROGEN CROSS-SECTION SETS:
COMPARISON OF NEUTRON AND SECONDARY-GAMMA-RAY TRANSPORT
CALCULATIONS WITH INTEGRAL EXPERIMENTS²⁵**

E. A. Straker²⁶ M. B. Emmett J. V. Pace III B. J. McGregor²⁷
R. W. Roussin¹ H. T. Smith²⁶ L. R. Williams¹

Two sets of cross sections for neutron interactions and secondary-gamma-ray production in nitrogen, one recently evaluated by P. G. Young and D. G. Foster and another assembled in 1968 by the author, have been tested in transport calculations corresponding to integral experiments. The experiments are Operation HENRE, during which measurements were made of the neutron and gamma-ray doses produced in the atmosphere by an accelerator emitting approximately 14-MeV neutrons, and two experiments in which liquid-nitrogen-filled dewars were pulsed with approximately 14-MeV neutrons. One of the nitrogen-dewar experiments, performed at Gulf Radiation Technology, yielded the energy spectra of fast and intermediate-energy neutrons and secondary gamma rays within the nitrogen, and the other, performed at Lawrence Livermore Laboratory, gave time-dependent count rates due to neutrons leaking from the nitrogen. The comparisons of the calculated and measured results showed that for Operation HENRE both cross-section sets were adequate for calculating the neutron doses but that only the old set correctly predicted the gamma-ray doses, the new set giving results that are 30 to 50% lower than the data. Conversely, the comparisons for the GRT nitrogen-dewar experiment showed that the new set gives gamma-ray spectral data that are in reasonable agreement with the experiments, whereas the old set overpredicts by as much as a factor of 2. For both nitrogen-dewar experiments, the new cross sections give better predictions of the neutron spectra and time-dependent neutron count rates than the old cross sections. Additional calculations with both sets of cross sections for an infinite air medium show that the two sets give identical neutron and secondary-gamma-ray doses for a fission source; they also give very similar neutron doses for a 12.2- to 15-MeV neutron source, but the secondary-gamma-ray doses are in disagreement, those obtained with the newer set being 30 to 50% lower. "Sensitivity" calculations indicate that for high-energy neutron sources most of the secondary gamma rays are produced by neutrons having energies greater than 10 MeV, and the greatest difference between the two cross-section sets is their gamma-ray production probabilities at high neutron energies. On the basis of the various comparisons, it appears that the new neutron cross sections give better predictions of neutron quantities but that a choice between the gamma-ray production cross sections is not obvious since each set agrees with one of the two gamma-ray experiments.

Sponsor: Neutron Physics Division

E. A. Straker

25. Abstract of ORNL-TM-3768 (August 1972).

26. Now at Science Applications, Huntsville, Ala.

27. On assignment from Australian AEC.

AMPX MODULE XLACS: A PROGRAM TO PRODUCE WEIGHTED MULTIGROUP CROSS SECTIONS FROM ENDF/B

J. E. White N. M. Greene J. L. Lucius R. Q. Wright

During the past year the following modifications and improvements have been made to XLACS,²⁸ which is the neutron cross section processing module of the AMPX system.^{29,30}

1. Revised neutron library format. Provisions have been made to allow an anisotropic representation for inelastic and $(n, 2n)$ scattering.

2. Implementation of additional weighting options. Cross sections can now be averaged over (a) an arbitrarily defined input weighting function, (b) a $1/E \sigma_t$ weighting function, and (c) a fission- $1/E$ -Maxwellian weighting function.

3. One-thermal-group treatment. In the past, the "hand-patched" one-thermal-group case has often caused some delay in processing the neutron cross sections. An allowance has been made to automatically treat the thermal group by weighting the ENDF/B File 3 thermal cross sections over a Maxwellian spectrum. The peak temperature is specified by an input parameter. This feature is in effect when the flux variation is assumed to be $1/E$. Alternatively, thermal values can be input on cards.

4. Inclusion of special built-in sources and response functions. Several response functions and sources can be automatically weighted (or integrated) over the problem group structure, including (a) Hurst dose factors, (b) Snyder-Neufeld dose factors, (c) conversion factors for neutron displacement in silicon, (d) conversion factors for neutron ionizations in silicon, and (e) several damage functions resulting from a study of neutron irradiation in stainless steel 304. A thermonuclear source is also included.

5. Improvement in code flexibility. In addition to specifying different logical units for the fast and thermal data sets, XLACS will now process ENDF/B data in any combination of logical unit number and tape mode (BCD or binary).

6. Improvement in resolved resonance treatment. New schemes pick optimal integration meshes in the resonance range. Doppler broadening is allowed. Any of the weighting functions, except $1/E \sigma_t$, mentioned in item 2 above can be used.

7. Analytic P_0 thermal treatment. To circumvent the time-consuming $S(\alpha, \beta)$ treatment, P_0 thermal scattering matrices can be generated analytically using modified subroutines taken from the THERMOS program.³¹

8. Modifications associated with ENDF/B format changes. The subroutine which averages the File 3 data now accommodates new and reactivated reaction type numbers.

XLACS can be obtained as a stand-alone code through the Radiation Shielding Information Center (RSIC) at ORNL or the Argonne Code Center at ANL. A report (ORNL-TM-3646) documenting the program is also available.

Sponsor: Neutron Physics Division

28. N. M. Greene et al., *XLACS: A Program to Produce Fine Group Averaged Neutron Cross Sections from ENDF/B*, ORNL-TM-3646 (April 1972).

29. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 62.

30. *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1972*, ORNL-4800, p. 30.

31. H. C. Honeck, *THERMOS: A Thermalization Transport Theory Code for Reactor Lattice Calculations*, BNL-5826.

DEVELOPMENT OF NITAWL, AN AMPX MODULE THAT PERFORMS RESONANCE CALCULATIONS AND PREPARES WORKING LIBRARIES

N. M. Greene J. L. Lucius

A segment of the XSDRN code³² that performs resonance calculations and processes neutron cross-section libraries was isolated and extended to meet the broader AMPX²⁹ requirement of processing coupled neutron and gamma cross-section libraries.

NITAWL has the capability of generating cross-section libraries directly for the ANISN,¹⁸ DOT,³³ and MORSE²⁴ codes in addition to preparing working libraries for processing by the XSDRN code.

Improved data storage techniques were designed and implemented which minimize core storage requirements.

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SMUG: THE AMPX SYSTEM MODULE THAT GENERATES GAMMA-RAY CROSS SECTIONS

J. L. Lucius W. E. Ford III

SMUG²⁹ has been modified to construct multigroup gamma-ray cross sections in the AMPX library format.²⁹ The ability to punch these cross sections directly into card libraries for codes such as ANISN¹⁸ and DOT³³ has been retained.

Input capabilities have been extended to accept basic cross-section library data from either the OGRE³⁴ or ENDF/B³⁵ libraries. Problem descriptive card input in the convenient free-form FIDO input format pioneered in the ANISN code is now accepted by SMUG, replacing a fixed-format input procedure.

The section of the code that calculates group tissue dose factors has been generalized to accept data from several sources. Several modifications have been completed to permit the code to function correctly in the AMPX system environment.

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C. E. Clifford
F. R. Mynatt

32. N. M. Greene and C. W. Claven, Jr., *XSDRN: A Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (July 1969).

33. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stevens, *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (1969).

34. D. K. Trubey and J. R. Stockton, *OGRE - General-Purpose Monte Carlo Gamma-Ray Transport Code System*, ORNL-3805 (1969).

35. M. K. Drake, ed., *Data Formats and Procedures for the ENDF Neutron Cross Section Library*, BNL-50274 (T-601), (ENDF 102, vol. 1) (October 1970).

LAPHFOR AND LAPHNGAS: MODIFIED VERSIONS OF LAPHANO, A P_0 MULTIGROUP PHOTON-PRODUCTION MATRIX AND SOURCE CODE FOR ENDF

W. E. Ford III J. L. Lucius

LAPHANO, a P_0 multigroup photon production matrix and source vector code for ENDF data developed by Dudziak et al.,^{36,37} has been modified as follows:

1. The CDC-6600 version was converted to run on the IBM 360 computer.
2. The code was flexibly dimensioned to remove the restrictions on the number of neutron fine and broad groups, number of gamma groups, number of zones, etc.
3. Program input was changed to the free-form FIDO input used in ANISN¹⁸ and many other ORNL nuclear codes.
4. The calculated secondary-gamma-ray production cross sections can now be punched in the format for input to the ASCC coupling code.³⁸
5. An option was provided to assume the following Maxwellian-weighted value for the thermal (n,γ) non-resonance neutron reaction cross section:³⁹

$$\bar{\sigma}_{th}^{MT=102} = \hat{\sigma} \frac{\pi T_0}{4 T},$$

where $\hat{\sigma}$ is the 2200-m/sec cross section for the (n,γ) reaction as determined from the ENDF MF = 3 data and $T_0 = 293.6^\circ\text{K}$. T , the mean temperature of the neutrons in the Maxwellian distribution, and the upper neutron energy for application of the assumption are input to the code.

6. The smooth fine-group weighting function can be normalized to an input value.
7. The code was modified to read ENDF/B data in both the binary and BCD formats.
8. Data management operations in the code have been made more efficient.

The code with the above modifications has been renamed LAPHFOR.

Requirements to produce secondary-gamma-ray production cross sections (SGRPXS's) and/or yield arrays for AMPX were met by using parts of LAPHFOR as the nucleus of the required module. This module has been designated LAPHNGAS. As a stand-alone module or as a step in the calculation of coupled neutron-gamma cross sections, LAPHNGAS calculates SGRPXS's from ENDF/B photon production data in a fine neutron-gamma-ray group structure. For a resonance neutron, LAPHNGAS calculates SGRPXS's for all given reactions except the (n,γ) and fission reactions and then calculates the photon yields for these two reactions. The SGRPXS's and/or yields are then passed to another AMPX module to have the yields combined with fine-group resonance neutron cross sections, to weight the SGRPXS's, and to collapse the SGRPXS's to the required broad neutron-gamma group structure.

36. D. J. Dudziak, A. H. Marshall, and R. E. Seamon, *LAPH: A Multigroup Photon Production Matrix and Source Vector Code for ENDF/B*, LA-4337 (1969).

37. D. J. Dudziak, R. E. Seamon, and D. V. Susco, *LAPHANO: A P_0 Multigroup Photon-Production Matrix and Source Code for ENDF*, LA-4756-MS (1972).

38. W. E. Ford III and J. S. Gillen, Appendix B in *The Testing of ^{238}U Secondary Gamma-Ray Production Data Sets from the POPOP4 Library*, ORNL-TM-3482 (1972).

39. C. H. Westcott, *The Specification of Neutron Flux and Effective Cross Sections in Reactor Calculations*, Atomic Energy of Canada Limited report CRRP-662 (1956).

Various options have been added to LAPHNGAS to weight the point neutron reaction ($MT = 3$) cross sections. In addition to the standard flat weighting, the module can also do $1/E_n$, $1/E_p$, tied to a fission spectrum, "exact" $1/E_n$, $1/(E_n \sigma_T)$, or arbitrary input weighting. These various weighting options are currently in the check-out phase.

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IMPLEMENTATION OF THE AMPX SYSTEM ON CONTROL DATA COMPUTERS

J. L. Lucius N. M. Greene

The AMPX system for generating coupled neutron and gamma-ray multigroup libraries²⁹ was developed on the IBM 360 series computers at ORNL. Conversion of the system by the ORNL staff to operational status on Control Data computers is a project requirement.

AMPX consists of over 20,000 source cards encompassing programming generated by several individuals over a period of years. No programming standards in the sense of exportability were observed, creating a significant conversion problem. The following steps were taken:

1. All source cards were placed on a 2314 disk and indexed by a file number and card number. No further reference was made to the source decks, the necessary modifications being made to the card images on the disk.
2. A program was written to convert the character set from EBCDIC to BCD, locate information between quotes, eliminate the quotes, and provide a count of Hollerith characters. Double precision, REAL*8 double precision function statements, and double precision constants were located and eliminated, since double precision arithmetic will not be required on Control Data equipment. The program also located doubly subscripted variables and flagged them for inspection and elimination by a programmer. STOP n type statements were examined and n converted to an octal constant if necessary.
3. An overlay structure compatible with CDC specifications was designed and implemented.

The converted system has been sent to an installation with CDC equipment, and ORNL staff members will go there to complete the implementation of the system.

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C. E. Clifford
F. R. Mynatt

PROCENDF: A POINT ENDF/B PROCESSING CODE

J. E. White E. M. Oblo¹

PROCENDF⁴⁰ was written to process neutron cross-section data in ENDF/B format and produce point cross-section libraries. Work has begun to convert PROCENDF for inclusion in the AMPX system. The revised version will (1) use a flexible dimensioning scheme to make optimal use of core storage, (2) use a better system for input-output management (the trigger to selectively suppress superfluous output will be retained; however, redundant input will be eliminated, and an efficient technique will be employed to scan

40. E. Holm and C. R. Weisbin, private communication.

BCD tapes), (3) use the free-form FIDO input routines, and (4) use a Z-MT scheme for identifying the different reaction processes for a given nuclide. In addition, the revised version of PROCENDF will be made fully compatible with ENDF/B Version III formats.

For present work, the Columbia version of PROCENDF has been made operational at ORNL to process several ENDF/B Version III materials (Fe, Na, ^{16}O , ^{14}N , Ca Si, ^{12}C , ^1H). The processed data are generally used in one-dimensional discrete-ordinates calculations.

Sponsor: Neutron Physics Division

A DETERMINISTIC METHOD FOR MULTIPLE SCATTERING CORRECTIONS

N. M. Greene R. L. Childs G. de Saussure¹ R. B. Perez¹

MSC⁴¹⁻⁴³ is a computer program which uses discrete-ordinates transport theory to calculate "foil responses" in the resonance energy region. Multiple scattering is treated explicitly in the discrete-ordinates calculation, where the resonance region is subdivided into very narrow energy groups. The "fineness" of the group structure sometimes creates serious problems in describing differential scattering cross sections with

41. N. M. Greene et al., *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1970*, ORNL-4592, p. 13.

42. N. M. Greene et al., *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1971*, ORNL-4705, p. 25.

43. N. M. Greene et al., *Neutron Phys. Div. Annu. Progr. Rep. May 31, 1972*, ORNL-4800, p. 14.

Fig. 7. The response function for the ^{238}U resonance at 821.5 eV, showing a "satellite" peak at 828 eV.

Legendre polynomial expansions. In some energy regions, multiple scattering "satellite" peaks are observed experimentally and are well described by Monte Carlo calculations. MSC generates cross sections with up to a P_3 expansion using analytical expressions. (Higher orders become impractical because of time considerations and significance difficulties with the IBM 360.) In the very fine group limit, differential group-to-group transfers are "spikes" which clearly cannot be fitted by the P_3 expansion. Figure 7 contrasts three calculations for a 23-mil ^{238}U foil. The curve labeled "MSC" uses a P_3 expansion. The "MSCA" curve from the latest code package was calculated by an analytic first-collision source technique for a source normal to an infinite slab.

The new programming will be worked into a fitting program that will allow the determination of resonance parameters from experimental data.

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PLOTting OF ENDF/B EVALUATED NEUTRON CROSS SECTIONS FOR GENERAL ORNL USE

R. Q. Wright M. B. Emmett

Three programs have been written in order to plot certain neutron cross sections from an ENDF/B³⁵ data tape.

The ORSIG program retrieves data from ENDF/B files 2 and 3 and performs the necessary calculations to place the data in the form required by the plotting program. The subroutines used have been borrowed from the SUPERTOG program.⁴⁴ The single-level Breit-Wigner formalism is used for calculation of cross sections in the resolved resonance region. The energy mesh is constructed by the program and includes 50 points for each resonance. Cross sections in the unresolved resonance region are computed by taking averages over suitable Porter-Thomas distributions of the neutron and fission widths. An energy mesh of 201 points equally spaced in lethargy over the unresolved resonance range is used. The resonance contributions are added to the smooth background cross section from ENDF/B file 3 to obtain the final cross sections. Doppler-broadened cross sections can be produced, if desired, using the method of the TEMPO program.⁴⁵ ORSIG generates point cross sections from ENDF/B for total, elastic, inelastic, fission, and capture.

The program ECSP produces the Calcomp plots of ENDF/B cross-section data. The program reads a specially prepared tape of cross sections vs energy produced by ORSIG. The plots are logarithmic and are 15 in. wide by 10 in. high. This program makes use of the modified INTRIGUE-360, which is described elsewhere in this report. The plots have been used by a number of individuals at ORNL, and a notebook containing all of the plots produced thus far is available for use.

SHAREN reads the data set generated by ORSIG. It will then, by input option, list, punch, or plot any desired reaction type (e.g., total cross section) for any material over any specified energy range. Plotting is accomplished using the BPLOT package for the CRT plotter. An option is available to get output in the ENDR/B format. This option has been used to transform an ENDF/B material that has resolved and/or

44. R. Q. Wright, N. M. Greene, J. L. Lucius, and C. W. Craven, Jr., *SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B*, ORNL-TM-2679 (September 1969).

45. K. Gregson and M. F. James, *TEMPO - a General Doppler Broadening Program for Neutron Cross Sections*, AEEW-M518 (1965).

unresolved resonance parameters to an equivalent material that has only point cross sections with no resonance parameters.

Sponsor: Neutron Physics Division

PLOTFC: A PLOTTING PROGRAM FOR ENDF/B DATA

R. Q. Wright

PLOTFC, a modified version of the program PLOTFB,⁴⁶⁻⁴⁸ utilizes the Calcomp (pen and ink) rather than the CRT plotter.

PLOTFC can also plot ENDF/B³⁵ point data and multigroup data on the same plot. The multigroup cross sections and the group structure are input on cards. This option has been very useful for checking multigroup cross sections and for determining if a given group structure is an adequate fit to the point data.

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R. W. Roussin

THE MAINTENANCE OF ENDF/B PROCESSING CODES EDITOR AND PLOTFB

J. E. White

Periodically, deficiencies in the Evaluated Nuclear Data File (ENDF) are rectified by creating new formats or modifying existing ones. As a consequence, the programs which edit, plot, or manipulate the data must be updated. During the past year, a few minor format changes were approved by the Cross Section Evaluation Working Group (CSEWG). These changes affected the ENDF/B edit⁴⁹ and plot⁵⁰ codes as follows:

1. EDITOR.

- a) Due to addition of new or reactivated reaction type numbers, the scheme for converting these reaction type numbers to their literal equivalent was revised. The new scheme will allow future additions to be made with relative ease.
- b) The smooth cross-section routines were modified to include the new LR flags, which indicate the mode of decay of the residual nucleus.
- c) The gamma-ray production files were modified to include the newly introduced LP flag, which indicates the origin of the gamma ray.

2. PLOTFB. The inclusion of the new MT numbers in the library of allowable reaction types was the only significant change.

In addition to the work created by the format changes, PLOTFB was triggered to plot the file 3 fission cross sections on a log-log graph and the file 4 angular distribution on a log-linear graph.

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46. Odelli Ozer, *Description of the ENDF/B Processing Codes and Retrieval Subroutines*, BNL-50300 ENDF-110 (revised June 1971).

47. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 60.

48. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 61.

49. C. L. Thompson et al., *EDITOR, a Processing Code for ENDF/B Format Data*, ORNL-TM-3266 (ENDF-142) (February 1971).

50. H. C. Honeck, *Description of the ENDF/B Processing Codes and Retrieval Subroutines*, BNL-13582 (ENDF-110) (revised September 1970).

UPDATING OF THE DLC-2 CROSS-SECTION LIBRARY

R. Q. Wright

Sixty-four materials in the ENDF/B³⁵ Version III library have now been processed by SUPERTOG,⁴⁴ and the DLC-2 100-group cross-section library⁵¹ has been updated.

The DLC-2 library was generated from nuclear data from ENDF/B. The explicit assumption was made that the flux (weighting function) has the shape of a fission spectrum joined at 0.0674 MeV by a $1/E$ tail. When resonance data were available, resolved and unresolved resonance contributions were calculated, using the infinite dilution approximation. DLC-2 consists of fine group constants such as one-dimensional reaction arrays (absorption, fission, etc.), P_n elastic scattering matrices, and inelastic and $(n, 2n)$ scattering matrices, which were generated, combined, and written on tape as card images in the ANISN format.¹⁸

DLC-2 uses a P_8 approximation to represent elastic scattering angular distributions. The data have a 100-group structure with energy group boundaries identical to those in the GAM-II library,⁵² with a group 1 upper boundary energy of 14.92 MeV and a group 99 lower energy of 0.414 eV. The group-to-group transfer matrices reflect only downscatter in energy, and group 100 serves as a thermal group.

The nuclides in DLC-2 are those which have been released as Category I ENDF/B by the National Neutron Cross Section Center, Brookhaven National Laboratory. The library contains data for H, D, He, ³He, ⁶Li, ⁷Li, ⁹Be, ¹⁰B, ¹¹B, ¹²C, ¹⁴N, ¹⁶O, ²³Na, Mg, ²⁷Al, Si, Cl, K, Ca, V, Cr, ⁵⁵Mn, Fe, ⁵⁹Co, Ni, Cu, ⁶³Cu, ⁶⁵Cu, Nb, Mo, ¹⁰⁷Ag, ¹⁰⁹Ag, ¹³⁵Xe, ¹³³Cs, ¹⁴⁹Sm, ¹⁵¹Eu, ¹⁵³Eu, Gd, ¹⁶⁴Dy, ¹⁷⁵Lu, ¹⁷⁶Lu, ¹⁸¹Ta, ¹⁸²Ta, ¹⁸²W, ¹⁸³W, ¹⁸⁴W, ¹⁸⁶W, ¹⁸⁵Re, ¹⁸⁷Re, ¹⁹⁷Au, Pb, ²³²Th, ²³³Pa, ²³⁴U, ²³⁵U, ²³⁸U, ²³⁸Pu, ²³⁹Pu, ²⁴⁰Pu, ²⁴¹Pu, ²⁴²Pu, ²⁴¹Am, ²⁴³Am, and ²⁴⁴Cm.

The DLC-2 Data Retrieval Program⁵³ was also updated for this version of the library.

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R. W. Roussin

CHECKER MODIFICATION

R. Q. Wright J. L. Lucius

A new version of the CHECKER program⁴⁶ was obtained from the National Neutron Cross Section Center, Brookhaven National Laboratory, and is now operational on ORNL computers. The purpose of CHECKER is to check the data on an ENDF/B³⁵ BCD card-image tape. Due to format modifications in ENDF/B Version III, two versions of CHECKER are now in use, one for Version II and one for Version III. CHECKER is used routinely by the Radiation Shielding Information Center to process ENDF/B and DNA cross section tapes.

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R. W. Roussin

51. DLC-2/100G: 100-Group Neutron Cross Section Data Based on ENDF/B, ORNL RSIC Data Library collection.

52. G. D. Joanou and J. S. Dudek, GAM-II: A B_3 for the Calculation of Fast-Neutron Spectra and Associated Multigroup Constants, USAEC report GA-4265, General Atomic (1963).

53. "DLC2RP: A Program to Edit or Convert SUPERTOG Output to Forms Suitable for Input to ANISN or DTF-IV," in DLC-2/100G: 100-Group Neutron Cross Section Data Based on ENDF/B, ORNL RSIC Data Library collection.

DOMINO: A GENERAL-PURPOSE DISCRETE ORDINATES TO MONTE CARLO COUPLING CODE FOR RADIATION TRANSPORT^{54,55}

M. B. Emmett C. E. Burgart⁵⁶ T. J. Hoffman

A method of coupling two-dimensional discrete-ordinates calculations with Monte Carlo calculations is incorporated in the DOMINO code. In particular, the DOT code,³³ a two-dimensional discrete-ordinates code, has been coupled with MORSE,²⁴ a Monte Carlo code.

The discrete-ordinates calculation is limited to an *r-z* geometry. Either the DOT boundary angular fluxes or the angular fluxes at internal surfaces may be input to DOMINO. Any amount of surface may be used in DOMINO, from all mesh points down to a portion of one interval. The radii, axes, and quadrature set must be read into DOMINO. Appropriate cumulative probability distributions are calculated from the angular fluxes and written on a DOMINO tape. Four different types of DOMINO tapes may be written for use in Monte Carlo codes — upward from a disk, downward from a disk, inward from a cylindrical surface, and outward from a cylindrical surface. The DOMINO tape contains all necessary coupling information for use by the Monte Carlo code. The MORSE calculation may utilize this data in four ways: (1) as a source for a forward MORSE case, (2) as a scoring function for an adjoint MORSE case, (3) as a source for an adjoint MORSE case, or (4) as a scoring function for a forward MORSE case.

A detailed discussion of the coupling operation as well as a sample problem are included in the appendices. Logical flow charts of the routines add to the understanding of the code.

Sponsor: Neutron Physics Division

C. E. Burgart

COUPLED DOT-MORSE (DOMINO) APPLICATIONS IN THE FTR SHIELD DESIGN

M. B. Emmett T. J. Hoffman

Many aspects of the Fast Test Reactor (FTR) shield design are best treated with discrete-ordinates methods. However, the geometric complexity of some components of the design requires the use of Monte Carlo techniques. The coupling of the discrete-ordinates calculations with the Monte Carlo calculations can be done with the DOMINO code.⁵⁷

One example of this procedure is the FTR stored-fuel calculation. This problem consisted in calculating the fission neutron production rate in 66 fuel elements located exterior to the core of the reactor but interior to the reactor vessel. This calculation utilized a forward DOT calculation³³ to obtain the angular fluxes leaking from the core and an adjoint MORSE calculation²⁴ where histories were initiated in the stored fuel. The adjoint Monte Carlo approach was taken due to the small size of the stored fuel volume and the large coupling surface.

Another example of coupled DOT-MORSE applications in the FTR design was the FTR head compartment calculation. In this calculation, neutron and gamma-ray doses were desired at several positions above the FTR. The large flanges in the head compartment made geometric compromises difficult; therefore, a DOT calculation was performed to a surface below the head. With the angular fluxes obtained from this calculation, a source tape for a Monte Carlo calculation was generated with DOMINO. A forward

54. Funded by Defense Nuclear Agency under Subtask PEO74-01.

55. Abstract of an ORNL report to be published.

56. Now at Science Applications, Inc., La Jolla, Calif.

57. M. B. Emmett, C. E. Burgart, and T. J. Hoffman, *DOMINO, a General-Purpose Discrete Ordinates to Monte Carlo Coupling Code for Radiation Transport*, ORNL report to be published.

MORSE calculation was then run with this source tape. The forward approach was taken in this problem since the effect of two responses (neutrons and gamma rays) was desired at several detector locations.

Sponsor: Neutron Physics Division

F. R. Mynatt

COMPARISON OF (n_{th}, γ) YIELDS FROM THE CURRENT ENDF/B-III DATA WITH PUBLISHED DATA⁵⁸

W. E. Ford III

As a first check of the ENDF/B photon production data available as of June 1972, the number of photons per thermal-neutron capture was calculated for 50-keV gamma-ray energy bins and compared with published data. This comparison was done for ^1H (MAT 1148), ^9Be (1154), ^{14}N (1133), ^{16}O (1134), ^{23}Na (1156), ^{27}Al (1135), Si (1151), Cl (1149), K (1150), Ca (1152), Fe (1180), and Pb (1136).

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THE TESTING OF ^{238}U SECONDARY-GAMMA-RAY PRODUCTION DATA SETS FROM THE POPOP4 LIBRARY⁵⁹

W. E. Ford III J. S. Gillen

The uranium nonfission capture, fission capture, and inelastic scattering data sets included in the POPOP4 library of neutron-induced secondary-gamma-ray yield and cross-section data were "tested" for use in the preparation of ^{238}U secondary-gamma-ray production cross sections (SGRPXS's). The data sets were "tested" over various neutron energy ranges by comparing calculated secondary-gamma-ray pulse-height spectra with previously measured spectra resulting from the exposure of a 30-mil-thick depleted uranium foil to bare, thermal, $\text{Cd-}^{10}\text{B-}$, $(\text{Cd-}^{10}\text{B-})$, and $(\text{Cd-}1.377^{10}\text{B-})$ -filtered neutron beams from the ORNL TSR-II reactor.⁶⁰

Uranium-238 nonfission capture data sets 928109, 928112, 928113 and the total SGRPXS data set 928901 are adequate for use in shielding calculations when used over the neutron and gamma-ray energy ranges for which the data are defined. In the absence of suitable ^{238}U fission capture and inelastic scattering data sets, ^{238}U data sets 925801 and 925301 were found to be adequate for these reactions in the preparation of ^{238}U SGRPXS's.

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THE TESTING OF PHOTON PRODUCTION DATA FROM ENDF/B-III MATERIAL 1135 (ALUMINUM)⁶¹

W. E. Ford III

Photon production data in the Evaluated Nuclear Data File (ENDF/B-III) for ^{27}Al (MAT 1135) were tested by (1) comparing the thermal-neutron capture gamma-ray yields calculated with MAT 1135 with

58. Abstract of ORNL-TM-3910 (ENDF-172) (August 1972).

59. Abstract of ORNL-TM-3482 (February 1972); also abstract of paper presented at the American Nuclear Society Winter Meeting, Miami, Fla., Oct. 17-21, 1971.

60. The measured spectra were obtained by the TSR-II staff under the direction of F. J. Muckenthaler (Neutron Physics Division).

61. Abstract of ORNL-TM-4032 (in press); also abstract of paper presented at the American Nuclear Society Winter Meeting, Washington, D.C., Nov. 13-17, 1972.

data from the literature, (2) comparing gamma-ray pulse-height spectra calculated with MAT 1135 with measured spectra, and (3) comparing the secondary-gamma-ray production cross sections calculated with MAT 1135 with cross sections from the literature.

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COMPARISON OF AVERAGE SECONDARY-GAMMA-RAY PRODUCTION CROSS SECTIONS FROM ENDF/B-III DATA WITH PUBLISHED CROSS SECTIONS⁶²

W. E. Ford III

As a means of obtaining a first-order check of the ENDF/B photon production data, LAPHFOR was used to calculate the average secondary gamma-ray production cross sections (SGRPXS's) for Al (MAT 1135), Si (1151), K (1150), Ca (1152), and Fe (1180). These SGRPXS's were then compared with experimentally determined data published by Maerker and Muckenthaler.⁶³ The experimental SGRPXS's were determined by exposing slabs of the materials of interest to a fission-like spectrum of fast neutrons. This neutron spectrum was obtained by placing a ^{10}B filter over the CRNL TSR-II reactor neutron beam port.

The point ENDF/B photon production data were first reduced to a set of SGRPXS's in 27 neutron fine groups ($0.0 \leq E_n \leq 14.9182$ MeV) and 13 gamma-ray groups ($1.0 \leq E_\gamma \leq 7.5$ MeV). For comparison with the published cross sections, the 27 neutron and 13 gamma group cross sections were then reduced to a single broad neutron group structure ($1.0 \leq E_n \leq 14.9182$ MeV) and the same 13 gamma groups by using the multigroup representation of the experimental ^{10}B -filtered neutron beam as a weighting function.

As examples of the results, the Al and Fe comparisons are shown in Tables 2 and 3. Also shown in the tables are previously published results from ref. 62. The total SGRPXS's from MAT 1135 and Maerker and Muckenthaler's data are compared graphically in Fig. 8.

Sponsor: Neutron Physics Division

NEUTRON CAPTURE GAMMA-RAY YIELDS IN IRON⁶⁴

J. E. White C. Y. Fu⁶⁵ K. J. Yost⁶⁶

Gamma-ray yields as a function of neutron energy from thermal to 1 MeV for iron have been generated with a combined experimental and theoretical approach. The theoretical part is to a large extent statistical; however, parameters are introduced to compensate for the nonstatistical behavior. Experimental data used to evaluate these parameters are the branching ratios among discrete levels and the gamma-ray primary transitions from thermal and available resonance capture. A discussion of the implications of additional resonance capture yield data, which were made available after the completion of the calculation, is included. The results have been compared with integral experiments, and the agreement is favorable.

62. Funded by the Defense Nuclear Agency under Subtask PEO74-02.

63. R. E. Maerker and F. J. Muckenthaler, *Gamma-Ray Spectra Arising from Fast-Neutron Interactions in Elements Found in Soils, Concretes, and Structural Materials*, ORNL-4475 (April 1970).

64. Abstract of paper submitted to *Nuclear Science and Engineering*.

65. University of Tennessee.

66. Purdue University.

Table 2. Comparison of Al (MAT 1135) average secondary-gamma-ray production cross sections with published data

Source	Cross section (mb) for gamma-ray energy range of													Total
	1- 1.5 MeV	1.5- 2 MeV	2- 2.5 MeV	2.5- 3 MeV	3- 3.5 MeV	3.5- 4 MeV	4- 4.5 MeV	4.5- 5 MeV	5- 5.5 MeV	5.5- 6 MeV	6- 6.5 MeV	6.5- 7 MeV	7- 7.5 MeV	
MAT 1135	197	34.3	120	35.2	44.4	7.2	6.5	9.6	3.5	2.5	1.8	1.1	0.7	463.8
Maerker and Muckenthaler ^a	181	36.3	102.5	26.3	42.4	8.8	5.8	6.9	4.9	2.0	<1.7	<1.5	<0.3	≤420
Celnik and Spielberg ^a	208	60.8	106	25.5	11.0	4.5	4.7	7.3	2.7	1.1	1.1	0.6	0	433

^aR. E. Maerker and F. J. Muckenthaler, *Gamma-Ray Spectra Arising from Fast-Neutron Interactions in Elements Found in Soils, Concretes, and Structural Materials*, ORNL-4475 (April 1970).

Table 3. Comparison of Fe (MAT 1180) average secondary gamma-ray production cross sections with published data

Source	Cross section (mb) for gamma-ray energy range of													Total
	1- 1.5 MeV	1.5- 2 MeV	2- 2.5 MeV	2.5- 3 MeV	3- 3.5 MeV	3.5- 4 MeV	4- 4.5 MeV	4.5- 5 MeV	5- 5.5 MeV	5.5- 6 MeV	6- 6.5 MeV	6.5- 7 MeV	7- 7.5 MeV	
MAT 1180	259.8	102.2	96.0	86.5	32.2	25.1	3.0	3.3	3.0	2.5	<0.7	<0.6	0.3	615
Maerker and Muckenthaler ^a	278	110	101	74	44	33	8.7	5.6	3.8	2.4	<2.1	<0.6	<1.5	≤665
Celnik and Spielberg ^a	307		198		78		14		8.5		2.0		0.4	608

^aR. E. Maerker and F. J. Muckenthaler, *Gamma-Ray Spectra Arising from Fast-Neutron Interactions in Elements Found in Soils, Concretes, and Structural Materials*, ORNL-4475 (April 1970).

Fig. 8. Comparison of weighted MAT 1135 SGRPXS's and Maerker and Muckenthaler's measured aluminum SGRPXS's for $1.0 < E_n < 14.9182$ MeV.

Considerable variations in the capture gamma-ray yields as a function of incident neutron energy are noticed.

Sponsor: Neutron Physics Division

CALCULATED NEUTRON AND SECONDARY-GAMMA-RAY LEAKAGE FROM THE ARMY PULSE RADIATION REACTOR

W. E. Ford III

Calculations of the neutron and secondary-gamma-ray leakage spectra from the Army Pulse Radiation Facility Reactor (APRF) have been completed for the reactor without the B_4C decoupling shroud. The APRF, which is located at Aberdeen Proving Ground, Maryland, is an unreflected and unmoderated nuclear reactor designed to produce fast-neutron and gamma radiation doses for the determination of radiation effects on materials. The reactor, shown schematically in Fig. 9, is an 8.900-in.-OD, 4.180-in.-ID, 7.960-in.-high annular cylinder made up of plates of a 90% uranium (93.2% ^{235}U)—10% molybdenum alloy. The plates, of several thicknesses, are held together by nine 9.494-in.-long, 0.787-in.-diam U-Mo bolts that thread into the bottom plate. Three of the bolts also attach the core to the reactor support structure. An 8.560-in.-long, 4.000-in.-OD, 2.688-in.-ID inner annulus of U-Mo, the safety annulus, having a mass of 16.7 kg, is attached to a central steel member that is coupled magnetically to a drive mounted above the core. The reactor is equipped with a pulse rod and with two 9.002-in.-long U-Mo control rods, called the

Fig. 9. The APRFR core assembly.

mass adjustment and regulating rods, having diameters of 0.631 and 1.006 in. respectively. The entire assembly contains about 125 kg of U-Mo alloy.⁶⁷ The glory hole was assumed to be void for this study.

Using a 39-group structure consisting of 21 neutron groups ($0.0 \leq E_n \leq 14.918$ MeV) and 18 gamma-ray groups ($0.01 \leq E_\gamma \leq 10$ MeV), coupled neutron-gamma cross sections were prepared for use in DOT⁶⁸ and ANISN⁶⁹ calculations of the required spectra. Spectrally weighted P_3 neutron cross sections were calculated with the XSDRN³² code and cross-section data from the "XSDRN 100-Group Library,"⁶⁹ secondary-gamma-ray production cross sections (SGRPX's) were prepared with the POPOP4 code⁷⁰ and data from the POPOP4 library,⁷¹ and P_3 gamma-ray cross sections were calculated with the MUG code.⁷² The secondary gamma rays were assumed to be emitted isotropically.

67. The APRF is described by J. T. Mihalcz, *Static and Dynamic Measurements with the Army Pulse Radiation Facility Reactor* ORNL-TM-2330 (1969).

68. F. R. Mynatt, *A User's Manual for DOT*, USAEC report K-1694 (to be published).

69. J. L. Lucius, J. D. Jenkins, and R. Q. Wright, *The INDEX Data System: An Index of Nuclear Data Libraries Available at ORNL*, ORNL-TM-3334 (1971).

70. W. E. Ford III and D. H. Wallace, *POPOP4 - a Code for Converting Gamma-Ray Spectra to Secondary Gamma-Ray Production Cross Sections*, USAEC report CTC-12 (1969).

71. W. E. Ford III, *The POPOP4 Library of Neutron-Induced Secondary Gamma-Ray and Cross Section Data*, USAEC report CTC-42 (1970).

72. J. R. Knight and F. R. Mynatt, *MUG - a Program for Generating Multigroup Photon Cross Sections*, USAEC report CTC-17 (1970).

The calculated differential neutron flux on the outer surface of the reactor is compared with Pickard and Williams' calculated results⁷³ in Fig. 10. Both calculations were made with ANISN. The above-described coupled cross sections were used in a P_3, S_8 calculation to obtain the present results, whereas Pickard and Williams used 100-group ENDF cross sections in a P_0, S_4 calculation. An additional example of the one-dimensional ANISN results is shown in Fig. 11, where the calculated differential neutron flux for the center of the glory hole is compared with Pickard and Williams' work.

Sponsor: Neutron Physics Division

73. P. S. Pickard and D. O. Williams, *Calculated Neutron Energy Spectra for the APRF Reactor*, unpublished memo for record (Apr. 28, 1970).

Fig. 10. Calculated neutron differential leakage flux spectra for APRF bare reactor.

Fig. 11. Calculated differential neutron flux spectra for APRF reactor center glory hole.

NEUTRON-ENERGY-DEPENDENT CAPTURE GAMMA-RAY YIELDS IN TANTALUM AND TUNGSTEN^{74,75}

K. J. Yost^{6,5} C. Y. Fu^{6,4} J. E. White W. E. Ford III

Gamma-ray yields as a function of neutron energy for tantalum and tungsten have been generated with a combined experimental and theoretical approach. The results are presented in a format that would facilitate use in coupled neutron-gamma-ray transport calculations. In the case of tungsten, pronounced variations in the capture yield spectra were noticed above 3.0 MeV. On the other hand, only slight variations in the yield spectra were evident for tantalum. The results have been compared with integral gamma-ray yield measurements, and the agreement is favorable.

Sponsor: Neutron Physics Division

A REEVALUATION OF NATURAL IRON NEUTRON AND GAMMA-RAY PRODUCTION CROSS SECTIONS

S. K. Penny W. E. Kinney¹

The cross sections for natural iron were reevaluated and placed in the ENDF/B format. The energy range of incident neutrons was extended to 20 MeV. Cross sections for $(n,2n)$, $(n,n'p)$, and $(n,n'\alpha)$ reactions were included as well as the gamma-ray production cross sections for inelastic scattering to the continuum. The important minima in the total cross section were changed to reflect recent measurements at ORELA. Direct interaction components were included in the energy distributions of neutrons that inelastically scatter to excite the continuum, and the representation of these energy distributions was changed to a form more convenient for multigroup cross-section processing codes.

Sponsor: Neutron Physics Division

F. G. Perey

CALCULATION OF GULF RADIATION TECHNOLOGY INTEGRAL EXPERIMENTS OF CARBON AND NITROGEN

S. N. Cramer E. M. Oblo¹

Calculations of the Gulf Radiation Technology integral experiments on carbon and nitrogen⁷⁶ for cross section testing have been performed using the MORSE Monte Carlo code.^{2,4} Reasonable agreement has been obtained for both neutron and gamma-ray time-dependent count rate. The calculations will be extended in the form of sensitivity studies with regard to different data sets, energy-group structure, anisotropic scattering expansion, and that type of analysis associated with the LLL pulsed-sphere program.⁷⁷

Sponsor: Neutron Physics Division

74. Funded by the Space Nuclear Systems Division of the Atomic Energy Commission.

75. Abstract of *Nucl. Sci. Eng.* 47, 209 (1972).

76. L. Harris, Jr., G. D. Trimble, and J. C. Young, *Integral Experiment to Test Carbon and Nitrogen Cross Sections*, Gulf-RT-A12292 (1972).

77. S. N. Cramer, R. W. Roussin, F. G. Perey, and E. M. Oblo, "Cross Section Sensitivity Studies for the LLL Pulsed-Sphere Experiments," this report.

CALCULATION OF ORELA CROSS-SECTION TESTING EXPERIMENTS

S. N. Cramer E. M. Oblow¹ G. L. Morgan¹ F. G. Perey¹

Several ORELA experiments are being performed on various materials such as C, Fe, and Al, and these experiments are being calculated by the MORSE²⁴ and O6R²³ Monte Carlo codes in order to test the cross-section data. A preanalysis of the carbon experiment⁷⁸ enabled the experimenters to choose an appropriate sample size, and the calculation of this experiment has been completed. Both time-dependent count rate and unfolded pulse-height spectra have been compared with calculations with good agreement. Calculations will continue on other materials and also in the form of sensitivity studies with regard to different data sets, energy group structure, anisotropic scattering expansion, and that type of analysis associated with the LLL pulsed-sphere program.⁷⁷

Sponsor: Neutron Physics Division

ANALYSIS OF LMFBR SHIELDING EXPERIMENTS

G. E. Whitesides M. B. Emmett

The MORSE Monte Carlo code²⁴ and SAMBO, its associated analysis package, have been used to analyze several LMFBR experiments done at the Tower Shielding Facility. One of these experiments was an axial shield measurement for an 18-in. stainless steel partial spectrum modifier. The source spectrum was from the 15 1/4-in. collimator at the TSF.⁷⁹ The point cross-section option in MORSE is implemented; that is, for certain groups the total cross section is taken from a table of point cross sections, and for other groups the multigroup total cross section is used. Several group structures including 218 group, 100 group, and 50 group were used in the calculations. Fluences were calculated for several types of detectors: an NE-213 detector, a hydrogen counter, and three sizes (3, 6, and 10 in.) of Bonner balls. Results were in good agreement with the experimental data.⁸⁰ Another experiment was a radial blanket shield measurement for a Westinghouse spectrum modifier consisting of a slab of 4 in. of stainless steel, 6 in. of sodium, and 1 in. of boral. Several group structures were used, including one combined 21-neutron-18-gamma group. Fluences were calculated for NE-213 detectors and Bonner ball detectors at various distances from the modifier. Both slab and general geometry packages were used. Results were in good agreement with experiment.⁸⁰

Sponsor: Neutron Physics Division

R. E. Maerker

THE DEVELOPMENT AND APPLICATION OF A DISCRETE-ORDINATES ADJOINT DIFFERENCE METHOD FOR ONE-DIMENSIONAL SHIELD WEIGHT OPTIMIZATION^{74,81}

R. L. Childs

An improved method for the weight optimization of one-dimensional layered shields has been developed. The radiation transport problem is represented by coupled neutron-gamma-ray discrete-

78. S. N. Cramer and G. L. Morgan, "Preanalysis of ORELA Cross-Section Testing Experiments," *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 59.

79. R. E. Maerker and F. J. Muckenthaler, *The Absolute Neutron Spectrum Emerging from the TSR-II Reactor through the 15 1/4 Inch Collimator at the Tower Shielding Facility*, ORNL-TM-4010 (November 1972).

80. *Fast Reactor Experimental Shielding Monthly Progr. Rep. August-September 1972*, ORNL-TM-4039; also *Fast Reactor Analytical Shielding Monthly Progr. Rep. August-September 1972*, ORNL-TM-4040.

81. Thesis submitted by R. L. Childs to the Department of Nuclear Engineering, University of Tennessee.

ordinates transport calculations. In the optimization procedure, forward and adjoint calculations are performed for the initial shield design. An approximate form of the perturbed adjoint is used in the adjoint difference approach to determine the effect of shield changes, and a simple closed-form optimization algorithm is used as in the ASOP code.

Three realistic shield optimization problems were solved to demonstrate the capabilities of the method. A comparison between the results obtained using this method and the ASOP code showed the agreement of the two methods to be very good and the new method to be significantly faster.

Sponsor: Neutron Physics Division

USE OF MONTE CARLO IN THE NEUTRON SHIELD DESIGN FOR THE SNAP 5-kW(e) SYSTEM

T. J. Hoffman J. R. Knight
W. W. Engle, Jr.¹

The SNAP 5-kW System neutron shield is a pear-shaped lithium hydride, shadow shield. In order to transport the reactor coolant (NaK) from the reactor to the radiator, tubes containing NaK were inserted in this shield. The effect of this inhomogeneity on the neutron flux at the dose plane is difficult to evaluate with discrete-ordinates methods. For this reason, a series of Monte Carlo calculations, using the multigroup code MORSE,^{2,4} were performed.

A discrete-ordinates calculation of the SNAP reactor was carried out with the code DOT.^{3,3} The angular fluxes from this calculation were input into the coupling code DOMINO^{8,2} to obtain the neutron source for the Monte Carlo calculations.

To improve the efficiency of the Monte Carlo calculation, path length stretching was used. The path length stretching parameter was optimized with a technique developed by Spanier.^{8,3}

Sponsor: Neutron Physics Division

W. W. Engle, Jr.

GEOMETRY DESCRIPTION OF SHIELDS FOR SPACE NUCLEAR SYSTEMS

J. R. Knight W. W. Engle, Jr.¹

Geometry descriptions for several designs of shields for space nuclear systems were prepared for use with the GEOM package from the OSR code.^{8,4} These geometry descriptions were used in Monte Carlo calculations to evaluate the effectiveness of the design for neutron shielding.

Sponsor: Neutron Physics Division

W. W. Engle

^{8,2} C. E. Burgart, M. B. Emmett, and T. J. Hoffman, *DOMINO - a General Purpose Discrete Ordinates to Monte Carlo Coupling Code for Radiation Transport*, CONF-720901 (1972).

^{8,3} J. Spanier, *A New Multi-Stage Procedure for Systematic Variance Reduction in Monte Carlo*, CONF-710302 (1971).

^{8,4} D. C. Irving, R. M. Freestone, Jr., and F. B. K. Kam, *OSR, a General-Purpose Monte Carlo Neutron Transport Code*, GRNL-3622 (February 1965).

MODIFICATIONS OF THE DUCT CODE FOR OPERATIONS ON IBM-360 EQUIPMENT

J. R. Knight W. W. Engle, Jr.¹

The DUCT code⁸⁵ determines the fluxes in ducts from angular fluxes generated by a DOT calculation.³³ Originally written in FORTRAN V for a Univac computer, it has been modified to operate on the IBM-360 model 75 or model 91. In addition to changes necessary to make the program compatible with FORTRAN IV on the IBM-360, several coding errors were found and corrected. A sample problem furnished with the code has been run using the modified version of the code.

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W. W. Engle

SILO ANALYSIS: IDENTIFICATION OF RADIATION STREAMING IN MINUTEMAN SILO EXPOSED TO THERMONUCLEAR SOURCE

T. J. Hoffman J. V. Pace III F. R. Mynatt¹ C. E. Burgart^{5,6}

This work represents part of a continuing study to determine the vulnerability of the Minuteman silo to radiation from a nuclear weapon. An investigation of radiation entering the silo through the silo cover has been completed.⁸⁶ The present effort is concerned with the effects of neutronic weak areas (streaming paths) in the silo design.

Four streaming paths, under several attack conditions, were investigated. Calculations were performed with the multigroup Monte Carlo Code MORSE²⁴ and the two-dimensional discrete-ordinates code DOT.³³ A report on this work is under preparation.

Sponsor: Neutron Physics Division

CSP: A PROGRAM TO CALCULATE CELL SURVIVAL PROBABILITIES RESULTING FROM NEUTRON OR CHARGED-PARTICLE IRRADIATION

K. C. Chandler T. W. Armstrong¹

The FORTRAN program CSP uses the cell inactivation model of Katz et al.⁸⁷ coupled with the transport codes HET⁸⁸ and O5R⁸⁹ to compute spatially dependent cell survival probabilities resulting from neutron or charged-particle irradiation. The cell survival calculations require the evaluation of integrals of the type

$$\sum_Z \int dE \Phi_Z(\bar{r}, E) R_Z(E; k, \sigma_0, D_0, m),$$

where $\Phi_Z(\bar{r}, E)$ is the fluence per unit energy of particles of charge Z at spatial point $\bar{r}$ (obtained from the HET and O5R calculations) and $R_Z(E; k, \sigma_0, D_0, m)$ is the response of the cell to particles of charge Z and

85. P. A. Reed, W. E. Selph, and R. J. Cerbone, *DUCT Code Manual*, GULF-RT-10654 (April 1971).

86. ORNL-TM-3599 (classified).

87. R. Katz et al., *Radiat. Res.* 47, 402 (1971).

88. K. C. Chandler and T. W. Armstrong, *Operating Instructions for the High-Energy Nucleon-Meson Transport Code HETC*, ORNL-4744 (1972).

89. W. A. Coleman and T. W. Armstrong, *The Nucleon-Meson Transport Code NMTC*, ORNL-4606 (1970).

energy E . The functional form for R_Z is provided by the Katz model. The radiosensitivity parameters k , σ_0 , D_0 , and m have been experimentally determined for a variety of cell types, for example, human kidney cells. The output from CSP also includes the relative biological effectiveness (RBE) and the oxygen enhancement ratio (OER) as a function of depth and radius.

Sponsor: Neutron Physics Division

HEAVY-ION CASCADE AND ANALYSIS CODES FOR COMPUTING NUCLEAR REACTIONS FROM BOMBARDMENT WITH HEAVY IONS

O. W. Hermann H. W. Bertini¹ T. A. Gabriel¹ R. T. Santoro¹

Code and model development is progressing in the effort to compute the residual nuclei and emitted particles, and their energies and momenta, which result from bombardment of a target with heavy ions.⁹⁰ The method, utilizing Monte Carlo techniques, consists of three parts.

The nuclear model used in the first part encompasses the description of collisions and interactions between the projectile and target nucleons and any ensuing π mesons and nucleons. This model uses a representation of the physics by free particle-particle collisions inside the nucleus, a premise first suggested by Serber.⁹¹ MECC-7,⁹² which has been used successfully to compute the cascade interactions of medium-energy incident nucleons, was tailored to represent the heavy-ion model. The relative position between an incident nucleon and target nucleus is chosen from a representative distribution. Then, the cascade interactions for each history are determined in the manner described earlier.^{93,94} The second half of the histories are done in the projectile-at-rest system. The first version of the code for computing the intranucleus cascade results is called HIC-1.

The second part involves analyzing the data to determine the evaporated particles and residual nuclei after decay from the excited state. An evaporation model, originally programmed by Dresner,⁹⁵ was modified to include the calculation of recoil momentum. Also, the initial nucleus excitation energy was directly calculated by using the particle-hole distribution remaining in the nucleus. Applying relativistic kinematics in processing the cascade code data and during the evaporation, final kinetic energy and momentum components of all products are determined. These are computed in EVAPHIC, the evaporation of heavy ions after cascade code.

The third part of the process involves analysis of the final data using ANHIC, the analysis of heavy-ion collisions code. It produces energy spectra or angular distribution cross sections of any desired isotope or emitted particle.

There was a somewhat limited quantity of experimental data with which calculated values were compared. The first total reaction comparisons were not definitive. While comparisons of spallation cross sections were somewhat favorable, larger errors were found in the computed production of individual isotopes within a small forward angle. The general pattern showed an overestimation of heavier isotopes, the reverse for lighter ones, and somewhat good comparison in the midrange. This result can be given a

90. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 48.

91. R. Serber, *Phys. Rev.* 72, 1114 (1947).

92. H. W. Bertini, M. P. Guthrie, and O. W. Hermann, *Instructions for the Operation of Codes Associated with MECC-3, a Preliminary Version of an Intranuclear-Cascade Calculation for Nuclear Reactions*, ORNL-4564 (1971).

93. H. W. Bertini, *Phys. Rev.* 131, 1801 (1963).

94. H. W. Bertini, *Phys. Rev.* 188, 1711 (1969).

95. L. Dresner, *EVAP -- a FORTRAN Program for Calculating the Evaporation of Various Particles from Excited Compound Nuclei*, ORNL-CP-61-12-30 (1961).

reasonable explanation in noting current work^{96,97} showing apparent effects of fission competition existing during the evaporation process and an associated discussion linking quantitatively the fission barrier with the excitation energy and angular momentum of the nucleus. If the heavier nuclei were found to be greatly reduced in quantity from fissioning compared with the light ones, it may substantially improve the results and justify effort needed in code modifications.

Preliminary results of the cascade-evaporation method described here have been currently presented,^{98,99} and it appears that this is a unique approach in the heavy-ion research in this country.¹⁰⁰ The results may be useful in areas of cancer research, space shielding, superheavy element theory, and other heavy-ion studies.

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R. G. Alsmiller, Jr.

HIGH-ENERGY TRANSPORT CODES

J. D. Amburgey

The main effort was directed in calculating energy depositions, fluxations, and ionization spectrometers. These devices were used to determine the energy of high-energy particles. The main codes used were HETC¹⁰¹ and an electron-photon code due to Beck.¹⁰² The analysis packages were modified to suit our particle needs.

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T. A. Gabriel

THE FERMI MOTION OF NUCLEONS ADDITION TO HECC, THE HIGH-ENERGY CASCADE CODE

O. W. Hermann H. W. Bertini¹

Fermi motion of the bound nucleons in the nucleus had not been implemented in the original HECC-1 version of the High Energy Cascade Code.^{93,94,103} Part of the work needed to add this modification was continued during the year. Two alternate approaches to the simulation of this mechanism and the derivation of the numerous equations required in describing the process were previously reported.¹⁰⁴ Since it was apparent that this addition would add considerably to the execution time in using the code, an analysis of the two approaches was first required. Although the physics is the same, the two methods differ in their solution to the problem. During one history, this solution might be needed hundreds of times at the

96. M. Blann and F. Plasil, "Limits on Angular Momentum in Heavy-Ion Compound-Nucleus Reactions," *Phys. Rev. Lett.* 29, 303 (1972).

97. J. B. Natowitz, "Complete-Fusion Cross Sections for Reactions of Heavy Ions with Cu, Ag, Au, and Bi," *Phys. Rev. C* 1, 623 (1970).

98. H. W. Bertini, "Calculation of High Energy Heavy-Ion Interaction by the Intranuclear Cascade Method," 1972 Gordon Research Conference on Nuclear Chemistry, Colby Junior College, New London, N.H.

99. T. A. Gabriel, "The Calculation of Heavy-Ion Interactions," paper presented at International Conference on Nuclear Solutions to World Energy Problems, vol. 15, No. 2, p. 968, Washington, D.C., November 1972.

100. Cascade-type method, for the forward case only, also being used by V. D. Tonzev et al., JINR, Dubna, USSR.

101. K. C. Chandler and T. W. Armstrong, "HETC, a Monte Carlo High-Energy Nuclear-Meson Transport Code," *RSIC Computer Code Collection*, CCC-178 (January 1972).

102. H. L. Beck, *A Monte Carlo Simulation of the Transport of High Energy Electrons and Photons in Matter*, HASL-213, USAEC Health and Safety Laboratory (1969).

103. *Math. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4515, p. 33.

104. N. B. Gove, H. W. Bertini, M. Feliciano, and A. H. Culikowski, *High Nuclear Cascades*, ORNL-TM-2627 (1970).

incident energies of 100 to 200 GeV, or more, which may be specified in typical cases. One approach applies the iterative method to a coarse mesh of intervals in the momentum magnitude and the cosine range of the bound nucleons. The other approach uses an analytic solution involving more complicated equations. Examining both methods for an estimate of the increase in execution time of each, it was found that the analytic approach would save considerable computer time for similar or better precisions. Also, the reported equations needed in these methods were determined again in order to help ensure a correct computation.

The derivation of additional distribution equations of both the momentum and the cosines was required for use in the Monte Carlo sampling. These are to be solved with an iterative method; however, the execution time should be relatively short, since they do not involve integration. Physically, there should exist only one root in the required range of the equations. A program was written which will check this premise when applied to all the input cross sections. Some of the subroutines in this testing code may eventually be utilized as a major part of the additions required in the HECC code. Other changes to the code, found to be necessary, either have been added or will be made soon.

Sponsor: Neutron Physics Division

H. W. Bertini

MONTE CARLO CALCULATIONS OF THE DOSE INDUCED BY CHARGED PIONS

T. W. Armstrong¹ K. C. Chandler

To test the validity of the transport code HETC^{8,9} for pion dose calculations, calculated results using HETC were compared with experimental data for the absorbed dose induced in water phantoms by a π^- beam of mean momentum 175 MeV/c and by π^- and π^+ beams of mean momentum 150 MeV/c. The calculated and experimental results for the depth dependence of the absorbed dose are in good agreement.

To provide data to aid in the design of the biomedical pion channel for the meson facility under construction at the Los Alamos Scientific Laboratory, HETC has been used to determine the spatial distribution of the absorbed dose produced in tissue by monoenergetic negative-pion beams. The calculations have been made for narrow (zero-width) monoenergetic pion beams normally incident on one side of a slab of tissue 60 cm thick. Beam energies of 53, 82, and 108 MeV (corresponding to ranges in tissue of approximately 10, 20, and 30 cm) were used.

The results for monoenergetic beams can be used to estimate the incident pion energy distribution needed to give a uniform absorbed dose over a specified depth interval. As an example, the calculated results for monoenergetic beams producing peak doses at 20 and 30 cm were used to synthesize approximately the incident pion energy spectrum needed to produce a uniform absorbed dose in the depth interval from 20 to 30 cm.

Sponsor: Neutron Physics Division

CALCULATION OF THE ABSORBED DOSE AND DOSE EQUIVALENT FROM HIGH-ENERGY NUCLEONS

K. C. Chandler T. W. Armstrong¹

Nucleon-meson cascade calculations using the transport code HETC^{8,9} have been carried out for monoenergetic neutrons and protons in the energy range from 3.5 GeV to 1.0 TeV. The neutrons and protons were taken to be normally incident over one side of a semi-infinite slab of tissue 30 cm thick. For

each energy considered (3.5, 10, 30, 100, and 1000 GeV), the absorbed dose and dose equivalent as a function of tissue depth were calculated. Analytic expressions for the resulting maximum and average fluence-to-absorbed-dose and fluence-to-dose-equivalent factors were obtained as a function of incident neutron or proton energy.

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CALCULATED RESPONSE OF THE TLND PERSONNEL DOSIMETER TO NEUTRONS WITH ENERGIES ≤ 400 MeV¹⁰⁵

J. Barish R. G. Alsmiller, Jr.¹

The TLND is an albedo-type neutron dosimeter designed by Hoy.¹⁰⁶ Awschalom¹⁰⁷ compared dose-equivalent data obtained with the TLND with dose-equivalent data obtained with a Bonner spectrometer and found the TLND to be quite accurate. To further test the reliability of this dosimeter, its response to monoenergetic neutron fluences with energies between thermal energies and 400 MeV has been calculated, and the results have been compared with the available low-energy (<10 MeV) experimental data.

Calculations have been carried out for very broad beams of neutrons both normally and isotropically incident on the face of the tissue that contains the TLND. The calculations were carried out using the discrete-ordinates code DOT³³ in the adjoint mode. The calculations show that over limited energy ranges the TLND can be used to obtain approximate values of the dose equivalent.

Sponsor: Neutron Physics Division

R. G. Alsmiller, Jr.

ENERGY DEPOSITION IN IONIZATION SPECTROMETERS

T. A. Gabriel¹ K. C. Chandler

The design of ionization spectrometers for measuring the energy of high-energy hadrons requires detailed information on the fluctuations in energy deposition induced by nucleon-meson and electromagnetic cascades. Calculations for different types of spectrometers have been carried out using HETC⁸⁶ to determine the nucleon-meson cascade. The photons from neutral-pion decay and the electrons and positrons from muon decay (calculated by HETC) were used as input to a slightly modified version of the code of Beck¹⁰² to determine the electromagnetic cascade. Calculations have been made for 28-GeV/c protons incident on a spectrometer consisting of plastic scintillators embedded in iron and 8-GeV/c negatively charged pions incident on a sodium iodide total absorption spectrometer.

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105. ORNL-TM-3984 (December 1972).

106. J. Hoy, *Personnel Albedo Neutron Dosimeter with Thermoluminescent ^6LiF and ^7LiF* , DP-1271, E. I. du Pont de Nemours and Co., Savannah River Plant (January 1972).

107. M. Awschalom, "The Radiation Safety Philosophy and Its Implementation at NAL," p. 1050 in *Proc. International Congress on Protection against Accelerator and Space Radiation, CERN, Geneva, Switzerland, April 25-30, 1971*, CERN-71-16 (1971).

**A CALCULATIONAL METHOD FOR PREDICTING PARTICLE SPECTRA
FROM HIGH-ENERGY NUCLEON AND PION COLLISIONS
(≥ 3 GeV) WITH PROTONS^{108,109}**

J. Barish T. A. Gabriel¹
R. T. Santoro¹

A calculational method for predicting the spectra from high-energy nucleon and pion collisions (≥ 3 GeV) with protons is described. The determination of nucleon-proton and pion-proton total, elastic, and nonelastic cross sections from experimental data is discussed, and procedures for obtaining nucleon and charged-pion spectra from the Ranft-Borak distributions are presented. A brief discussion of the computer program logic is also included.

Sponsor: Neutron Physics Division

T. A. Gabriel

**COUPLED CALCULATIONS OF THE TRANSPORT OF NEUTRONS AND SECONDARY
GAMMA RAYS THROUGH CONCRETE FOR NEUTRON SOURCES
WITH ENERGIES BETWEEN 15 AND 75 MeV¹¹⁰**

J. Barish R. W. Roussin¹
R. G. Alsmiller, Jr.²

Coupled neutron and gamma-ray transport calculations have been carried out for monoenergetic neutrons normally incident on an infinite slab shield of concrete with 5.5% water by weight. The production of gamma rays from interactions of neutrons with energy greater than 15 MeV was ignored. For the 50- and 75-MeV incident neutron energies, the gamma-ray dose equivalent was found to be no more than 5% of the total dose equivalent. For the 15- and 25-MeV incident neutron energies, the gamma-ray dose equivalent dominates at greater depths into the slab. A conservative estimate of the effect of including gamma rays produced by interactions of neutrons having energies greater than 15 MeV indicates that the calculated total dose equivalent would increase by no more than 5%.

Sponsor: Neutron Physics Division

R. G. Alsmiller, Jr.

**CALCULATION OF THE NEUTRON FLUX SPECTRA IN THE EARTH'S ATMOSPHERE
INDUCED BY GALACTIC COSMIC RAYS**

T. W. Armstrong¹ R. G. Alsmiller, Jr.¹ K. C. Chandler J. Barish

Calculations have been previously carried out to obtain the neutron flux spectra in the earth's atmosphere due to galactic protons.¹¹¹ At some geomagnetic latitudes, galactic alpha particles contribute significantly to the neutron flux spectra. Therefore, the code HETC⁸⁸ was modified to include, in an approximate manner, alpha-particle transport. This required the incorporation of a model¹¹² to treat high-energy alpha-particle-nucleus interactions. The modified code has been used to determine the

108. Work partially funded by National Aeronautics and Space Administration under order H-38280A.

109. Abstract of ORNL-TM-3615 (Nov. 1, 1971).

110. Abstract of paper to be published in *Nuclear Engineering and Design*.

111. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 50.

112. T. A. Gabriel, R. T. Santoro, and R. G. Alsmiller, Jr., "An Approximate High-Energy Alpha-Particle-Nucleus Collision Model," *Nucl. Sci. Eng.* 44, 104-110 (1971).

contribution of galactic alpha particles to the neutron flux spectra induced by galactic cosmic rays at various depths in the atmosphere.

Sponsor: Neutron Physics Division

SPAR: A FORTRAN PROGRAM FOR COMPUTING STOPPING POWERS AND RANGES

K. C. Chandler T. W. Armstrong¹

A computer program has been written to calculate stopping powers and ranges for muons, charged pions, protons, and heavy ions in any nongaseous medium at essentially all energies (0–1 TeV). In computing the stopping powers, a different calculational procedure is used in each of three (β , z) regions, where β is the speed of the particle relative to the speed of light and z is the nuclear charge of the particle. At high energies ($\beta > 0.04z^{2/3}$), where the particles can be considered to be completely ionized, Bethe's theory^{1 13} with shell and density effect corrections is used. At intermediate energies ($0.0046z^{1/3} < \beta \leq 0.04z^{2/3}$), where charge reduction is important but energy losses from elastic nuclear Coulomb collisions can be ignored, an empirical expression^{1 14} for the charge reduction is used in conjunction with Bethe's theory. At low energies ($0 \leq \beta \leq 0.0046z^{1/3}$), where both charge reduction and nuclear Coulomb stopping are important, the theory of Lindhard et al.^{1 15} is used. At all energies the ranges are obtained by numerical integration of the stopping power.

Sponsor: Neutron Physics Division

TRAPP: A COMPUTER PROGRAM FOR THE TRANSPORT OF ALPHA PARTICLES AND PROTONS WITH ALL NUCLEAR REACTION PRODUCTS NEGLECTED^{116,117}

J. Barish F. S. Alsmiller¹ R. T. Santoro¹ R. G. Alsmiller, Jr.¹

TRAPP is a FORTRAN IV program primarily intended for carrying out studies of the shielding required to protect astronauts against Van Allen belt protons and against solar-flare protons and alpha particles. The program treats the transport of protons and alpha particles through a homogeneous shield and tissue with the assumptions that all nuclear reaction products may be neglected and all particles travel in a straight line and undergo a continuous slowing down. The geometry considered is that of a spherical shell shield with a tissue sphere at its center. For an isotropically incident proton or alpha-particle flux per unit energy with maximum energy ≤ 3 GeV, the program gives the particle flux per unit energy, the absorbed-dose rate, and the dose-equivalent rate at the center of the tissue sphere as a function of the spherical-shell-shield thickness.

Sponsor: Neutron Physics Division

R. G. Alsmiller, Jr.

¹¹³. B. Rossi, *High Energy Particles*, Prentice-Hall, Englewood Cliffs, N.J., 1952.

¹¹⁴. W. H. Barkas, *Nuclear Research Emulsions*, Academic, New York and London, 1963, p. 371.

¹¹⁵. J. Lindhard, M. Scharff, and H. E. Schiott, "Range Concepts and Heavy Ion Range: (Notes on Atomic Collisions, II)," *Kgl. Dan. Vidensk. Selsk., Mat.-Fys. Medd.* 33, No. 14 (1963).

¹¹⁶. Work funded by National Aeronautics and Space Administration under order H-38280A.

¹¹⁷. Abstract of ORNL-4763 (August 1972).

SHIELDING CALCULATIONS FOR A 400-MeV ELECTRON ACCELERATOR

J. Barish R. G. Alsmiller, Jr.¹

In a series of previous papers,¹¹⁸⁻¹²⁰ the results of neutron-transport calculations carried out for a variety of neutron source energies ≤ 400 MeV by the method of discrete ordinates were presented. In the present work, similar results have been obtained for the neutron source spectrum produced when 400-MeV electrons are normally incident on thick copper targets. These calculations are being carried out to aid in the design of the shielding for the 400-MeV electron accelerator under construction at the Massachusetts Institute of Technology.

In the previous papers, shields of soil and concrete block were considered. In the present work, shields of soil, concrete, ilmenite, iron, and iron followed by soil are considered. The geometry considered in the present calculations is that of a point isotropic source at the center of the sphere shield.

Sponsor: Neutron Physics Division

R. G. Alsmiller, Jr.

SHIELDING OF MANNED SPACE VEHICLES AGAINST PROTONS AND ALPHA PARTICLES^{121,122}

R. G. Alsmiller, Jr.¹ H. C. Claiborne¹²³ R. T. Santoro¹ J. Barish

Preparation of a space shielding handbook, which summarizes the available information on the shielding of manned space vehicles against protons and alpha particles in space, has been completed. The handbook is intended primarily for nonexperts and is expected to be most useful to mission planners who must decide with little effort whether a radiation hazard is likely to exist during a specific mission. It will also serve as a useful starting point for obtaining more adequate information about the shielding required when a radiation hazard is thought to exist on a specific mission.

Many space shielding calculations have been published and are available, but to ensure uniformity and consistency throughout the handbook, a large majority of the calculated results contained in the handbook were generated specifically for this publication. The calculational model used is that of a 300-cm-ID spherical shell shield of a specified material and thickness with a 30-cm-diam tissue sphere at the center. This configuration simulates only very approximately a manned space vehicle, but it does serve to illustrate many of the significant features in spacecraft shield design.

Sponsor: Neutron Physics Division

R. G. Alsmiller, Jr.

118. R. G. Alsmiller, Jr., F. R. Mynatt, J. Barish, and W. W. Engle, Jr., "High Energy (<400 MeV) Neutron Transport Using the Method of Discrete Ordinates," *Nucl. Sci. Eng.* 36, 251 (1961); also ORNL-TM-2420 (1968).

119. R. G. Alsmiller, Jr., F. R. Mynatt, J. Barish, and W. W. Engle, Jr., "Shielding against Neutrons in the Energy Range 50 to 400 MeV," *Nucl. Instrum. Methods* 72, 213 (1969); also ORNL-TM-2554 (1969).

120. R. W. Roussin, R. G. Alsmiller, Jr., and J. Barish, "Calculations of the Transport of Neutrons and Secondary Gamma Rays through Concrete for Incident Neutrons in the Energy Range 15 to 75 MeV," ORNL-TM-3659 (revised) (1972); to be published in *Nuclear Engineering and Design*.

121. Research funded by the National Aeronautics and Space Administration under orders H-38280A and H-79272A.

122. R. G. Alsmiller, Jr., R. T. Santoro, J. Barish, and H. C. Claiborne, *Shielding of Manned Space Vehicles against Protons and Alpha Particles*, ORNL-RSIC-55 (November 1972).

123. Advanced Planning Group, Chemical Technology Division, ORNL.

OPERATIONS DIVISION

UNFOLDING OF NEUTRON SPECTRA

F. W. Stallman F. B. K. Kam¹

An iterative method has been developed for determining the neutron spectrum of a reactor from saturation activities. The measured saturation activities $\tilde{\alpha}_i$, $i = 1, n$, are related to the unknown spectrum $\phi(E)$ through the integral

$$\alpha_i = \int_0^{\infty} \phi(E) \sigma_i(E) dE + \epsilon_i, i = 1, n. \quad (1)$$

The $\sigma_i(E)$ are cross sections at energy E , and the ϵ_i are measuring errors which have an estimated variance of s_i .

Formula (1) represents an undetermined system of equations for $\phi(E)$. To make it definite, a prior estimate $\psi(E)$ of the spectrum is made, and the solution $\tilde{\phi}(E)$ of (1) is determined which minimizes the integral norm

$$S^2 = \int_0^{\infty} \left[\frac{d}{dE} \left(\frac{\tilde{\phi}}{\psi} \right) \right]^2 w(E) dE, \quad (2)$$

with some suitably chosen positive weight function $w(E)$, subject to the condition that the mean square error

$$f = \sum_{i=1}^n \left(\frac{\epsilon_i}{s_i} \right)^2 \quad (3)$$

remains less than a given tolerance limit.

A general method for solving this problem is given in ref. 2. Frequently, however, some of the values of $\tilde{\phi}(E)$ obtained in this manner become negative, in contradiction to the physical realities. To avoid this, the a priori function $\psi(E)$ is changed in the following manner: if some values of $\tilde{\phi}(E)$ are negative, the tolerance limit f in (3) is increased until $\tilde{\phi}(E)$ is close enough to $\psi(E)$ to be positive. This function is then used as a new a priori estimate, and the procedure is repeated until a positive solution $\tilde{\phi}(E)$ appears which has the prescribed tolerance limit (3).

Such a solution of (1) may not exist at all, in which case the procedure will not converge. In numerical experiments, however, using data from reactor experiments, the procedure converged rapidly to reasonable solutions using a wide variety of initial choices of $\psi(E)$. It may be pointed out that these solutions do not necessarily represent the true spectrum but only a reasonable estimate produced from the limited information in (1). For the same reason, no firm error bounds can be given for $\tilde{\phi}(E)$.

Sponsor: Operations Division

1. Operations Division.

2. F. W. Stallmann, *Numer. Math.* 15, 297-305 (1970).

STUDIES OF THE EFFECTS OF HEAVY-WATER AND BERYLLIUM REFLECTORS ON THE THERMAL-NEUTRON FLUX THROUGH DUCTS FROM THE BSR

J. R. Knight P. A. McCarty F. B. K. Kam¹

The KENO Monte Carlo code³ was used to determine the effects of heavy-water and beryllium reflectors on the thermal-neutron flux through ducts from the BSR. Calculations were made for varying thicknesses and placements of the reflectors. Variations of the type and location of materials in the ducts were also evaluated. The purpose of the calculations was to determine the conditions for optimum generation of thermal-neutron flux in the duct.

Sponsor: Operations Division

F. B. K. Kam

HFIR REACTOR POWER DENSITY

M. R. Patterson F. D. Hammerling R. D. Ellison

Techniques previously developed^{4,5} to analyze the azimuthal symmetry of power density data were applied to the HFIR reactor. Modifications to the program were made to allow the user to select independently the number of harmonics allowed for the inner and outer annular regions of the reactor. Provision was made to extract only the constant term if data for only one value of the azimuthal angle are available. The Runberg integration scheme previously used to normalize the power density over the reactor volume took considerable machine time. Consequently, the three-dimensional integration was changed to a much faster adaptive-Simpson-rule routine, furnished by R. H. Fowler.

Sponsor: Operations Division

F. B. K. Kam

FEDEN: FUEL ELEMENT DENSITY DETERMINATION

C. C. Webster

A program has been developed for use at a remote terminal to use the measurements made on irradiated materials within a remote facility and determine the density, volume, and mass with their variation (when several measurements are made) for the irradiated specimens. The program stores a table of the weight correction values and updates them at the user's discretion. Adjustments are made for humidity and temperature effects to achieve five-place accuracy in the results. An important feature of the program is the display of the input data and the calculated output in a format that can be utilized directly.

Sponsor: Operations Division

S. Dismuke

3. G. E. Whitesides and N. F. Cross, *KENO - a Multigroup Monte Carlo Critically Program*, CTC-5 (September 1969).
 4. M. R. Patterson and F. D. Hammerling, *Fourier Analysis of Unequally Spaced Data*, ORNL-TM-3547 (September 1971).
 5. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, pp. 66-67.

ORNL-NSF ENVIRONMENTAL PROGRAM

ORRMIS: OAK RIDGE REGIONAL MODELING INFORMATION SYSTEM

R. C. Durfee

A geographically oriented information system is being developed for the Regional Environmental Systems Analysis Group at ORNL. The system was described very briefly in last year's annual report.¹ This system is being designed to operate either as a stand-alone inquiry-retrieval system or as a communications supervisor for use within a simulation model. The development of the Oak Ridge Regional Modeling Information System (ORRMIS) has been divided into three phases. The first phase, which has now been completed, consisted in designing and implementing the basic storage-retrieval system, which, at its lowest level, recognizes the existence of individual cells within a given geographical area. Final emphasis in phase 1 is being placed on some specialized routines for the East Tennessee Development District land-use model.²

Phase 2, currently under way, involves the development and use of a generalized record structure that will support complex hierarchical data structures. The record structure decided upon for use by the Regional Environmental Systems Analysis Group is the ADSEP generalized record format³ used within the Mathematics Division at ORNL. Although the data bases developed by the Regional Environmental Systems Analysis Group will use this ADSEP format, it should be pointed out that the Phase 1 routines can be used with any type of record structure.

Phase 3 of ORRMIS covers development of a user-oriented question-answer language to communicate with the information system in the stand-alone mode (perhaps interactively) or as a driver for the various simulators. In the stand-alone mode, the user could retrieve, display, and update information within the various data bases. He might also ask simple questions which involve searching algorithms and statistical calculations. Although no basic design for Phase 3 exists, a review of the literature is under way to study the various types of command languages that are available.

Actual data for the East Tennessee Development District are presently being loaded into an ORRMIS data base that contains approximately 30,000 records. This data base may eventually occupy as much as 16 million bytes of disk storage.

Sponsor: Regional Environmental Systems Analysis Group,
ORNL-NSF Environmental Program

C. W. Craven, Jr.

DEVELOPMENT OF SPECIAL FACTOR AND CLUSTER ANALYSIS ROUTINES TO ANALYZE SPATIALLY DISTRIBUTED DATA

R. C. Durfee

We are currently developing two statistical packages which use factor and cluster analysis to analyze spatially distributed data over a geographical region. The primary requirement for using these two techniques is that the geographical region under study be described with a set of variables measured for a group of cells or parcels covering the region. One of the purposes of factor and cluster analysis, in this case, is to combine these variables or cells into meaningful and distinct groups. Once these groups have been

1. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 72.

2. J. L. Liverman, research proposal submitted to the National Science Foundation - Regional Environmental Systems Analysis, ORNL, Feb. 1, 1972.

3. A. A. Brooks, *Adoption of Generalized Record Format*, ORNL-CF-71-1-9 (January 1971).

formed. it is then necessary to identify, describe, and display them geographically. In order to accomplish these goals, it has been necessary to develop and add special routines to the traditional factor and cluster analysis programs^{4,5} previously used with nonspatial data.

In the case of factor analysis, we have added routines which enable us to

1. quickly identify the factors,
2. calculate factor scores,
3. print out the factor scores in map form,
4. plot the factor scores as three-dimensional perspective plots.

In the case of cluster analysis, we have added routines which enable us to

1. cluster large numbers of cells (2000–10,000),
2. calculate cluster profiles,
3. rank the variables in each cluster,
4. rank the clusters,
5. display the location of each cluster on the ground.

The development and use of these two statistical packages are described in more detail in the report "The Use of Factor and Cluster Analysis in Regional Modeling."⁶

Sponsor: Regional Environmental Systems Analysis Group,
ORNL-NSF Environmental Program

C. W. Craven, Jr.

SUBREGIONAL SELECTION IN THE EAST TENNESSEE DEVELOPMENT DISTRICT

R. C. Durfee C. R. Meyers, Jr.⁷

The Regional Environmental Systems Analysis Group at ORNL has chosen as its study region the East Tennessee Development District (ETDD). This area is comprised of 16 counties in upper East Tennessee that surround and include Knoxville. One of the first tasks facing this group has been to divide the ETDD study region into smaller units (subregions). The selection of these subregions, if done properly, should satisfy certain requirements such as homogeneity and compactness. The subregions, once chosen, may be defined geographically by groups of cells or parcels within a grid system superimposed upon the region. The parcels which make up each subregion should have characteristics common to themselves but different from their neighbors.

In choosing subregions, many analysts accept existing areas such as those defined by political boundaries, or at best, they divide the region into subunits through some subjective procedure. We are attempting to solve this problem through the use of factor and cluster analysis techniques. The strategy has been to (1) gather for each parcel those variables which are considered important to subregional selection, (2) group these variables into factors which are then more meaningful and reliable, and (3) finally cluster

4. R. C. Durfee, *Multiple Factor Analysis*, ORNL-TM-1798 (March 1967).

5. Edward E. Cureton, L. W. Cureton, and R. C. Durfee, "A Method of Cluster Analysis," *Multivariate Behav. Res.* 5, 101–116 (1970).

6. R. C. Durfee, *The Use of Factor and Cluster Analysis in Regional Modeling*, ORNL-TM-3720 (September 1972).

7. ORNL-NSF Regional Planning Consultant.

the parcels based upon the previous factors found. These clusters will then represent the subregions being sought. Of course, the final step is to define each cluster as to what makes it unique and different from its neighbors.

Sponsor: Regional Environmental Systems Analysis Group,
ORNL-NSF Environmental Program

C. W. Craven, Jr

ACQUISITION AND USE OF 1970 CENSUS DATA FOR THE EAST TENNESSEE DEVELOPMENT DISTRICT

R. C. Durfee V. A. Singletary R. Kemper⁸

We have extracted approximately 200 different variables from the 1970 Census tapes and prepared them for use with certain statistical programs. The information was extracted from the first, second, and fourth Count Tapes for the East Tennessee Development District (ETDD), an area consisting of 16 counties around Knoxville. The information from the first and second Count Tapes was retrieved for 796 different Enumeration Districts which completely cover ETDD. The fourth Count Tapes contained information at two higher levels, the County Civil Division (CCD) and the Census Tract. There are 108 County Civil Divisions which completely cover ETDD. However, the Census Tracts, of which there are about 89 in ETDD, exist only inside certain cities such as Knoxville and Oak Ridge. Areas outside these cities and elsewhere are not tracted. Thus, the hierarchy of census districts, although incomplete, goes from Enumeration District to Census Tract to County Civil Division.

In order to spatially analyze the information from these three levels simultaneously, it was necessary to have a common spatial unit for all variables. The unit which was chosen consisted of County Civil Divisions for all of ETDD, except inside those cities which were tracted. In those cities the Census Tracts were used. The final set of spatial units covering all of ETDD contained 170 different parcels (88 Census Tracts and 82 CCD's).

In order to statistically compare one spatial unit with another, it was necessary to transform many of the variables from raw counts into variables on a common scale. For example, the count of houses using oil heat was converted into the percentage using oil heat. The population counts were converted into the number of people per square mile, etc. After aggregating and transforming all the original items, the final set of data contained 199 variables for each of the 170 different parcels.

Sponsor: Regional Environmental Systems Analysis Group,
ORNL-NSF Environmental Program

C. W. Craven, Jr.

TWO-DIMENSIONAL MAP PRINTING ROUTINES FOR GEOGRAPHICAL DATA

R. C. Durfee

We have developed a routine for outputting spatially distributed data on the line printer in map form. The geographical region under study must be overlaid with a grid, and the data to be mapped should be digitized for each cell within the grid. (A special program has been written to allow easy digitization of certain types of maps.) These digitized values, after being scaled to integers in the range -99 to 999, may then be printed as shown in Fig. 12. This computer map shows the distribution of brooks and streams over

8. Civil Defense Research Section, Health Physics Division.

ORNL-DWG 73-1328

(0-9) — 28 x 32 GRID

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	
1	1							1	0	0	1	3	0	0	1	1	2	3	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2						0	0			0	0	0	0	0	3	2	0	4	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0
3						0	0	0	0	0	0	0	0	0	0	2	3	1	3	2	3	0	0	0	0	0	0	0	0	0	0	0	0
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NO. OF VALID CELLS = 826 - RANGE OF MAP SCORES = 0 TO 9 - AVERAGE MAP SCORE = 2.467 - STDDEV OF MAP SCORES = 2.773

Fig. 12. Presence of brooks and streams by percentage of cell occupied.

a 35,000-acre region overlayed with a 28×32 grid. Each numerical value represents the percentage of the cell containing brooks or streams (0 = 0%, 1 = 10%, 2 = 20%, etc.). As shown in this example, a border may be drawn around a nonrectangular study region, with the unused cells outside being blanked out. Those cells within the map which contain similar numerical values may be outlined together to correspond to the different colored areas on the original source map. The user may control the way in which this outlining is done. Other options, such as automatic rescoring of certain numerical values or suppressing printout for those cells which are zero, are available to the user. This routine may, of course, be used with any type of spatially distributed data, not just geographical maps.

Sponsor: Regional Environmental Systems Analysis Group,
ORNL-NSF Environmental Program

C. W. Craven, Jr.

ACQUISITION AND DISPLAY OF A GEOGRAPHICALLY ORIENTED DATA BASE

D. L. Wilson L. J. Campbell R. L. Stephenson T. C. Tucker A. H. Voelker⁹

We have continued development of techniques and computer codes for the geographic portion of the data base for Regional Environmental Systems Analysis.¹⁰ This work is also being done, as a joint task, for the Biome and Regional Synthesis Group of the Environmental Sciences Division.

We continued work on codes used for collecting data with the Hough-Powell line scanner. We modified existing programs to refine the techniques used to locate the map within the scanner and to make location assignments for the data obtained. We wrote new codes to correct errors in line-scanner digitization, to separate composite maps, to aggregate data to various levels, and to enter data into ORRMIS.¹

We have worked on techniques for using a manually positioned x-y digitizer to take data from printed maps. The output from the digitizer we have used is a punched paper tape containing, essentially, x-y-z data at more or less random locations. (The z data are entered manually prior to digitizing a collection of corresponding x-y pairs.) We read the paper tape on the PDP-10, interpret the new data, and punch the x-y-z triples into cards. (We anticipate replacing the punched cards with magnetic tape when the computer algorithms using the data become better defined.) The random x-y-z data must be distributed to the grid or cell locations used.¹¹ We have used the SYMAP program¹² to interpolate elevation data. Figure 13a shows a contour map which we digitized using this technique, and Fig. 13b shows the contour map drawn by CR3CON¹³ from the resultant grid data. While the gross characteristics of the original survived, too much detail has been lost. We believe that the interpolation algorithm is the major source of error, and we have begun work on advanced techniques for interpolation.

We have increased our library of subroutines for calculating map projections.

We have generated a large number of miscellaneous maps throughout the year, including one computer-generated motion picture. This showed the residential development of a region over a period of 35 years of recorded history and 8 years of simulation. Housing density was shown by drawing houses of varying size and intensity on a perspective drawing of the region. We drew approximately 1100 individual

9. Director's Division.

10. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 70.

11. ORNL-CF-71-10-29; also *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 70.

12. *Users' Reference Manual for Synagraphic Mapping "SYMAP" Version V*, Laboratory for Computer Graphics, Harvard University (June 1968).

13. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 68.

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Fig. 13. Comparison of original and computer-drawn contour maps. (a) Original contour map. (b) Computer-drawn contour map.

frames using about 2 hr of 360/75 time, 80 magnetic tapes, 12 hr of CRT plotter time, and about 40 hr of programming.

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C. W. Craven, Jr.

ANALYSIS AND DISPLAY OF TOPOGRAPHIC DATA

T. C. Tucker

We have continued and expanded the studies in digital topography which were reported previously.^{1,2}

The subroutine for making perspective and isometric drawings, PERSPX, has been expanded into a package of similar subprograms.^{1,4}

Although perspective drawings are a good means for sensing shape, they do not show elevation or in some cases even slope. We wrote a subprogram, PERCON, to superimpose contours on the perspective drawing PERSPX. Since different logic for locating contours was desirable in CR3CON and PERCON, we wrote an additional plane contour program CR4CON, which is consistent with PERCON.

We are continuing the study of hydrological properties determined by topography. Additionally, we are designing computer programs to determine slope and aspect, local horizon, and incident solar radiation.

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C. W. Craven, Jr.

SOCIOECONOMIC ANALYSIS

G. W. Westley R. J. Olsen^{1,5}

Since analysis and projection of population and employment are frequently the foundation for major planning decisions, the goal of the Socioeconomic Analysis is the development of systematic procedures (a model) for forecasting and predicting changes in population and employment for a geographic region consisting of an urban core with substantial rural fringes (e.g., the East Tennessee Development District). The model must be able to make "base-line" forecasts of population and employment as well as forecasts "conditioned" on inclusion of the specific public or private project being examined. The impact of the project is thus the difference between conditional and base-line forecasts.

A macrosocioeconomic model of the region as a whole is being considered that is sensitive to the relative attractiveness of the model area in comparison with other areas similarly defined, and of central importance to this macro model is an export-base model of the region.

The export-base approach argues that so much of the economic activity within small geographic regions (such as ETDD) is oriented toward serving markets outside the region that, in a very real sense, the activities of the export-oriented industries form the basis or foundation for the remaining locally oriented industries. In its crudest form, export-base analysis establishes a ratio between locally oriented service employment and export employment. Any change in export employment is multiplied by this ratio to estimate the impact on service employment. The total impact of a change in export employment is then the sum of the changes in export and service employment.

Since the export-base approach has been criticized, thought has been given to the possibility of using a more elaborate macroeconomic and/or interindustry approach. However, the paucity of meaningful

14. T. C. Tucker, *CATCH: Computer Assisted Topography, Cartography, and Hypsography; Part III, PERSPX, a Subroutine Package for Perspective and Isometric Drawings*, ORNL-TM-3790 (in press).

15. ORNL-NSF Environmental Program.

time-series data for a region such as the model area (ETDD) has led to a more pragmatic approach where all flows are measured in terms of people as members of the population or as employees. Thus, the socioeconomic submodel as a whole can be interpreted as an attempt to simulate the dynamics of labor supply (including population) and demand for the modeling area (or region). Labor demand is then the center of the model which is export-base in nature. In the model, the labor supply is derived from the product of the population and labor participation components. The labor demand is made up of the sum of the locally oriented employment and regional export employment components. The model as a whole then uses an iterative procedure to reconcile the labor supply and demand results for each year.

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C. W. Craven, Jr.

AIR POLLUTION PATTERNS IN THE VICINITY OF A STEAM PLANT

M. T. Mills N. E. Bolton¹⁶ R. I. Van Hook¹⁷

Air pollution calculations employing the Gaussian plume model are being performed for comparison with soil and air quality measurements now under way in the vicinity of the TVA Allen Steam Plant near Memphis, Tennessee. With a knowledge of the amount of pollution from the stacks and detailed atmospheric data for the Memphis area, we will be able to predict deposition rates of heavy-metal contaminants from the combustion of coal.

Sponsor: ORNL-NSF Environmental Program

R. Rabin

AIR POLLUTION MODEL FOR A WATERSHED

M. T. Mills M. Reeves S. Hanna¹⁸

A program is being written to calculate deposition rates within a watershed for airborne pollutants generated from area and point sources. Given the latitude and longitude of sampling points, point sources, and area source centroids, along with area source dimensions, precipitation data, wind speed and direction measurement, and atmospheric stability data, the ground-level air concentration for each pollutant is calculated by use of the Gaussian plume model.¹⁹ The source strengths, dry deposition velocities, and rainfall washout coefficients are then used to find the deposition rates for input to the hydrological transport model (HTM),²⁰ which will trace the flow of contaminants into the stream and groundwater.

Sponsor: ORNL-NSF Environmental Program

R. Rabin

AN ELECTRICITY SUPPLY-DEMAND PREDICTION SYSTEM

T. J. Tyrrell L. D. Chapman²¹ T. Mount²²

We are beginning the third year of our investigation of factors influencing electricity demand growth.²³ We have developed logical, statistically significant models of electricity demand for the three major

16. Health Division.

17. Environmental Sciences Division.

18. Consultant, Atmospheric Turbulence and Diffusion Laboratory, Oak Ridge, Tenn.

19. F. Pasquill, *Atmospheric Diffusion*, D. Van Nostrand, London, 1962.

20. N. H. Crawford and R. K. Linsley, *Digital Simulation in Hydrology*, technical report No. 39, Department of Civil Engineering, Stanford University (1966).

21. Resource economist, Cornell University.

22. Econometrician, Cornell University.

23. This project began in the fall of 1969; see *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 16.

consumer classes (residential, commercial, and industrial). These are logarithmic in form and specify demand as a function of electricity, gas, and electrical appliance prices, population, and per capita income. Demand has a lagged relationship to the explanatory variables (demand is a function of current values as well as past values of all variables), and regional constants define unique regional trends.

We have worked with many different functional forms. One of particular interest at the moment is a log-inverse-log model in which the log of demand is a function of the log of each variable as well as its exponentiated inverse. This implies that the elasticity of demand with respect to income, for example, is a function of the level of income. Preliminary findings give the appealing result: small changes in income exert greater influence on demand growth in low-income areas than in high-income areas.

The residential log-inverse-log model:

$$\text{LRDE}_{jt} = \text{RG}_j + \sum_{i=t}^n 0.898^{t-i} \left[-0.177\text{LPE}_t - 1.127\left(\frac{1}{\text{PE}_t}\right) + 0.052\text{LPI}_t + 86.3\left(\frac{1}{\text{PI}_t}\right) + 0.050\text{LPOP}_t - 21.3\left(\frac{1}{\text{POP}_t}\right) + 0.003\text{LPG}_{t-1} - 1.84\left(\frac{1}{\text{PG}_{t-1}}\right) + 0.359\text{LPA}_{t-1} + 0.484\left(\frac{1}{\text{PA}_{t-1}}\right) \right],$$

where

RDE_{jt} = residential demand for electricity in time period t for census region j ,

RG = a regional constant,

PE = the average price of electricity,

PI = personal income,

POP = population,

PG = the average price of gas,

PA = an electric appliance price index.

An "L" preceding a variable name indicates the log of that variable [$\text{LPE} = \log(\text{PE})$]; the index i runs from the current period t back to some initial period n . The explicit lag (0.898) of this model enables us to calculate long-run as well as short-run elasticities.

Regression results. For 1128 observations, $R^2 = 0.99$, $F > 10,000$, the Von Neumann statistic is 1.9, and all coefficients are significant at the 99.5% level with one exception (0.003 PG).

Results of our work have been reported this year at the Sierra Club Conference on Power and Public Policy²⁴ and the Cornell-NSF Workshop on Energy and the Environment.²⁵ By request we submitted testimony to the U.S. House of Representatives Subcommittee on Science, Research, and Development.²⁶

In addition to our model building, we have made projections of electricity demand. One set of these was requested jointly by the Federal Power Commission and the U.S. Water Resource Council;²⁷ another set can be found in a paper to be published in *Science* in early 1973.²⁸

Sponsor: Energy Group, ORNL-NSF Environmental Program

R. S. Carismith

24. L. D. Chapman and T. J. Tyrrell, "Alternative Assumptions about Life Style, Population, and Income Growth: Implications for Power Generation and Environmental Quality," presented at Johnson City, Vt., Jan. 14-15, 1972.

25. L. D. Chapman, T. Mount, and T. J. Tyrrell, "Predicting the Past and Future in Electricity Demand," presented at San Juan, P.R., Feb. 22-24, 1972.

26. L. D. Chapman, T. J. Tyrrell, and T. Mount, "Electricity Demand Growth: Implications for Research and Development," testimony submitted to the Subcommittee on Science, Research, and Development of the Committee on Science and Astronautics of the U.S. House of Representatives, June 16, 1972.

27. T. J. Tyrrell and L. D. Chapman, *Demand for Electricity: The Ohio Test Region and the United States* (August 1972).

28. Based primarily on Subcommittee testimony, this was accepted for publication Aug. 4, 1972.

AN ALGORITHM FOR DETERMINING SHORTEST PATHS IN DIRECTED GRAPHS

T. C. Tucker

An important characteristic of any site considered for some kind of development is the distance from that location to other sites which interact with it. For example, a fire station should be as near as possible (in travel time) to every part of its service area. While this siting problem may be relatively simple, others involve large numbers of points and an even larger number of interconnecting paths.

We have coded an algorithm, MOORE,²⁹ to determine a minimum-length path to each point in a network from one of a collection of specified points called roots. The algorithm operates on directed (one-way) paths. It determines the length of the shortest path from a root to each point that can be reached and the description of one such path. It should be noted that the path and root may not be unique but that there is no shorter path to any root.

This algorithm is a correction and translation to FORTRAN IV of an ALGOL procedure published in the *Communications of the Association for Computing Machinery*. The correction was necessary because the published version failed whenever a point could be reached but not left.

Sponsor: ORNL-NSF Environmental Program

C. W. Craven, Jr.

DEFILE: A DYNAMIC DEFINE FILE ROUTINE FOR FORTRAN DIRECT-ACCESS DATA SETS

R. C. Durfee

We have written a FORTRAN subroutine, DEFILE, to define FORTRAN direct-access data sets exactly like the DEFINE FILE statement does. The advantage in using DEFILE is that the file parameters, such as the block size or logical unit number, may be variables defined at execution time rather than integer constants defined at compile time.

Sponsor: Regional Environmental Systems Analysis Group,
ORNL-NSF Environmental Program

C. W. Craven, Jr.

PACK, UNPACK: TWO ROUTINES FOR PACKING AND UNPACKING ADSEP RECORDS WITH INTEGER DATA

R. C. Durfee

We have written two subroutines, PACK and UNPACK, to pack and unpack ADSEP records³⁰ which contain integer data. The purpose for such packing is to decrease the amount of disk space required to store ADSEP records. These routines may, in some cases, reduce the size of the records to one-fourth of their original size. Because of this decrease in record size, the overall execution time may also decrease, even though each record must undergo this packing-unpacking process. These two routines may actually be used with any type of record, ADSEP or otherwise, and data elements may be of any type, although integers work best.

Sponsor: Regional Environmental Systems Analysis Group,
ORNL-NSF Environmental Program

C. W. Craven, Jr.

29. Robert B. Dial, Algorithm 360, "Shortest-Path Forest with Topological Ordering," *Commun. ACM* 12(11), 632-33 (1969).

30. A. A. Brooks, Jr., *Adoption of Generalized Record Format*, ORNL-CF-71-1-9 (Jan. 8, 1971).

PHYSICS DIVISION

PROPORTIONAL WIRE CHAMBER DATA ANALYSIS PROGRAM

M. T. Mills W. M. Bugg¹ R. D. McCulloch J. J. Lucas

An effort is currently under way to write a data analysis package for the proportional wire chamber system now being installed upstream from the bubble chamber at the National Accelerator Laboratory. Nine planes consisting of 48 parallel wires spaced 2 mm apart are set at different orientations and distances from the center of the bubble chamber so that a series of wire firings initiated by the passage of a highly relativistic charged particle will give a much better measure of the particle trajectory than would be possible from bubble chamber measurements alone.

The first section of the upstream counter data analysis package uses wire-firing information from straight-through beam tracks to determine the displacement of five of the wire chambers with respect to the other four. Once these displacements are determined, a nine-plane fit is carried out to extract the trajectory parameters, which are then correlated with bubble chamber measurements to find the transformation coefficients from the bubble chamber coordinate system to the proportional wire chamber system. This information, along with downstream wire firings, will enable us to determine scattering angles for events in the bubble chamber.

Sponsor: Physics Division

H. Cohn

COMPUTER CODES FOR HEAVY-ION REACTIONS

L. W. Owen G. R. Satchler²

The nuclear reaction codes DWUCK,³ QUACK,⁴ and HELENE⁵ and the "global" search code Genoa, written by F. G. Perey of the Neutron Physics Division, have been modified to calculate heavy-ion reactions. Since the wave number k can be quite large in a typical heavy-ion reaction, it was necessary to greatly increase the maximum permissible number of partial waves and radial mesh points. In addition, since the Coulomb parameter η can be large as well, a new Coulomb function generator⁶ that is accurate in the entire (η, ρ) plane was added to the above codes. Further modifications and improvements are planned as we gain experience in analyzing these reactions.

Sponsor: Physics Division

THE BRUECKNER-HARTREE-FOCK APPROXIMATION TO THE NUCLEON-NUCLEUS OPTICAL POTENTIAL

L. W. Owen M. R. Patterson R. L. Becker²

Pauli-corrected two-body nuclear reaction matrix elements, computed from realistic nuclear interactions, are being used to calculate matrix elements of a two-body optical-model potential in an oscillator

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1. Consultant, Physics Department, University of Tennessee.
 2. Physics Division.
 3. P. D. Kunz, University of Colorado report COO-535-606 (1969).
 4. R. M. DeVries, private communication.
 5. S. K. Penny, *HELENE - a Computer Program to Calculate Nuclear Cross Sections Employing the Hauser-Feshbach Model, Porter-Thomas Width Fluctuations and Continuum States*, ORNL-TM-2590 (1969).
 6. C. Bardin et al., *Comput. Phys. Commun.* 3, 73 (1972).

representation.⁷ The projectile energy is assumed to be low enough that the optical potential is real. Either unit or fractional occupation probabilities and either purely single-oscillator or Hartree-Fock wave functions may be used for the normally occupied single-particle states of the target nucleus. The present code will calculate the optical potential for spherical nuclei, and generalization to deformed nuclei is planned.

We are collaborating with John Philpott, of Florida State University, who is using our optical potential matrix elements to calculate the scattering of low-energy nucleons by ^{16}O .

Sponsor: Physics Division

RENORMALIZED FINITE-NUCLEAR BRUECKNER THEORY

M. R. Patterson R. L. Becker²

The collaboration begun last year with R. C. Braley and W. F. Ford of the NASA Lewis Research Center⁸ has yielded Hartree-Fock calculations of intrinsic states having permanent deformation. These calculations yield estimates of binding energies, size, separation energies, electromagnetic transition rates, moments, and electron scattering form factors for several light nuclei, based on a density-dependent Hartree-Fock theory.⁹ The application of this technique to ^{12}C using the Hamada-Johnston interaction has been described elsewhere.¹⁰

A code to perform such Hartree-Fock calculations has now been written locally. Its major purpose is to allow mixing of all available m states so that odd- A nuclei can be considered. A secondary purpose has been to extend the range of A that can be computed to heavier nuclei than were previously possible. It has been successfully applied to nuclei with $A \leq 16$ in check-out runs and will be extended to larger nuclei as the work progresses.

Sponsor: Physics Division

COULOMB REPULSION ENERGY FOR TWO SPHEROIDS

R. H. Fowler G. S. McNeilly

A program has been written to calculate the Coulomb repulsion energy of two overlapping coaxial spheroids. The code calculates integrals of the form

$$I = \iint \frac{\rho(\vec{x}) \rho(\vec{x}')}{r} d^3x d^3x',$$

where r is the distance between volume elements d^3x and d^3x' . In the case of azimuthal symmetry the integral is easily reduced to a fivefold integral.

Sponsor: Physics Division

H. W. Schmitt

1. R. L. Becker, A. D. MacKellar, and B. M. Morris, *Phys. Rev.* 174, 1264 (1968).

8. *Math. Div. Annu. Prog. Rep.* Dec. 31, 1971, ORNL-4761, p. 75.

9. W. F. Ford et al., *Deformed Brueckner-Hartree-Fock Calculations*, NASA TM X-68134 (1972).

10. R. L. Becker et al., *Deformed Renormalized Brueckner-Hartree-Fock Approximation and Its Application to ^{12}C* , ORNL-TM-3951 (September 1972).

PDP-9 PROGRAMS FOR ACQUISITION AND ANALYSIS OF FISSION PHYSICS DATA

L. W. Gilley

Essentially two programs have been written. One accepts data from the buffered tape buffer of a ND 3300, makes a number of calculations using the data, and displays it on a CRT. The second program takes data from up to four ADC's in either multiparameter or single-parameter modes, writes the data on Dec tape, and displays a selected buffer on a scope interfaced to the PDP-9.

Sponsor: Fission Group, Physics Division

H. Schmitt

CONFLUENT HYPERGEOMETRIC FUNCTION

N. M. Larson I. J. Lucas

A code is being developed to evaluate the second form¹¹ of the confluent hypergeometric function $U(a, b, z)$ for nonnegative values of z , using the appropriate formulas (exact or asymptotic). This function is used in normalization of the wave functions of the double oscillation potential. Previous versions of the function failed at large z .

Sponsor: Physics Division

M. G. Mustafa

LEVEL SCHEME PLOTTING PROGRAM

M. Feliciano C. C. Webster

The program as it existed when described in the last annual report¹² has been modified to include improvements in the plotting routine. The program has been modified with the addition of subroutines giving the capability of using the input data as presented on cards used previously as well as the new version of the input data cards. The input data can be presented in either keV or MeV, and the user has the option as to which energy range will appear on the output plot.

Sponsor: Nuclear Data Project, Physics Division

D. Horen

11. M. Abramovitz and I. A. Stegun, *Handbook of Mathematical Functions*, National Bureau of Standards, pp. 504 ff. (1965).

12. *Math Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 66.

REACTOR DIVISION

REACTOR SITING

P. R. Coleman C. C. Webster

A program has been developed to compare the population distribution around potential reactor sites with that of existing reactor sites. This program is based on the method used in the PANS program¹ for

1. P. R. Coleman and A. A. Brooks, *PANS: A Program to Tally Population by Anuli and Sectors*, ORNL-TM-3923 (October 1972).

population distribution. The main application has been to show the population distribution at each point of a grid system for use in determining suitable locations for power parks and offshore reactors.

Sponsor: Reactor Division

Otto Klepper

A PROGRAM FOR THE EQUILIBRIUM FUEL CYCLE OF REACTORS

J. D. Amburgey

GAFFOY² is a one-dimensional equilibrium cycle reactor burnup program that calculates the characteristics of the equilibrium fuel cycle of large power reactors in considerable detail. GAFFOY was programmed in FORTRAN V for the Univac 1107/1108 computer series with a 64K memory. Extensive reprogramming was required to convert the program from the Univac FORTRAN V language to the IBM 360 FORTRAN IV language. The program made extensive use of variable dimensions, subroutine subprograms, and other features of FORTRAN V not compatible with FORTRAN IV.

Sponsor: Reactor Division

L. L. Bennett

EXPANSION OF POWER PLANT MAINTENANCE PROGRAM

J. D. Amburgey

The program arranged power plant maintenance schedules so that there is always sufficient power available while certain power plants are down. Extensive modifications were necessary to allow the program to handle 62 power plants concurrently in contrast to the original 31 plants.

Sponsor: Reactor Division

L. L. Bennett

HETEROGENEITY EFFECTS IN THE ZPR-III ASSEMBLY 48 BY MONTE CARLO³

S. N. Cramer

Geometric heterogeneity effects in the standard drawer of ZPR-III Assembly 48 have been investigated by Monte Carlo. Results are given for one-, two-, and three-dimensional mockups of the drawer and compared with one-dimensional discrete-ordinates calculations. Full core eigenvalue evaluations are also presented. The Monte Carlo calculations were performed with a version of the ESP code which allows the exact description of the plate-drawer assembly through the use of the fictitious scattering transport model and a generalized array geometry routine.

Sponsor: Reactor Division

2. H. Kraetsch, C. George, and M. Wagner, *GAFFOY*, Gulf General Atomic (Aug. 18, 1970).

3. Abstract of ORNL-TM-3730.

ESP: A GENERAL MONTE CARLO REACTOR ANALYSIS CODE⁴

S. N. Cramer R. S. Carlsmith⁵
 G. W. Morrison G. W. Perry⁶
 J. L. Lucius

The ESP code is a general-purpose steady-state Monte Carlo reactor analysis code. It covers the complete energy range of interest in reactor calculations and is designed for both eigenvalue and fixed-source reactor and reactor cell calculations. Basic data are accepted only in the ENDF/B format. In addition to smooth data, the cross-section preparation includes a detailed treatment of resolved and unresolved resonances and the free gas and $S(\alpha, \beta)$ thermal models. The collision and source routines utilize the ENDF/B nonelastic secondary distributions, the anisotropic scattering data, and the fission spectra. The energy range may be divided into as many as 25,000 intervals, and over each interval the appropriately averaged cross sections are used as constant point-energy values. A general geometry description is available, as well as several specialized geometries. Use of fixed-source options allows calculations on nonmultiplying systems.

ESP may be run in its entirety with only one problem setup and computer pass. No subroutine or tape preparation is necessary. The analysis of neutron histories is performed in computer core for many quantities of interest usually wanted in reactor calculations. Included among these are neutron fluxes, reaction rates, and cross sections, averaged over arbitrary energy and spatial regions.

Sponsor: Reactor Division

CALCULATION OF NUCLIDE-DEPENDENT AVERAGE CROSS SECTIONS BY MONTE CARLO

S. N. Cramer J. L. Lucius J. R. Trinko⁷

The ESP code⁸ has been modified to produce nuclide-dependent energy group and spatial region averaged cross sections in addition to average cross sections for mixtures of nuclides. The resolved and unresolved resonance cross-section treatment has also been modified in order to more efficiently give some nuclides very detailed resonance treatment. The changes in ESP are part of a Monte Carlo evaluation of the molten salt breeder reactor.

Sponsor: Reactor Division

A TREATMENT OF DOUBLE HETEROGENEITIES IN REACTOR FUEL CELLS

G. L. Ragan⁹ N. M. Greene O. L. Smith⁹ J. L. Lucius

A method¹⁰ has been developed for calculating resonance self-shielding effects that attempts to take into account double heterogeneities in reactor lattices of fuel rods that contain dispersions of grainy materials.

4. Abstract of ORNL-TM-3164.

5. ORNL-NSF Environmental Program.

6. TVA, Chattanooga, Tenn.

7. Ebasco Services, New York, N.Y.

8. S. N. Cramer, G. W. Morrison, R. S. Carlsmith, G. W. Perry, and J. L. Lucius, "ESP: A General Monte Carlo Reactor Analysis Code," this report.

9. Reactor Division.

10. G. L. Ragan et al., "Estimates of Resonance Self-Shielding Effects in Doubly Heterogeneous Systems," *Trans. Amer. Nucl. Soc.* 15(1), 453 (1972).

Tests indicate that for many systems other effects are of greater importance and "better" results are obtained by homogenizing the grainy material in the resonance calculation.

Sponsor: Reactor Division

UPDATING OF THE GAM-II AND 100-GROUP XSDRN CROSS-SECTION LIBRARIES

R. Q. Wright

Fifty-four materials in the ENDF/B Version III library¹¹ have been processed by SUPERTOG,¹² and GAM-II and XSDRN libraries^{13,14} have been updated. Most materials with resonance parameters appear on these libraries in two forms, as an infinite-dilution nuclide and also as a resonance nuclide requiring an additional resonance calculation. The materials processed included 54 infinite-dilution nuclides and 37 resonance nuclides.

Sponsor: Reactor Division

J. D. Jenkins

USE OF MORSE FOR CALCULATION OF REACTION RATES FOR A STANDARD MODEL FOR COMPARISON OF NEUTRONICS CODES

Margaret B. Emmett D. Steiner⁹ S. K. Penny

Work has continued on the previously reported¹⁵ MORSE¹⁶ calculation of reaction rates for a standard blanket model. Some more recent cross sections for ⁶Li, ⁷Li, and niobium were used in the calculations. The differences between the MORSE and ANISN¹⁷ results have been resolved through use of larger quadrature sets in the ANISN runs and correction of an error in the calculation of the source variables in MORSE.

Sponsor: Reactor Division

D. Steiner

EVALUATION OF NEUTRON CROSS SECTIONS IN ENDF/B FORMAT FOR TEN ISOTOPES OF CURIUM, BERKELIUM, AND CALIFORNIUM

R. Q. Wright N. M. Greene

Partial cross-section evaluations for ²⁴⁴Cm, ²⁴⁵Cm, ²⁴⁶Cm, ²⁴⁷Cm, ²⁴⁸Cm, ²⁴⁹Bk, ²⁴⁹Cf, ²⁵⁰Cf, ²⁵¹Cf, and ²⁵²Cf were performed, and the data were compiled in ENDF/B format.¹¹ The reactions included were fission, capture, and ν (the number of neutrons per fission). Resolved and/or unresolved reso-

11. M. K. Drake, ed., *Data Formats and Procedures for the ENDF Neutron Cross Section Library*, BNL-50274 (T-601) (ENDF 102, vol. 1) (October 1970).

12. R. Q. Wright, N. M. Greene, J. L. Lucius, and C. W. Craven, Jr., *SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B*, ORNL-TM-2679 (September 1969).

13. G. D. Joanou and J. S. Dudek, *GAM-II: A B_3 Code for the Calculation of Fast-Neutron Spectra and Associated Multigroup Constants*, GA-4265 (1963).

14. N. M. Greene and C. W. Craven, Jr., *XSDRN: A Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (July 1969).

15. *Math Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 76.

16. E. A. Straker et al., *The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585 (1970).

17. W. W. Engle, Jr., *A User's Manual for ANISN - a One Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1693 (1967).

nance parameters were used to specify the cross sections below 10 keV. In the energy range 15 MeV–10 keV a point-by-point representation was used. In the thermal region a $1/V$ cross section was assumed up to 0.625 eV.

The ENDF/B data were then processed by the SUPERTOG code¹² to produce group-averaged cross sections in the GAM-II¹³ 99-group structure. These cross sections were then used to update an XSDRN¹⁴ cross-section tape for use in a subsequent XSDRN calculation.

Sponsor: Reactor Division

O. L. Smith

CASDAR: A CROSS-SECTION AND SPECTRUM DIRECT-ACCESS RETRIEVAL PROGRAM

G. W. Cunningham J. D. Jenkins⁹

The work on CASDAR¹⁸ has been completed. The direct-access data files may contain up to 2000 cross sections $[\sigma(E)]$ and 2000 neutron spectra $[\Phi(E)dE]$. All data are stored in a standard 123-group structure. Input data are always converted to the 123-group structure regardless of the input form. The plotting options in CASDAR use the ORGRAPH package.¹⁹ There is now a provision in the program to update the neutron data on an ORIGEN library tape.²⁰ A report is not currently planned; however, an input description is available on a listing of computer cards.

Sponsor: Reactor Division

REACTOR DIVISION COOPERATIVE CODE DEVELOPMENT – THE VENTURE PROGRAM

G. W. Cunningham T. B. Fowler⁹ D. R. Vondy⁹

The AEC Division of Reactor Development and Technology is interested in facilitating the exchange of computer codes between installations involved in the Liquid Metal Fast Breeder Reactor Program. Representatives of the various installations have met to study the problem and recommend programming and data standards. A set of standard interface files evolved, which, hopefully, contains sufficient data to describe a reactor calculation (using either diffusion theory or SN transport theory). In addition, a standard free-form input processor for card input was proposed. A restraint on computer memory use of 50K words was adopted. Modular codes written at various installations are to be executed under the control of a supervisory program, with communication between the modules being through the standard interface files.

ORNL is participating in this effort by developing a multigroup, multidimensional finite-difference diffusion-theory neutronics program called VENTURE. The iterative procedure is basically that of CITATION²¹ but allows solution of much larger problems with less computer memory by increasing the amount of data stored on external devices.

Sponsor: Reactor Division

18. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 87.

19. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 29.

20. M. J. Bell, "ORIGEN – the ORNL Isotope Generation and Depletion Code, to be published.

21. T. B. Fowler, D. R. Vondy, and G. W. Cunningham, *Nuclear Reactor Core Analysis Code: CITATION*, ORNL-TM-2496, rev. 2 (July 1971), suppl. 3 (July 1972).

A COMPUTER PROGRAM FOR OUT-OF-PLANE BENDING OF NOZZLE-TO-CYLINDER ATTACHMENT

S. G. Bozeman R. E. Funderlic

A computer program, in the developmental stage, has been written to determine the stresses in the region of the intersection of a cylinder-to-cylinder geometry. This geometry models the nozzle-to-shell attachment commonly used in pressure vessels. The arrangement consists of one cylinder intersecting another at right angles so that the center lines of each intersect and the ratio of the radii is less than $\frac{1}{3}$. A bending moment is applied to the nozzle so that it is deflected out of the longitudinal plane of the geometry. Eight compatibility equations which are functions of angle were given to describe the conditions at the intersection. In practice, it is necessary to use the compatibility equations at a very large number of angles in order to determine the coefficients of the series solutions of the two cylinders. This leads to very large least-squares problems, for example, 12,000 rows by 72 columns. The programs GLSQ and HSEBLK, described elsewhere in this report, have been used for the least-squares solution. Programs by D. A. Arnurius and V. A. Singletary that calculate Bessel functions along the 45° angle in the complex plane have also been implemented in the code.

Sponsor: Reactor Division

A. Edmundson²²

CREEP-PLAST: A TWO-DIMENSIONAL FINITE-ELEMENT PROGRAM FOR ELASTIC-PLASTIC-CREEP ANALYSIS

J. S. Crowell J. A. Clinard⁹ P. G. Fowler

This program was developed for ORNL and the LMFBR industry by General Electric for analyzing metal structures operating at high temperatures.^{23,24} The program was made operational on the IBM 360. Extensive testing of the program is being carried out, and many corrections and modifications have been made. Distribution of the program to interested FFTF and LMFBR component vendors has begun. The program is being released with the understanding that changes and modifications will be coordinated with ORNL. This will allow everyone to benefit from any corrections or extensions made to the program. An ORNL user's manual²⁴ for the program is being prepared to update and extend the information contained in the original CREEP-PLAST user's manual.²⁵

Sponsor: Reactor Division

J. M. Corum

PLOTting PROGRAMS FOR CREEP-PLAST

P. G. Fowler J. S. Crowell

Two programs have been written to aid users in analyzing the voluminous results output from the elastic-plastic-creep finite-element program CREEP-PLAST.^{23,25} The first of these programs gives

22. Mechanical Engineering Department, University of Tennessee, consultant to Reactor Division.

23. Y. R. Rashid, *Part I, Theory Report for CREEP-PLAST Computer Program*, AEC research and development report GEAP-10546 (January 1972).

24. J. A. Clinard and J. S. Crowell, *ORNL User's Manual for CREEP-PLAST Computer Program*, ORNL-TM-4062, in preparation.

25. Y. R. Rashid, *Part II, User's Manual for CREEP-PLAST Computer Program*, AEC research and development report GEAP-13262 (March 1972).

immediate plots of displacements, stresses, and strains for user-selected nodes and load histories. The second program will plot detailed information such as stress contours, nodal displacements, and stress trajectories at user-specified times of interest in the analysis. These latter plots require minimal polishing to be of report quality.

Sponsor: Reactor Division

J. M. Corum

FINITE-ELEMENT ANALYSIS OF B16.9 TEE JOINTS

J. S. Crowell P. G. Fowler

Three programs that perform stress analysis, transient heat-flow analysis, or thermal stress analysis of B16.9 piping tees have been implemented on the IBM 360. The stress-analysis programs use linear elasticity theory and include geometry-generating facilities to simplify the input. The programs use an eight-node modified isoparametric finite element.

Sponsor: Reactor Division

S. E. Moore

FINITE-ELEMENT PERSPECTIVE PLOTTING

P. G. Fowler J. S. Crowell

A program has been written that produces perspective plots of three-dimensional shell surfaces and of temperature and stress contours on the surfaces. The program has been used to display experimental and finite-element results for tee joints.

Sponsor: Reactor Division

S. E. Moore

EPACA: AN ELASTIC-PLASTIC-CREEP FINITE-ELEMENT ANALYSIS PROGRAM FOR THREE-DIMENSIONAL THICK-SHELL STRUCTURES

S. K. Iskander O. W. Russ J. S. Crowell P. G. Fowler

This program was developed for ORNL and the LMFBR industry by Franklin Institute Research Laboratories.²⁶ The program has been made operational on the IBM 360. There are at present in the program eight different types of finite elements that may be chosen for structural analysis: four types of flat elements and four types of curved isoparametric elements. With these elements, elastic, plastic, creep, buckling, and dynamic analyses may be performed. Mesh generation capabilities reduce the input data requirement, with special generators for tee- and elbow-type structures. This program's different capabilities are now being tested, and the output is being compared with available experimental and theoretical results.

In the near future, a thermal analysis capability is planned for this program.

Sponsor: Reactor Division

J. M. Corum

AIR POLLUTION STUDY OF FUEL COMBUSTION JOINT SOURCES

C. H. Gard

Using data provided by the Office of Air Programs for the cities of New York, Buffalo, and Philadelphia, a computer program has been written to produce tables of the following variables: the annual

26. Z. Zudans et al., *Theory and Users' Manual for EPACA*, F-C3038, Franklin Institute Research Laboratories (June 30, 1972).

fuel consumption (coal in thousands of tons, residual oil in millions of gallons, and distilled oil in millions of gallons), heat input (the rated heat capacity, the operating average, and the yearly average in millions of Btu per hour), and the emissions (SO_2 and dust in tons per day). Sums are given for each SIC (standard industrial classification) within each 10-km-square grid.

Sponsor: Reactor Division

J. K. Delson

THERMAL ANALYSIS OF THE HIGH-TEMPERATURE GAS-COOLED REACTOR

I. I. Siman-Tov W. D. Turner

The transient temperatures which will develop in a high-temperature gas-cooled reactor (HTGR) in the event of a partial or total loss of coolant flow are needed in the safety evaluation of the HTGR. We are developing models and modifying some of our existing heat-transfer codes to use in this analysis.

Sponsor: Reactor Division

J. P. Sanders

STUDY OF WATERTUBE OR HEAT-RECOVERY BOILERS

C. H. Gard

For the nongenerating units, a pressure (psig)—capacity (thousands of pounds per hour) report was prepared for each SIC (standard industrial classification) for the years 1965–1971. This report was also prepared for each state. Steam capacity was compared with electrical capacity for the generating units. A special study was made of the units with a capacity greater than 250,000 lb/hr. Data were provided by the American Boiler Manufacturers Association.

Sponsor: Reactor Division

J. K. Delson

GAS BEHAVIOR IN MOLTEN-SALT REACTORS

T. C. Tucker L. W. Gilley H. A. McLain⁹

The program to calculate Xe, I, Te, and Sb concentrations in the fuel-salt loop of a molten-salt reactor has been completed.²⁷ A program to calculate tritium concentrations in the fuel-salt loop and coolant-salt loop is currently being written.²⁷

Sponsor: Reactor Division

H. A. McLain

MOLTEN-SALT REACTOR INFORMATION SYSTEM

R. B. Hofstra

We completed the work reported last year²⁸ in regard to preparing the file of references for the Molten-Salt Reactor Information System. This was used to prepare a new document.²⁹ Abstracts are given

27. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 80.

28. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 92.

29. D. W. Cardwell and P. N. Haubenreich, *Indexed Abstracts of Selected References on Molten-Salt Reactor Technology*, ORNL-TM-3595 (Dec. 3, 1971).

for 321 reports and articles which provide an introduction to MSR technology and describe major developments since 1960. Three indexes are provided: by key word, by author, and by subject category. Revised hard-copy bibliographic reports will be forthcoming.

Sponsor: Reactor Division

D. W. Cardwell

CONVERSION OF OTHER DATA BASES TO ADSEP FORMAT

F. D. Hammerling

Two bibliographic data bases. NDIC (Nuclear Desalination Information Center) and NDMA (Nuclear Desalination Materials Abstracts), were converted from the format used at the CTC Information Systems Department to the ADSEP input format.³⁰ This required writing a PL/I program to read the 7090 binary tapes; perform the necessary editing, conversions, and translations; and write the resulting data in the ADSEP input format.

Sponsor: Nuclear Desalination Information Center

K. O. Johnsson

30. A. A. Brooks, *ADSEP - an Automated Data Set Editing Program*, CTC-34 (May 12, 1970).

REACTOR CHEMISTRY DIVISION

ACIDITY MEASUREMENTS AT ELEVATED TEMPERATURES AND THE DISSOCIATION OF WATER

R. E. Funderlic

The self-dissociation of water was studied in potassium chloride media over the temperature range 0 to 300°. The experimental and theoretical basis of this work was carried out by the same investigators who reported related work.¹ This analysis led to a nonlinear least-squares problem with three different functional forms, with some of the unknown least-squares parameters in common. Numerical derivatives were used for one of the functional forms, the least-squares calculation, and for the calculation of thermodynamic quantities for the dissociation reaction.

Sponsor: Reactor Chemistry Division

R. E. Mesmer

1. R. E. Mesmer, C. F. Baes Jr., and F. H. Sweeton, "Acidity Measurements at Elevated Temperatures. IV. Apparent Dissociation Product of Water in 1 *m* Potassium Chloride up to 292°," *J. Phys. Chem.* 74, 1537-42 (1970).

SOLID STATE DIVISION

A COMPLETE SYSTEM FOR CONTROLLING AN AUTOCORRELATION NEUTRON TIME-OF-FLIGHT SPECTROMETER

S. H. Merriman

Two new input-output devices have been added to the DEC PDP-15/30 which controls the time-of-flight spectrometer at the HFIR.¹ A new RS09 DEC disk has replaced DEC tape as the system

1. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 88.

device. All system and user programs now reside on the disk, and the DEC tape units are used only for data storage and backup. A COMLOT plotter was also added to the configuration, and the necessary software was written.

A preliminary study was made to determine the feasibility of adopting a new real-time executive system, RSX-15, to replace the Advanced Monitor V5A currently in use.

Sponsor: Solid State Division

H. A. Mook

THERMONUCLEAR DIVISION

LARGE-SCALE PLASMA SIMULATION

H. R. Hicks H. K. Meier¹

A $2\frac{1}{2}$ -dimensional detailed simulation of a confined plasma is a large-scale problem on present computers, even when the simulated entities of the plasma are really aggregates of many particles so that the number of entities is of the order of 10^6 . As a computational problem, the storage requirements are large (several 2314 disk packs), and the run time is essentially open-ended.

The strategy is to retain in core the arrays containing information on electric and magnetic fields at mesh points. Quantities associated with the particles are paged from the disk, using triple buffering. Maximum channel separation is attempted in order to get the greatest transfer rate.

Advantage is taken of some functional characteristics of the 360/91. The innermost loops are written in assembly language. Wherever possible, loads and stores are interleaved with condition setting and conditional branches, loop mode is entered as often as possible, simultaneous access of different storage modules is performed, and other techniques are used to gain speed.

Sponsor: Thermonuclear Division

H. K. Meier

MICROINSTABILITIES IN INHOMOGENEOUS PLASMAS

H. R. Hicks C. O. Beasley¹

A program has been written for the determination of unstable electrostatic oscillations in a model mirror-confined plasma with a Gaussian density variation along the magnetic field. A formal solution to the collisionless Boltzmann equation is obtained for a plasma confined in a parabolic well. Using this solution, one may solve Poisson's equations to obtain eigenfunctions (perturbed potentials) and eigenvalues (densities) of the system for a given complex frequency. The program now includes Landau damping, drift cone effects and magnetic field variations with thermal effects.

Sponsor: Thermonuclear Division

C. O. Beasley

SYNCHROTRON RADIATION TRANSPORT IN FUSION REACTORS

R. H. Fowler J. F. Clarke¹

A one-dimensional synchrotron radiation model has been developed in which the radiation is transported by a diffusion process in regions with a large self-absorption coefficient α_ω , while that in

1. Thermonuclear Division.

regions of low self-absorption is lost by free radiation. The power/volume lost by synchrotron radiation can be written as

$$\frac{\partial P}{\partial V} = \frac{1}{r} \frac{\partial}{\partial r} r D_R \frac{\partial T_e}{\partial r} - \dot{n}_R T_e,$$

where D_R is a modified Rosseland diffusion coefficient and $\dot{n}_R$ represents an equivalent density of photons per second lost by free radiation.

An explicit scheme is used to solve the eight partial differential equations — six density equations plus two power-balance equations for the ions and electrons.

Sponsor: Thermonuclear Division

J. F. Clarke

NEOCLASSICAL FUSION REACTOR STUDIES

R. H. Fowler J. F. Clarke¹ J. F. Etzweiler²

A numerical model has been used to calculate the dynamic behavior of a plasma following ignition. The fusion energy production is balanced against radiation losses. It is assumed that the reactor operates in a regime in which heat conductivity and particle diffusion can be neglected compared with radiation. The model consists of six density equations, corresponding to electrons, hydrogen, deuterium, tritium, ³He, and ⁴He, and two power-balance equations for the electrons and ions. The model includes neutral injection heating and fueling, synchrotron and bremsstrahlung radiation losses, and heat transfer to ions by classical Coulomb collisions.

Without injection, we find that β limitations at practical magnetic field levels limit the free burning time to less than 200 sec. However, the judicious use of neutral injection allows burn times of up to 700 sec and a beneficial power flattening with only a slight penalty in recirculating power.

Sponsor: Thermonuclear Division

J. F. Clarke

MHD EQUILIBRIA AND MAGNETIC FIELD COMPUTATIONS

R. H. Fowler R. A. Dory¹

An equilibrium code originally developed to study MHD equilibria in Tokamaks has been generalized for several geometries. The code applies an SOR method in cylindrical coordinates (R, ϕ, Z) to solve

$$\frac{R}{\partial R} \frac{\partial}{\partial R} \left(\frac{R^{-1}}{\partial R} \frac{\partial \psi}{\partial R} \right) + \frac{\partial^2 \psi}{\partial Z^2} = -4\pi R^2 \frac{dP}{d\psi} \frac{-F dF}{d\psi}.$$

where F and P are, in general, nonlinear functions of $\psi(R, Z)$; ψ is constant on the boundary. For Tokamak studies, the solution is found in the region $(R - R_0)^2 + Z^2 \leq a^2$. Other geometries which have been considered are ellipses, doublets, triangles, and triangulated ellipses.

2. Summer Participant, University of Wisconsin, Madison.

We have used this code to solve the problem $\text{curl } \mathbf{B} = 4\pi\mathbf{J}$, where $\mathbf{J} = \hat{\phi}J_0$ is specified and the boundary condition is $\hat{n} \cdot \mathbf{B} = 0$. The magnetic field components are given by

$$B_R = \frac{-1}{R} \frac{\partial \psi}{\partial Z}, \quad B_Z = \frac{1}{R} \frac{\partial \psi}{\partial R}.$$

Sponsor: Thermonuclear Division

R. A. Dory

LONG-FIELD EXPERIMENT DESIGN STUDY

C. S. McNeilly

Studies of the magnetic field configuration for the proposed LFX device to optimize plasma confinement are under way. In order to enhance usability, additions and modifications to an existing code which calculates the longitudinal adiabatic invariant have been completed.

Sponsor: Thermonuclear Division

G. R. Haste

BEAM PROBE DESIGN CALCULATIONS

G. S. McNeilly

Heavy-ion beam probe calculations for the ORMAK and EBT devices have been performed. The purpose was to optimize the source-detector geometry and ion energy required to produce desirable detector lines. This work is reported in detail in ORNL-4834.

Sponsor: Thermonuclear Division

C. F. Barnett

CURRENT LOOP CALCULATION

G. S. McNeilly

An explicit expression for the magnetic field due to a current loop has been derived, in terms of complete elliptic integrals. The formula is useful in magnetic field calculations. This work is reported in detail in ORNL-TM-4023.

Sponsor: Thermonuclear Division

G. R. Haste

PROGRAM FOR ASSESSING THE HYDROMAGNETIC STABILITY OF A LOW- β PLASMA CONFINED BY THE MIRROR EFFECT

J. D. Amburgey

Modifications were made to the contour plotting portion of this computer program. The original procedure was to plot contours using a different energy for each contour while holding the flux moment and matrix values constant. The program was modified to plot contours from a matrix with fixed energy and flux moments. In general the plotting package was made more efficient, especially for finer grids, where an interpolation scheme is now present.

Sponsor: Thermonuclear Division

C. E. Parker

A REEVALUATION OF VANADIUM NEUTRON AND GAMMA-RAY PRODUCTION CROSS SECTIONS³

S. K. Penny L. W. Owen

The cross sections for vanadium were reevaluated with the emphasis placed on adding gamma-ray production files. The starting basis was the ENDF/B evaluation material 1017. The newly evaluated cross sections are in the ENDF/B format.

Sponsor: Thermuclear Division

D. Steiner⁴

3. Abstract of ORNL-TM-4007, November 1972.

4. Reactor Division.

INTERDIVISIONAL PROJECTS

COMPUTER-AIDED PREPARATION OF BIBLIOGRAPHIES

F. D. Hammerling	R. Slusher
D. L. Wilson	C. Gard
D. W. Altom	A. F. Joseph

During the past year, several bibliographies were prepared for publication using the computer programs within the ORCHIS system.¹ The programs were used to enter and update the information, to produce a page format suitable for publication, and to produce indices, both simple and permuted. The publications included the following topics: Energy-RANN, Mercury, PCB's, Regional Modeling, Vols. 2 and 3, Environmental Law, Vol. 2, Plutonium, Thermal Effects, Ecological Models, and the International Biological Program Abstract Journal.

Sponsors: Environmental Information Systems Office
ORNL-NSF Environmental Program
Environmental Sciences Division
National Library of Medicine

KWIC AND OTHER INDICES FOR ADSEP DATA SETS

D. L. Wilson

Several modifications were made to the indexing system² which interfaces KWIC³ with the ADSEP⁴ format, to produce a KWIC (key word in context) index on any field or group of fields for photoreduction and publication. Parameters control page size, page format, and page number and title to be printed at the top of each page.

1. A. A. Brooks, ed., *ORCHIS Interim Technical Report - Collected Memos and Cumulative Bibliography*, ORNL-TM-3727 (August 1972).

2. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 17.

3. G. K. Haeuslein and Ann S. Klein *The Oak Ridge National Laboratory KWIC Index*, ORNL-4536 (May 1970).

4. A. A. Brooks, *ADSEP - an Automated Data Set Editing Program*, CTC-34 (May 12, 1970).

Other indices can also be produced on word lists from any two arbitrary fields for photoreduction and publication. The indices are produced in either of two formats: (1) one column of indices per page or (2) two columns of indices per page. Input parameters control the page format, page size, and page number and title to be printed at the top of each page. There are other options available which perform various editing functions on the fields before the index is produced.

Sponsors: Environmental Sciences Division
Environmental Information Systems Office

MODIFICATIONS TO ADSEP AND RELATED PROGRAMS

C. H. Gard

The ADSEP program was modified in order that blanket partial corrections can be made to any field of a data base. It is also possible to have character string input enter as it is with no checking for blanks at the end of a card image, so that words can be split across a card image. Other features and request commands have been implemented to increase the ease of updating a data base.

A program has been written to sort a string correction file or a string add file that has the record numbers before processing the file through ADSEP. It is possible to change the ADSEP record numbers of a data base to correspond to the text of any field which can be converted to integer.

A program has also been written so that a "\$" in a field for string input to ADSEP will be replaced by the text of that field in the previous record.

Sponsors: Environmental Sciences Division
Biology Division

ATOMIC MASS ADJUSTMENT

N. B. Gove A. H. Wapstra⁵ K. Bos⁵

About 4000 nuclear reaction Q values and spectroscopic doublets are combined in a least-squares program to determine best values for the 1800 atomic masses. We reported on this project last year.⁶ This year a table of Q values for heavy-ion reactions is being published.⁷ A new mass adjustment was made this year in order to take account of the high-precision results of the new technique of rf mass spectroscopy. We redesigned the program to use the GETCOR subroutine.⁸ Now a test run requires only 270K of core space instead of the former 600K.

Sponsors: Instituut voor Kernfysisch Onderzoek, Amsterdam
Nuclear Data Project
Mathematics Division

5. Instituut voor Kernfysisch Onderzoek, Amsterdam, Netherlands.

6. *Westh Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 5; A. H. Wapstra and N. B. Gove, "The 1971 Atomic Mass Evaluation," *Nucl. Data Tables* 9, 267-468 (1971); N. B. Gove, A. H. Wapstra, and K. Bos, "Evaluation of Atomic Masses from Experimental Data," *Bull. Amer. Phys. Soc.* 16(12), 1418 (December 1971).

7. N. B. Gove and A. H. Wapstra, "The 1971 Atomic Mass Evaluation. Part V. Nuclear Reaction Q -Values," *Nucl. Data Tables* 11, 128-280 (1972).

8. R. C. Durfee, *FORTRAN Dynamic Storage Allocation*, ORNL-CF-70-8-59.

NUCLEAR MOMENT OF INERTIA

N. B. Gove M. Schmorak⁹

The variable moment of inertia model¹⁰ relates the energies of rotational bands in nuclei to a ground-state moment of inertia I_0 and a restoring force constant C :

$$E(J) = \frac{1}{2}C(I - I_0)^2 + \frac{1}{2}J(J+1)/I.$$

Here, J is the spin of the level and I is the moment of inertia. I may be different for each level and is determined by minimizing the energy: $dE/dI = 0$. This leads to a cubic equation for each level:

$$CI^3 - CI_0I^2 - \frac{1}{2}J(J+1) = 0.$$

For trial values of C and I_0 , this equation is solved for each I at each level. From the I 's are calculated the values of $E(J)$ and then

$$(N-2)\chi^2 = \sum_i (E_{\text{exp}} - E_{\text{calc}})^2/U^2,$$

where N is the number of levels and the U 's are the uncertainties of the level energies. The C and I_0 which minimize χ^2 are determined using G. Westley's subroutine LEARCH.¹¹

We applied this model to ground-state rotational bands in even-even U, Pu, Cm, and Cf, and Cf nuclei.¹²

Sponsors: Physics Division
Mathematics Division

BETA DECAY STATISTICAL RATE FUNCTIONS

N. B. Gove M. J. Martin⁹ S. Raman⁹

We calculated the $\log f$ values for positron decay, negatron decay, and electron capture. Tables were prepared to cover every atomic element number Z from 6 to 95 and energies from 0.01 to 10 MeV.¹³

The statistical rate functions are described in ref. 13.

The confluent hypergeometric functions were calculated with a subroutine due to C. W. Nestor. The bound-state wave functions and exchange factors were computed with the ORNL atomic function code.¹⁴

9. Physics Division.

10. M. A. J. Mariscotti, G. Scharff-Goldhaber, and B. Buck, *Phys. Rev.* 178, 1864 (1969).

11. G. W. Westley and J. A. Watts, CTC-39 (1970).

12. M. Schmorak, C. E. Bemis, Jr., M. J. Zender, N. B. Gove, and P. G. Dittner, "Ground State Rotational Bands in Doubly Even Actinide Nuclei," *Nucl. Phys.* A178, 410 (1972).

13. N. B. Gove and M. J. Martin, Log- f Tables for Beta Decay," *Nucl. Data Tables* 10, 206-317 (1971).

14. S. Raman, N. B. Gove, J. K. Dickens, and T. A. Walkiewicz, "Log ft Values for Second-Forbidden β -Transitions and the Decay of ^{24}Na ," *Phys. Lett.* 40B, 89 (1972).

The $\log f$ values are used in the determination of $\log ft$, where t is the half-life of the transition in question. The $\log ft$ values are related to nuclear matrix elements and are sometimes useful in categorizing transitions as allowed, first-forbidden, first-forbidden unique, etc., which in turn helps in making spin and parity assignments to nuclear levels. A literature survey and several experiments were done in the course of this work.^{14,15}

Sponsors: Physics Division
Mathematics Division

SUPERTOG: A MULTIGROUP NEUTRON CROSS-SECTION GENERATOR

R. Q. Wright

The current version of SUPERTOG,^{16,17} designated as SUPERTOG-III, is in production use at ORNL. This version of SUPERTOG is also available externally and is distributed by the Radiation Shielding Information Center.

The principal changes are:

1. SUPERTOG now includes the effects of Doppler broadening in the resolved resonance region through the ordinary psi and chi functions.
2. A table look-up and interpolation method to evaluate the J function has been added so that Doppler broadening can be accounted for in the unresolved resonance calculation.
3. A new subroutine, OUT6, which prints and punches all the 1-D cross sections generated by SUPERTOG has been added.
4. Subroutine GOUT has been modified to allow making GAM-II update data for hydrogen.
5. An additional input card is now required in subroutine SNOUT to read in σ_A , $\nu\sigma_F$, σ_t , and $\sigma_{g \rightarrow g}$ for the thermal group.

SUPERTOG-III has been used to process all of the ENDF/B-III materials and most of the DNA library.

Sponsors: Neutron Physics Division
Reactor Division

MAINTENANCE OF ENDF/B AND DNA EVALUATED NEUTRON CROSS-SECTION DATA AND RELATED COMPUTER PROGRAMS ON THE NUCLIB DISK PACK

R. Q. Wright

NUCLIB is a permanently mounted 2314 disk pack which is shared by both the 75 and 91 computers. Three neutron cross-section data sets in ENDF/B format¹⁸ are presently maintained on NUCLIB:

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15. N. B. Gove and S. Raman, "Log $f_1 t$ Values for First-Forbidden Unique β -Transitions and the Decay of ^{90m}Y ," *Bull. Amer. Phys. Soc.* 17(10), 905 (October 1972).
 16. R. Q. Wright, N. M. Greene, J. L. Lucius, and C. W. Craven, Jr., *SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B*, ORNL-TM-2679 (September 1969).
 17. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 92.
 18. M. K. Drake, ed., *Data Formats and Procedures for the ENDF Neutron Cross Section Library*, NBL-50274 (T-601) (ENDF 102, vol. 1) (October 1970).

1. LMP.ENDFB2
2. LMP.ENDFB3
3. RQW.DNA.DATA

LMP.ENDFB2 contains 10 materials in ENDF/B Version II format which are not available in the ENDF/B Version III library.

LMP.ENDFB3 contains 73 materials in ENDF/B Version III format which have been released as Category I ENDF/B by the National Neutron Cross Section Center, Brookhaven National Laboratory.

RQW.DNA.DATA contains the 13 materials in the current version of the Defense Nuclear Agency Working Cross Section Library, which is distributed by the Radiation Shielding Information Center.

A number of ENDF/B processing codes are also available on the NUCLIB disk to read and/or write data in the ENDF/B format. These include checking codes, editing and plotting codes, and multigroup cross-section processing codes.

Sponsors: Neutron Physics Division
Reactor Division

DEXTR DATA REDUCTION PROGRAMS

O. W. Russ, Jr.

Programs for UN-4, -5, and -6 and MINT-1 fuel capsule experiments in the ORR were completed to print, punch, and Calcomp plot the data over selected operating time periods.

Program modifications for HTGR HRB-3 fuel capsule experiments in the HFIR were completed, and additional programming was begun for HRB-4 and -5 fuel capsules for similar printing and Calcomp plotting of operating cycle data.

Programming for the LMFBR-FFM test bundle 2 at 9201-3, Y-12, was completed to include the larger number of inputs for optional printing and punching of daily operating data. A program was completed for similarly handling test bundle 1B data, and additional programming will be required for a new test bundle 3A, to be installed in the next test sequence. Programming was begun for the thermal stress tee test at 9204-1, Y-12, to optionally print out and punch the temperatures and strain units at selected angular locations along the branch and run sections of the tee unit. A program for the weldment creep-rupture test, also at 9204-1, was completed for optional daily printing and punching of temperatures and pressures of the four specimen test furnaces.

Sponsors: Reactor Division

Metals and Ceramics Division
Instrumentation and Controls Division

S. E. Bolt	W. G. Dodge
P. A. Gnadt	W. J. McAfee
B. H. Montgomery	L. F. Parsly
R. L. Senn	A. M. Smith
K. R. Thoms	J. L. Wantland
B. Feischer	
R. M. Burnett	R. L. Durall
R. F. Hyland	

SMOOTHING PION DOSE DATA

V. E. Anderson

A method for smoothing pion dose data was developed. This will be used for making isodose curves which will serve as an aid to the radiologist in cancer therapy. Mesons produced at Los Alamos Scientific Laboratory will be used for irradiating the malignant tumors, and the isodose curves will indicate how the pion beam must be oriented relative to various parts of the tumor for maximum effect.

Sponsors: Health Physics Division
Neutron Physics Division

LINEAR LEAST SQUARES

S. G. Bozeman R. E. Funderlic M. T. Heath
B. W. Rust M. H. Noojin¹⁹

A number of new linear least-squares routines have been written and new features incorporated into existing codes. Perhaps the most commonly used linear least-squares program at ORNL is ALSQ.²⁰ This code, however, has no provision for returning important statistical information about the quality of the fit. Therefore, a new version, called LSQCOV, has been written which returns the covariance matrix of the fitted parameters, thus allowing the user to determine standard deviations, cross correlations, etc. Another disadvantage of ALSQ is that it requires the entire least-squares matrix to be available in machine memory. An algorithm is being developed which will carry out the Householder reduction on successive blocks of the least-squares matrix, greatly reducing core requirements. Another solution to this problem is Givens' method, which has been implemented in a time-sharing program for the PDP-10 which reads in the least-squares matrix one row at a time. This routine is also available as a callable FORTRAN subroutine for the IBM 360.

Sponsors: Mathematics Division
Reactor Division

GRAIN-BOUNDARY DIFFUSION THEORY

G. Young²¹ R. E. Funderlic

The theory of diffusion in grain boundaries was initiated by Fisher,²² using an idealized model in which a poorly diffusing half-space (the crystal) is bisected by a thin well-diffusing slab (the grain boundary), with a fixed concentration of diffusing material suddenly established at the free surface. He found that the depth to which a given concentration has penetrated in the grain boundary apparently increases as the fourth root of the elapsed time, rather than the familiar square-root dependence in a uniform half-space.

19. Formerly employed by Union Carbide Nuclear Division; now with IBM.

20. G. W. Westley and J. A. Watts, eds., *Computing Technology Center Numerical Analysis Library*, CTC-39 (October 1970).

21. Director's Division.

22. J. C. Fisher, "Calculations of Diffusion Penetration Curves for Surface and Grain Boundary Diffusion" *J. Appl. Phys.* 22, 74 (1951).

In his analysis Fisher made several simplifying assumptions. Whipple²³ later gave a complicated exact solution for the thin slab problem; approximations are customarily made in its numerical evaluation.^{24,25}

Current work has generalized Whipple's solution to include anisotropic diffusion in the crystal, plus other changes. It now contains both the original Whipple result and an improved Fisher result as special cases, and displays explicitly the effect of the different assumptions. A double-precision version of a Clenshaw-Curtis quadrature²⁶ routine was developed and used to evaluate the integrals involved in the solution. This automatic quadrature routine proved to be extremely effective and superior to the adaptive Simpson routines on our library system.²⁰

Sponsors: Director's Division
Mathematics Division

PANS: A PROGRAM TO DETERMINE THE POPULATION DISTRIBUTION BY ANNULI AND SECTORS ABOUT A SET OF ARBITRARY POINTS

P. R. Coleman A. A. Brooks

A program to tally the population by sectors and annuli located about a set of arbitrary points on the earth has been completed and documented.^{27,28}

The program has been used to study several siting problems, especially those of reactors.

Sponsors: Mathematics Division
Health Physics Division

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- 23. R. T. P. Whipple, "Concentration Contours in Grain Boundary Diffusion," *Phil. Mag.* **45**, 1225 (1954).
 - 24. V. E. Wood, A. E. Austin, and F. J. Milford, "Theoretical Solutions of Grain-Boundary Diffusion Problem Approximations and Interpretation of Experiments," *J. Appl. Phys.* **33**, 3574 (1962).
 - 25. A. D. LeClaire, "The Analysis of Grain-Boundary Diffusion Measurements," *Brit. J. Appl. Phys.* **14**, 351 (1963).
 - 26. W. Morven Gentleman, "Clenshaw-Curtis Quadrature," *Commun. ACM* **15**, 353 (1972).
 - 27. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 90.
 - 28. P. R. Coleman and A. A. Brooks, *PANS: A Program to Tally Population by Annuli and Sectors*, ORNL-TM-3923 (October 1972).

INTERNATIONAL NUCLEAR COMPANY

SHIPPING CONTAINER EVALUATION FOR THE INTERNATIONAL NUCLEAR COMPANY

N. F. Cross J. R. Knight

KENO¹ and ANISN² were used to evaluate the FL-10-1 shipping container used for shipping uranyl nitrate and plutonium nitrate. The uranyl nitrate was found to be the most reactive, so it was used in the ANISN study to determine the change in k -infinity vs boron content in the phenolic foam. A similar ANISN study was made of the water density in the phenolic foam vs the k -infinity. A KENO calculation was made using the values of boron and water from the ANISN studies, and the container was found to be safe. Several more KENO calculations were then done to determine the effect of plutonium precipitation from the plutonium nitrate fuel. No increase in reactivity was observed.

Sponsor: International Nuclear Company

W. R. Housholder

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- 1. G. E. Whitesides and N. F. Cross, *KENO - Multigroup Monte Carlo Criticality Program*, CTC-5 (September 1969).
 - 2. W. W. Engle, Jr., *A Users' Manual for ANISN*, K-1693 (Mar. 30, 1967).

NATIONAL LEAD INDUSTRIES

SHIELDING CHARACTERISTICS OF THE PWR AND BWR FUEL ELEMENT SHIPPING CASKS

J. R. Knight G. E. Whitesides L. B. Shappert¹ H. C. Claiborne¹

The DOT discrete-ordinates transport code² was used to determine the effectiveness of the National Lead Industries design of a cask for shipment of spent BWR and PWR fuel elements. Both neutron and gamma-ray dose rates were determined at various points around the cask. It was found that the proper distribution of the space mesh intervals was important for obtaining useful results.

Problem areas appear to be near the ends and rims of the cask. The highest dose rates from both neutrons and gamma rays were observed in these regions.

Sponsor: National Lead Industries

L. B. Shappert¹

1. Chemical Technology Division.

2. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stephens, *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding*, CTC-INF-952 (1969).

NATIONAL LIBRARY OF MEDICINE

CHEMICAL NAME MATCH

H. J. Hamilton D. W. Altom¹
 C. A. Giles K. L. Kannan
 A. H. Culkowski A. H. Tindell
 A. F. Joseph

During calendar year 1972 the implementation and modification of the first phase of the CAS Name-Match System was completed. The major goal of this project was the development of an efficient system (in the ORNL environment) for the retrieval of chemical-structure-related information. The streamlining process was accomplished by both modifications to existing programs and the development of new ones. The major revision was the elimination of all processes in the system which are nonessential in a retrieval-only system. Improvements were made by the incorporation of several new and desirable features. These additions included new options for user-specified data content and format of retrieval results, more error-checking and diagnostic capabilities, and new routine techniques for information flow. The most significant enhancement to the system was the development of a new program, written in PL/I, which provides a wide variety of output formats and data content of output units.

Sponsor: National Library of Medicine

CONVERSION OF ADSEP DATA BASES TO OTHER FORMATS

F. D. Hammerling

A PL/I program was written to convert ADSEP data bases² to any format desired by the user. The fields to be processed and some control parameters are input to the program. The program requires that the

1. Now with Technical Information Center, USAEC.

2. A. A. Brooks, *ADSEP - an Automated Data Set Editing Program*, CTC-34 (May 12, 1970).

user supply a processing procedure which will perform the necessary initialization, process each field, and output the resulting data in the desired format. Two data bases have been converted using the program:

1. The CTCP (Clinical Toxicology of Commercial Products) file was converted to the Wylbur format for the University of Rochester.
2. The Hayes file on pesticides received from EPA was converted to the STIMS format for the National Library of Medicine.

Sponsor: National Library of Medicine

NATIONAL SCIENCE FOUNDATION

SWEDISH WATERSHED MODEL

D. E. Fields I. J. Lucas

A FORTRAN listing of the Stanford watershed model¹ was obtained from the Royal Institute of Technology, Stockholm, Sweden. A deck was punched from this listing, errors were corrected, missing subroutines and initialization commands were inserted, and a sample data deck was generated. Test runs have been made, which were apparently successful, and revision of the Swedish plot routines allowing use of our local Calcomp plotter is near completion. After checking this code for numerical accuracy by comparison of our results with output which we have requested from the Swedish group, we hope to use it in our Toxic Metals in the Environment (TME) modeling and to make it available to others.

Sponsor: National Science Foundation

R. Rabin

HYDROLOGICAL TRANSPORT MODEL

A. A. Brooks J. K. Munro
M. R. Patterson R. D. Ellison

The Stanford watershed model¹ evolved by Crawford and Linsley was modified by Dale D. Huff² and collaborators at the University of Wisconsin to include the water transport of such materials as radioactive elements. We have proposed to use Huff's code as the basis of a comprehensive transport code for toxic materials.

Huff's code was written in FORTRAN V to run on the Univac 1108 using drum storage. This type of FORTRAN has many incompatibilities with FORTRAN IV, the similar language accepted by the IBM 360 computers available at ORNL. A translation to FORTRAN IV of Huff's code has begun. Many of the original incompatibilities, including such things as different word lengths for literals, substitution of disk storage for drum storage, and character string manipulation, have been resolved.

The ORNL version of this code presently executes three of the four major links of the program; however, the detailed output does not yet match that of the Wisconsin 1108. The ORNL program is under intensive study, and the debugging process is expected to be completed near the end of the year.

Sponsor: National Science Foundation

R. Rabin

1. N. H. Crawford and R. K. Linsley, *Digital Simulation in Hydrology*, Technical Report No. 39, Department of Civil Engineering, Stanford University (1966).

2. D. D. Huff and E. H. Dettman, *Section V, Lake Winona Ecosystem Study Annual Report, 1969-1970*, University of Wisconsin.

ORGDP

SAFEGUARD GAMMA TRANSPORT CODE

T. J. Hoffman L. M. Petrie

As part of the Safeguard Program, a computer code has been written to calculate the uncollided response of a uniformly distributed radioactive source in a pipe. The detector, assumed to be a point detector, can be located an arbitrary radial distance outside the pipe. The detector response function can vary with the angle between the incoming particle direction and a vector normal to the pipe.

In order to obtain the detector response for many pipe configurations with a given response function, a Gaussian quadrature option is available. With this option, the angular flux is only calculated for the directions required by the quadrature. For response functions with a Gaussian shape, this option will yield a very accurate integral response with few flux calculations. The Gaussian quadrature parameters can be input or calculated by the program. A trapezoidal integration option is also included.

Sponsor: ORGDP

Jack C. Bailey

PORTSMOUTH GASEOUS DIFFUSION PLANT

PORTSMOUTH CRITICALITY SAFETY ANALYSIS

N. F. Cross R. J. Hinton

A variety of safety calculations were performed using the KENO code.¹ Most of the work was concerned with the following systems:

1. Study the effects of both water and concrete reflection on 8- and 12-in.-diam UF_6 cylinders arranged in various arrays.
2. Determine the criticality safety considerations involved in the cleaning of 8- and 12-in.-diam UF_6 containers.
3. Investigate the effect of enrichment on various storage arrays.
4. Evaluate 48-in. UF_6 cylinders at 4.5% and 5.0% enrichment both dry and with coolant at the ERP Station and in the tails area.
5. Evaluate arrays of 30-in. cylinders of UF_6 at 5% enrichment.
6. Investigate the criticality safety aspects of a UF_6 gas cooler.

Sponsor: Portsmouth Gaseous Diffusion Plant

J. L. Feuerbacher

1. G. E. Whitesides and N. F. Cross, *KENO - Multigroup Monte Carlo Criticality Program*, CTC-5 (September 1969).

TENNESSEE VALLEY AUTHORITY

MTX: A PROGRAM TO CALCULATE MULTIGROUP NEUTRON CROSS SECTIONS FOR THE MUFT AND THERMOS CODES

J. L. Lucius N. M. Greene
R. Q. Wright

The XLUX code,¹ described in last year's annual report, has been renamed MTX. MTX prepares multigroup neutron cross sections for the MUFT² and THERMOS³ codes by processing ENDF/B data.⁴ MTX was developed by revising XLACS⁵ resonance, inelastic scattering, elastic scattering, and thermal treatments. XSDRN⁶ cross-section library updating procedures were deleted and replaced by similar procedures for the MUFT and THERMOS codes.

Major effort in 1972 has been in the area of validation, routine maintenance, improving treatments, documentation, and consultation with Tennessee Valley Authority staff members.

Sponsor: Nuclear Engineering Branch, Tennessee Valley Authority, Chattanooga, Tennessee

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1. *Math. Div. Annu. Progr. Rep. Dec. 13, 1971*, ORNL-4761, p. 96.
 2. H. Bohl, Jr., E. M. Gelbard, and G. M. Ryan, *MUFT-4 Fast Neutron Spectrum Code for the IBM-704*, WAPD-TM-72 (1957).
 3. H. C. Honeck, *THERMOS - a Thermalization Transport Theory Code for Reactor Lattice Calculations*, BNL-5826 (1961).
 4. M. K. Drake, ed., *Data Formats and Procedures for the ENDF Neutron Cross Section Library*, BNL-50274 (October 1970).
 5. N. M. Greene, J. L. Lucius, J. E. White, R. Q. Wright, C. W. Craven, Jr., and M. L. Tobias, *XLACS: A Program to Produce Weighted Multigroup Neutron Cross Sections from ENDF/B*, ORNL-TM-3646 (AMPX-2) (April 1972).
 6. N. M. Greene and C. W. Craven, Jr., *XSDRN: A Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (July 1969).

U. S. ARMY MATERIAL COMMAND

CONVERSION OF MODCRAFT PROGRAMS

O. W. Russ

Modification, debugging, and testing of the U.S. Veteran's Administration's MODCRAFT Calcomp plotting programs for hospital floor plan layouts was completed to convert them for use by the U.S. Army Material Command as design tools for aircraft maintenance depot floor plan layouts.

Sponsor: Maintenance Support Center, U.S. Army Material Command

F. B. Hubler

U.S. ARMY MISSILE COMMAND

SPECTROSCOPIC FACTORS FROM THE REACTIONS $^{12}\text{C}(d,n)^{13}\text{N}$ AND $^{12}\text{C}(d,p)^{13}\text{C}$ USING THE WBP MODEL

G. W. Morrison G. W. Westley

Spectroscopic factors have been extracted from weakly bound projectile model calculations for the reactions $^{12}\text{C}(d,p)^{13}\text{C}$ (ground state and 3.09-MeV state) and $^{12}\text{C}(d,n)^{13}\text{N}$ (ground state). The values for S

were obtained by minimizing the quantity

$$X^2 = \sum_i (S\sigma_T - \sigma_E)_i / (\sigma_E^2)_i$$

where σ_T is the theoretical cross section and σ_E is the experimental cross section. The summation extends over all the experimental points.

The linearly constrained nonlinear programming procedure of Westley¹ was used to minimize X^2 over five variables which included the radius parameter, r , of the captured neutron and the diffuseness, a , of the outgoing particle

Sponsor: Physical Sciences Laboratory, U.S. Army Missile Command, Huntsville, Alabama

1. G. W. Westley, *A Linearly Constrained Nonlinear Programming Algorithm*, ORNL-4644 (January 1971).

U.S. ATOMIC ENERGY COMMISSION

MODIFICATIONS TO THE HEATING HEAT TRANSFER PROGRAMS

I. I. Siman-Tov W. D. Turner

HEATING4, the latest version in the family of HEATING heat transfer codes, is identical with HEATING3¹ except that it has change of phase capabilities. During the past year we have modified HEATING4 to allow the following:

1. The input parameters involving forced convective, radiative, and natural convective boundary conditions and the specified heat flux across a boundary may be a function of position, temperature, and time. Normally, these parameters are calculated by products of tabular and analytical functions supplied by the code. However, the user may specify the calculational technique used to evaluate any of the parameters by supplying a subroutine defining the respective quantity.
2. The maximum and minimum temperatures and their locations may be tabulated as a function of time for transient calculations and as a function of iteration number for steady-state problems.
3. The temperatures at user-specified nodes may be tabulated as a function of time or iteration number.

Additional input/output improvements are currently being programmed to make the code more informative and easier to use.

Sponsor: Directorate for Materials Licensing, USAEC

R. H. Odegarden

THE ADDITION OF TEMPERATURE MAP PRINTOUTS TO THE HEAT TRANSFER CODE HEATING4

R. C. Durfee R. L. Stephenson
W. D. Turner

We have added a new output capability to the heat transfer code HEATING4 (the latest version of HEATING3).¹ This capability allows temperature distributions to be printed in a maplike framework, as in Fig. 14, rather than in tabular form. This allows the user to quickly and easily see what his temperatures are

1. W. D. Turner and M. Siman-Tov, *HEATING3 - an IBM 360 Heat Conduction Program*, ORNL-TM-3208 (February 1971).

		NODAL TEMPERATURES AFTER 155 TIME STEPS											
REGION	NODE	1	2	3	4	5	6	7	8	9	10	11	12
1	1	201.46	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00
	2	201.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00
	3	201.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00
	4	201.01	20.01	20.01	20.01	20.01	20.01	20.01	20.01	20.01	20.00	20.00	20.00
	5	201.01	20.01	20.01	20.01	20.01	20.01	20.01	20.01	20.01	20.01	20.00	20.00
2	6	201.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.01	20.00	20.00
	7	201.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.01	20.00	20.00
	8	201.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.01	20.00	20.00
	9	201.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.01	20.00	20.00
	10	201.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.02	20.01	20.00	20.00
3	11	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	12	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	13	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	14	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	15	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
4	16	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	17	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	18	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	19	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	20	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
5	21	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	22	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	23	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	24	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
	25	201.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.03	20.02	20.01	20.00
FIRST =		0.00	1.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	11.00
		12.00	13.00	14.00	15.00	16.00	17.00	18.00	19.00	20.00	21.00	22.00	23.00

Fig. 14. A cylindrical shipping cask with an internal heat source.

EVALUATION OF THE NEUTRON AND GAMMA-RAY SHIELDING OF THE IF-300 SHIPPING CASK

J. R. Knight G. W. Morrison
R. H. Odegaarden³

The ANISN one-dimensional transport code⁹ was used to evaluate the effectiveness of the neutron and gamma-ray shielding of the IF-300 shipping cask. Coupled neutron-gamma-ray cross sections with 22 neutron and 18 gamma groups were used for the calculations, and some results were also compared with 21 neutron and 18 gamma-ray group cross sections. Neutrons and gamma-ray sources originating from BWR and PWR spent fuel elements were used to obtain fluxes, neutron dose rates, and gamma-ray dose rates at various distances from the edge of the cask. The effect of secondary gamma rays generated by neutron captures was included.

Highest dose rates were encountered under the accident conditions, for which the loss of all water from the cask was assumed. The results from two different sets of neutron and gamma-ray dose factors showed no important effect on the results. Since these calculations are all for one dimension only, no effects of the ends of the cask were included in the results.

Sponsor: Directorate for Materials Licensing, USAEC

R. H. Odegaarden

A COUPLED NEUTRON AND GAMMA-RAY MULTIGROUP CROSS-SECTION LIBRARY FOR USE IN SHIELDING CALCULATIONS

G. W. Morrison E. A. Straker⁵
R. H. Odegaarden³

A state-of-the-art library of coupled neutron and gamma-ray cross sections has been compiled for several elements that are commonly used for shielding calculations. The coupled cross sections have been expanded in a P_3 Legendre expansion and are given in the ANISN format, which permits their usage in the discrete-ordinates codes ANISN⁹ and DOT⁸ as well as the three-dimensional Monte Carlo code MORSE.⁶

Calculations of the neutron and gamma-ray fluence from several shielding problems have been performed using this library.

Sponsor: Directorate for Materials Licensing, USAEC

RECON

A. A. Brooks	A. H. Culkowski	N. B. Gove
G. K. Haeuslein	C. E. Hammons	S. M. Kaplan
W. B. Malthouse	R. E. Plemens	D. G. Taylor

This is the second year of ORNL operation of the RECON system.¹⁰ RECON (remote console) is an information retrieval program for interactive searching of large bibliographic files. Queries are typed in at a keyboard; answers come to a CRT screen. There are now 11 terminals (LBL, TIC, Bettis-Pittsburgh, ORNL-Math, AEC-Washington (?), Westinghouse-Pittsburgh, ORNL-Y-12, ORNL-CRL, LLL, KAPL).

9. W. V. Ziegler, *A User's Manual for ANISN*, K-1693 (March 1967).

10. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 97.

The searchable data base consists of subject and author key words from 4½ years of *Nuclear Science Abstracts*.

The retrieval program obtained from Lockheed has been replaced by a locally written program which runs substantially faster. Several improvements in the ORNL version are programmed and being tested.

We put on special demonstrations of RECON for an Environmental Protection Agency conference in Cincinnati and an American Society for Information Science symposium in Washington.

Sponsor: Office of Information Services, USAEC

LINK BETWEEN ORCHIS AND RECON

W. B. Malthouse

A program, READSEP, was written to convert a file in the ADSEP internal format into a corresponding RECON input file. A small bibliographic data base (Mercury in the Environment) was converted and displayed on RECON. The program is driven by tables created from free-form input, which specify which ADSEP fields are to be included in the RECON linear file and which are to be included in the inverted file. Attempts to use READSEP on nonbibliographic files revealed some limitations. For example, the program does not allow complete generality of field names. Some recoding is being done to remove these limitations.

Sponsor: Office of Information Service, USAEC

UNIVERSITY OF TENNESSEE

REENTRY VEHICLE RADIATION VULNERABILITY STUDIES

T. J. Hoffman

To study the radiation damage to a reentry vehicle under many attack conditions, it is desirable to divide the calculation into two parts. One part of the calculation should involve only the reentry vehicle and the type of damage under investigation. The second part of the calculation should involve only the radiation source and the reentry vehicle environment. This division of the problem is possible through the use of adjoint-forward coupling techniques.^{1,2}

In this work, asymmetric damage to a reentry vehicle was analyzed. The geometric complexity of the problem required Monte Carlo methods. Two adjoint-forward coupling techniques, the surface integral¹ and the adjoint difference,² were applied. A report on the results of this work is being prepared.

Sponsor: University of Tennessee

P. F. Pasqua

1. G. E. Hansen and H. A. Sandmeier, "Neutron Penetration Factors Obtained by Using Adjoint Transport Calculations," *Nucl. Sci. Eng.* 22, 315-20 (1965).

2. T. J. Hoffman, J. C. Robinson, and P. N. Stevens, "The Adjoint Difference Method and Its Application to Deep-Penetration Radiation Transport," *Nucl. Sci. Eng.* 48, 179-88 (1972).

Y-12 PLANT

MODIFICATIONS AND IMPROVEMENTS IN KENO

N. F. Cross L. M. Petrie

Several improvements that have been made in the KENO code¹ to increase its flexibility and usability are described below.

1. The geometry capabilities have been extended through the addition of a "hemicylinder" geometry package. A hemicylinder is a half cylinder (divided lengthwise) whose length lies along the coordinate axis and whose center line lies on that same axis. The origin of the coordinate system must fall along the center line (or the extension of the center line). A hemicylinder exists entirely in the plus or minus X , Y , or Z direction.

2. The option of being able to calculate the matrix k -effective of a system has been added. Other information that is available as a result of this option includes the fission probability matrix by unit, the average unit self-multiplication, cofactor k -effective by position, the box-type k -effective, the fission probability matrix by box type, the source for each box type, and the cofactor k -effective by box type. This information can be useful in determining the relative importance of different positions in an array of fissile units.

3. The option of being able to restart a problem without losing the benefit of the previous run has been added. If a problem is to be restarted at some subsequent time, a key is set to tell how often the data pertinent to restarting must be written out. These data are then saved on some device (disk or tape). At the time of restarting, these data are read in and the problem is continued.

4. A new search type has been added to the KENO search package.² This search type searches for convergence using a small number of histories and, upon achieving that convergence, continues to search using a larger number of histories. This is quite useful when a poor starting guess has been made.

5. KENO has been altered to allow for different albedo materials to be specified on each face of an array. Thus up to six different albedos may be used on a problem – a different one on each face for which albedos have been specified. Previously, the same albedo had to be used on all the faces for which albedos were specified.

6. KENO input has been changed to read data in a free format. A repeat factor was added so that the same number could be repeated several times by just specifying the number of repeats and the number.

7. KENO has been modified so that it can run an adjoint problem by merely setting an input flag.

Sponsors: Critical Experiments Facility, Y-12
Aerojet Nuclear, Idaho Falls, Idaho
Directorate for Materials Licensing, USAEC

J. T. Thomas
W. Morrison
R. H. Odegarden

1. G. E. Whitesides and N. F. Cross, *KENO – a Multigroup Monte Carlo Criticality Program*, CTC-5 (September 1969).
2. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 106.

MONTE CARLO CRITICALITY STUDIES

N. F. Cross R. J. Hinton P. G. McCarty J. T. Thomas³

A variety of problems pertaining to nuclear criticality safety in the storage of fissile materials were explored using the KENO code¹ with the Hansen-Roach cross-section sets.⁴

One set of calculations designed to display the influence of reflected array shape on the criticality of water-reflected arrays is also being used to determine if a set bias exists between the results from full water tracking and albedos. The matrix k -effective option of KENO has been used to investigate the effect of double batching on the array criticality⁵ and to study the coupling between various unit positions within an array.

Sponsor: Critical Experiments Facility, Y-12

J. T. Thomas

CALCULATIONS OF AN ARRAY OF URANIUM (5.0) METAL RODS IN A 5.0% URANYL FLUORIDE SOLUTION USING 123-GROUP ENDF III CROSS SECTIONS

L. M. Petrie R. J. Hinton E. B. Johnson³

Using the CHERIE code⁶ (a multigroup Monte Carlo code with a geometry package which allows specification of fairly intricate configurations), calculations were performed on an array of 121 uranium(5.0) metal rods suspended in a 5.0%-enriched uranyl fluoride solution (296 g of uranium per liter) by a Plexiglas frame and surrounded by the solution on the sides and bottom. The metal rods were approximately 0.3 in. in diameter and were set on a pitch of 0.81 in. Cross sections used were an XSDRN 123-group ENDF (Version III) set.⁷ Although the array was experimentally critical as described, the code gave a value of k_{eff} that was approximately 4% high.

Sponsor: Critical Experiments Facility, Y-12

CALCULATIONS OF REFLECTED AND BARE URANIUM METAL SPHERES USING XSDRN 123-GROUP ENDF VERSION III CROSS SECTIONS

L. M. Petrie R. J. Hinton D. W. Magnuson³

Using the XSDRN code,⁸ critical radius searches and k_{eff} calculations were performed using 123-group cross sections produced by XSDRN from the ENDF/B Version III data.⁷ The geometries considered were bare spheres and spheres reflected by 30 cm of polyethylene. Using these cross sections, k_{eff} calculations were also carried out on the KENO code¹ for rectangular-shaped cores reflected by polyethylene.

Sponsor: Critical Experiments Facility, Y-12

3. Critical Experiments Facility, Y-12.

4. G. E. Hansen and W. H. Roach, *Six and Sixteen Group Cross Sections for Fast and Intermediate Critical Assemblies*, LAMS-2543 (1961).

5. J. T. Thomas, *Double Batching Cell Loadings in Storage Arrays of Fissile Materials*, YDR-36.

6. L. M. Petrie, unpublished Monte Carlo code.

7. H. C. Honeck, *ENDF/B - Specifications for an Evaluated Nuclear Data File for Reactor Applications*, BNL-50066 (ENDF-10?) (May 1966) (revised July 1967).

8. N. M. Greene and C. W. Craven, Jr., *XSDRN: A Discrete Ordinates Spectral Averaging Code*, ORNL-TM-2500 (1969).

STUDIES OF GADOLINIUM STEEL PLATES IMMERSSED IN URANYL FLUORIDE AND URANYL NITRATE SOLUTIONS

L. M. Petrie R. J. Hinton E. B. Johnson³

In order to study the usefulness of thin plates of gadolinium steel as absorbers for use in a forthcoming experiment involving containers of uranium salt solutions, calculations were performed using the KENO Monte Carlo code¹ and the ANISN discrete-ordinates code.⁹ Assuming the plate thickness to be $\frac{1}{8}$ in., calculations were run for 93.2%-enriched uranyl nitrate solutions of 100 and 411 g/liter and for 5.0%-enriched uranyl fluoride solutions of 650 and 905 g/liter. The dimension search options of ANISN and KENO were deployed in an effort to determine the distance between plates which would produce a critical value for k_{eff} for equally spaced plates immersed in cylindrical containers of solution. (Note: this was the case for the KENO calculations; for the ANISN calculations, the plates were treated as equally spaced infinite slabs surrounded by solution.) These "critical spacing" searches were repeated for varying numbers of plates from one to ten plates, and in the case of the KENO calculations, the cylinder diameters ranged from 8 to 15 in. These studies indicated that the gadolinium steel plates were not nearly as good absorbers as had been presumed, since the critical solution height increased quite slowly as the number of plates increased.

Sponsor: Critical Experiments Facility, Y-12

MONTE CARLO STUDY OF THE EFFECT OF DOUBLE HETEROGENEITIES ON CRITICALITY

L. M. Petrie P. G. McCarty E. B. Johnson³

A study of experimentally critical doubly heterogeneous systems¹⁰ is under way, using the KENO multigroup Monte Carlo code.¹ The principal effect studied so far is the effect of the second heterogeneity on the average multigroup cross sections in the resonance energy range of ^{238}U . The doubly heterogeneous systems consist of lattices of 5%-enriched uranium rods in water in which the rods are grouped in clusters separated by various thicknesses of water. The number of clusters, the number of rods per cluster, and the spacing between clusters have all been varied. Reflecting the assemblies with heavy metals instead of water and interspersing steel instead of water between the clusters are also being studied. So far, the study has shown that it is important to account for the different average cross sections of the rods around the edge of a cluster relative to those of the rods in the center.

Sponsor: Critical Experiments Facility, Y-12

E. B. Johnson

MONTE CARLO ANALYSIS OF CRITICAL ASSEMBLY EXPERIMENTS

T. J. Hoffman J. R. Knight

Several experiments performed at the Critical Experiments Facility were analyzed with the multigroup Monte Carlo code MORSE.¹¹ Effects of interest include the effective multiplication constant, fixed-source

9. W. W. Engle, Jr., *A Users' Manual for ANISN, a One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1693, CTC (1967).

10. E. B. Johnson, personal communication.

11. E. A. Straker, P. N. Stevens, D. C. Irving, and V. R. Cain, *The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585 (1970).

multiplication, reactivity, fixed-source importance, generation time, lifetime, and variation of neutron density with time. These calculations were performed with 100-group P_3 cross-section sets.

Sponsor: Critical Experiments Facility, Y-12

J. T. Mihalczko

THE EFFECTS OF STACKED LAYERS OF VARIOUS MATERIALS ON CRITICALITY

J. R. Knight D. W. Magnuson³

The KENO Monte Carlo criticality code¹ was used to determine the effect of various layer arrangements of Plexiglas, polyethylene, steel, and voids on the criticality of uranium-containing arrays. Variations of the thickness and placement of these materials within the arrays were evaluated. Comparisons between the results from exact geometry descriptions and from geometries where several of the layers were homogenized were made for some of the arrays. Direct comparison between calculated and experimental results was made for some of the arrays studied, and the agreement was good in most cases.

Sponsor: Critical Experiments Facility, Y-12

D. W. Magnuson

CALCULATED CONCENTRATIONS FOR CRITICAL MIXTURES OF WATER-MODERATED MIXTURES OF URANIUM AND PLUTONIUM COMPOUNDS

J. R. Knight D. W. Magnuson³

The ANISN transport code⁹ was used to determine critical mixtures of water-moderated uranium and plutonium compounds. The mixtures studied were oxides and nitrates of uranium and plutonium. The effects of variations in the enrichment of the uranium and plutonium compounds and the effects of variations in the fissile element to water ratio were studied. In a few cases, calculations were made for low enrichments below which no critical concentrations of the compounds considered were found. It was noted that the nitrates required higher concentrations for criticality than the oxides.

Sponsor: Critical Experiments Facility, Y-12

D. W. Magnuson

CALCULATION OF ROCKY FLATS PIPE INTERSECTION EXPERIMENTS

N. F. Cross R. J. Hinton G. E. Whitesides

KENO¹ and CHERIE⁶ were used to calculate ten critical experiments reported in ref. 12. These systems were calculated using both 16-group Hansen-Roach cross sections⁴ and 123-group XSDRN cross sections. The experiments were done at Rocky Flats using a square central column and cylindrical arms filled with aqueous solutions of uranyl nitrate (about 93% enriched) and having a density of 450.8 g of ²³⁵U per liter. The central column was made of 1/8-in. stainless steel with internal dimensions of 7.0 X 7.0 in. The arms were 54 in. long. All the experiments were considered to be unreflected. The average values of the k -effectives for the whole set of problems were 0.9923 ± 0.0055 for the 123-group XSDRN cross sections and 0.9772 ± 0.0030 for the 16-group Hansen-Roach cross sections. This work is part of a

12. B. B. Ernst and C. L. Schuske, *Empirical Method for Calculating Pipe Intersections Containing Fissile Solutions*, RFP-1197 (September 1968).

continuing study we have under way to help write a guide for the design of nuclearly safe pipe intersections containing solutions of fissile materials.

Sponsor: Critical Experiments Facility, Y-12

E. B. Johnson

MONTE CARLO REACTIVITY CALCULATIONS USING A PERTURBATION SOURCE

T. J. Hoffman L. M. Petrie N. F. Cross

A Monte Carlo method for the calculation of the change in the multiplication constant due to cross-section perturbations in a nuclear reactor has been developed. Although this method is similar to that employed by Matthes,¹³ it is not limited by the first-order perturbation requirement. The removal of this requirement does not significantly increase computational time and may significantly improve results.

The method was implemented in the multigroup Monte Carlo code MORSE¹¹ and applied to two one-dimensional test problems. For these test problems, a significant improvement over Matthes' approach and a correlated sampling technique was observed.

Current effort involves implementation in the Monte Carlo codes KENO¹ and ESP,¹⁴ improved selection from the perturbation source, and analysis of various experiments.

Sponsors: Critical Experiments Facility, Y-12
Criticality Safety Section,
Radiation Safety Department, Y-12

E. B. Johnson
G. R. Handley

CALCULATIONS OF THE TIME-DEPENDENT BEHAVIOR OF FAST CRITICAL SYSTEMS

J. R. Knight J. T. Mihalczo³

The time-dependent ANISN code¹⁵ was used to study the time behavior of fast critical systems consisting of bare plutonium metal spheres. The fission neutron density resulting from an initial ²⁵²Cf source at the center was determined as a function of time and position inside the sphere. The effects of variation in the size and number of time steps on the results were evaluated. The 16-group cross-section set from Hansen and Roach⁴ was used in the calculations. Additional calculations using 15-group cross sections obtained from ENDF/B Version III data are planned.

Sponsor: Critical Experiments Facility, Y-12

J. T. Mihalczo

TABULATED CRITICALITY OF REFLECTED CUBIC ARRAYS DEFINED BY SURFACE-DENSITY PARAMETERS

N. F. Cross J. T. Thomas³

A program was written to generate criticality data from surface-density parameters. Four tables are made for each set of data on the basis of the number of units and six different cell sizes. The tables are

13. W. Matthes, *Nucl. Sci. Eng.* 47, 234 (1972).

14. S. N. Cramer et al., *ESP - a General Monte Carlo Reactor Analysis Code*, ORNL-TM-3164 (January 1972).

15. W. W. Engle and F. R. Mynatt, "One-Dimensional Time-Dependent Discrete Ordinates," *Trans. Amer. Nucl. Soc.* 12, 400 (1969).

made in such a way that each page can be put directly into a report without alteration. The data generated for the tables are

1. the radius of spherical units centered in cubic cells of water-reflected critical cubic arrays,
2. the mass of spherical units centered in cubic cells of water-reflected critical cubic arrays,
3. the mass of spherical units and corresponding transport index for units centered in cubic cells of water-reflected subcritical cubic arrays at a k -effective not exceeding 0.85,
4. the mass of spherical units centered in cubic cells of water-reflected cubic arrays having a k -effective not exceeding 0.93.

The same tables can be generated for cylindrical or cuboidal geometries. A total of 648 tables were generated.

Sponsor: Critical Experiments Facility, Y-12

J. T. Thomas

COUPLED REACTOR POWER EQUATIONS

M. Reeves L. W. Owen

A code has been written which solves a system of coupled reactor power equations. These are first-order differential equations for the power of prompt neutrons, the power of up to ten delayed neutron groups, and the reactor temperature (the Ricatti nonlinear equation) as a function of time. The system of stiff equations is solved by assuming that for a sufficiently small time interval Δt , the equations may be uncoupled and the coupling terms set equal to constants. Reasonable accuracy is obtained with $\Delta t \sim 0.1$ sec.

Sponsor: Critical Experiments Facility, Y-12

J. T. Mihalczo

CONTINUED USE AND MODIFICATIONS OF X-RAY ANALYSIS CODES

O. W. Hermann

X-ray analysis codes INDOCX,¹⁶ POWD2R, XCHART,¹⁷ and others^{18,19} have been used in varying degrees throughout the year. These codes perform treatment on x-ray crystalline data, including refinement of lattice constants, indexing crystals from reflection spacings, calculating diffraction patterns from pertinent parameters, plotting the patterns, and plotting Kikuchi and Kossel lines. Although the codes are used primarily by the project sponsors, several new or unusual applications were requested. POWD2R was revised to handle larger problems and is currently being corrected to avoid a rare execution abnormality. Input modifications to INDOCX were made, and others are being considered.

Sponsor: Development Division, Y-12

D. A. Carpenter
C. E. Holcombe

16. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 102.

17. D. K. Smith, *A Revised Program for Calculating X-Ray Powder Diffraction Patterns*. UCRL-50264 (1967).

18. *Math. Div. Annu. Progr. Rep. Dec. 31, 1970*, ORNL-4661, p. 108.

19. B. T. M. Loh and K. H. G. Ashbee, *A General Program for Constructing Maps of Kikuchi and Kossel Lines*, ORNL-TM-3557 (1971).

MODIFICATION OF CONTOUR, A CODE FOR PLOTTING X-RAY INTENSITY CONTOURS TO ACCEPT UNALTERED DATA FROM NEW INSTRUMENT

O. W. Hermann

An x-ray analysis code processing diffractometer data with the CONTOUR subroutines²⁰ has been in use during the past several years. The code produces a plot of equal-intensity lines similar to elevation contours shown on geographical maps. These plots enhance metallurgical analysis of the specimens used in the diffractometer measurements. The data, representing x-ray counts, are recorded automatically on punched paper tape at points covering a desired area of the sample. The previous diffractometer used a locus defined by radii including equal angles and a spiral. The new diffractometer uses more complexly derived points on concentric circles that approximately represent equal areas of the surface being analyzed. Examination of the code, in particular the data smoothing treatment and matrix scanning technique, indicated that the new form of accepting data could be properly transformed within the code. The revisions have been completed and given a preliminary test. More testing will be made with additional data.

Sponsor: Development Division, Y-12

W. E. Baucum

VISUALIZATION OF THE ELECTRON BEAM IN AN ELECTRON BEAM WELDER

T. C. Tucker

Optimal use of an electron beam welder requires sharp focusing of the electron beam at the weld point. The Metallurgy Department of the Y-12 Development Division measured the beam of a typical welder at various stations in the welding zone. The data indicated that the electron beam had a rotating elliptical cross section of varying size. We used a modification of the PERSPX perspective plotting subroutine²¹ to facilitate visualization of the beam. Figure 15 assumes linear interpolation between ten sampling positions. The roughly axial lines are spaced at equal fractional distances around the perimeter of each ellipse.

Sponsor: Development Division, Y-12

D. G. Scott

20. E. E. Branstetter, *CONTOUR, a Fortran Subroutine for Producing Contour Maps*, ORNL-4031 (1966).

21. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 68.

Fig. 15. Perspective drawing of the beam in an electron beam welder.

Systems Programming

SYSTEM/360 HISTORY

T. D. Calton	J. D. McDowell
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L. P. Helton	R. P. Rannie
R. P. Leinius	C. P. Walker
R. O. Williams	

During 1972 the IBM 360/91 and 360/75 computers operated under ORNL-modified versions of the IBM MVT operating system. The ORNL-modified HASP system continued to be the major subsystem used to handle input and output for the computers. Use of shared direct-access devices has continued to increase, not only in the area of on-line data storage but also as a means for improving the system maintenance features of the ORNL computer operation. During the past year, which has been a period of increasing demand on the computer facilities, there have been changes in controlled memory allocation (CMA) techniques on both computers. These changes, in addition to a restructuring of the ORNL job class definitions and the addition of machine-independent automatic timing features, have resulted in greater throughput and significantly better machine utilization. There has been a successful effort in the development of system maintenance techniques which are unique to ORNL and which have greatly reduced the dependency of ORNL on IBM system maintenance techniques. Use of the ORNL techniques not only has reduced the lost production time formerly used by IBM for system maintenance but also has enabled ORNL systems development and testing to be carried out with a smaller impact on production operations. A major avenue for improving the operating systems continues to be informal liaison with numerous other computing organizations. With the notable exception of the RECON and CRBE systems, the number of terminals being served by the computers has not increased, although there have been increases in the transmission data rates used on several of the terminals. There has also been an increase in the number of jobs submitted to the 360 computers from remote locations. The newly developed ability of the 360/91 computer and the 360/75 computer to transmit jobs between themselves via the PDP-10 has been a major factor in the increased remote computing load.

System Monitoring

A number of measurements of system activity were carried out by IBM in August using the IBM System Measurement Instrument (SMI) hardware monitor.

Measurements made on the 360/91 showed an overall utilization of the central processing unit (CPU) of approximately 80%, with second- and third-shift utilizations of approximately 70%. CPU utilization on the first, or daytime, shift was found to be approximately 90%. No significant problems were found in the channel loadings, nor were any significant contention problems found in the use of direct-access devices

that were shared between the two 360 computers. The result of this study, in conjunction with other considerations, led to the decision not to request an additional 2 million bytes of memory for the 360/91 computer, since the nature of the ORNL operations indicates that even with the present memory the 360/91 central processor is nearly fully utilized.

Measurements made on the 360/75 indicated an overall CPU utilization of approximately 60%. The large core storage (LCS) on the 360/75 was found to be busy approximately 60% of the time the CPU was busy. This indicates that the LCS was busy approximately 36% of the time. The lower CPU utilization on the 360/75 computer would be expected, due to the large number of telecommunications handling programs which operate in the slow memory (LCS) on the 360/75. The lower utilization is also due to the smaller computational load on the 360/75. This is a direct result of the small amount of fast memory (512K bytes) available on the 360/75. As a result of this study and other data, a change in the CMA program was made that checked to see if a job running in LCS was CPU bound (or at least not input-output bound). All CPU-bound jobs running in LCS were run at a reduced priority in order to better assure that the fast memory of the 360/75 would receive the maximum utilization. Efforts to obtain further fast memory for the 360/75 have been supported by the results of this study, and such efforts are continuing.

Other System/360 Activities

Time-sharing option (TSO). A large amount of time was expended on the installation of the IBM TSO system on the 360/75, but a production version of TSO is not yet available. Once in production, TSO is expected to add a new teleprocessing dimension to the 360/75.

The version of TSO available under the current operating system has proven unreliable; an attempt to integrate an improved version into the operating system is under way.

Enhancements by other TSO installations have been evaluated, and some will be incorporated into the ORNL system.

Tests indicate that performance of the ORNL ORLOOK inquiry subsystem when controlled under TSO will be improved. The Argonne SPEAKEASY mathematical subprogram package will also be evaluated under the control of TSO.

Conversational Remote Batch Entry (CRBE). Approximately 180 persons are enrolled as users of the ORNL CRBE system. An average of 2700 terminal sessions are processed and 2300 jobs are submitted each month. The leading CRBE application areas are data base preparation and data inquiring programs. Minor modifications were made to the system.

In terms of response time and disk storage space, CRBE is viewed as a near-saturated system. Performance degradation will likely preclude any further significant expansion.

Task execution monitor. A program has been developed which allows for the execution time monitoring of any system or user task executing on the IBM 360/75 or IBM 360/91 computer system. The program breaks down the region assigned to each module of a specified task into subregions, or "windows," of equal length. These "windows" may vary from 8 bytes to approximately 80 bytes, depending upon the size of the task being monitored. The output includes an activity breakdown for each module. For each subregion in which there was activity, the associated total activity count is given, along with that subregion's absolute address and its address relative to the beginning of the task.

System log compression and recording. A program has been developed for the management of the data present in the system output logs for the IBM 360/75 and 360/91 computer systems. These data, comprised of records pertaining to all system and user activity, are compressed, encoded, and written into a cyclically reusable data set. A printer copy of the log will still be produced. The principal advantage of the compression/recording process is that, in addition to the printer copy of the log, there will be available an

on-line concise copy from which programmed analysis of system/user activity and error occurrences may be made.

Card utility program. A utility program has been written for the IBM/360 which can be used to reproduce or convert (BCD to EBCDIC or EBCDIC to BCD) card images. Input and output may be via card decks, magnetic tapes, or direct-access volumes. The routine is available as a load module which can be executed by invoking a cataloged procedure. Various options can be specified by the user.

TELEPROCESSING USING REMOTE CRT STATIONS ON A POLLED LINE

G. K. Haeuslein A. H. Culkowski

We reported on this project last year.¹ We wrote our own version of the RECON program, which can readily be adapted to changes in the data bases such as removal of linear files. This program, RECONX, has been in daily operation since September 1972.

Since the code is quite sizable, it has become difficult to add new features, so we are presently in the process of breaking up the program into smaller and more easily modifiable modules.

PDP-10 SYSTEMS PROGRAMMING

PDP-10 Monitor

C. E. Hammons M. M. Goodman D. R. Winkler

The 505-level monitor was installed in the Intermediate Analysis and Coordinating Computer (IACC). This involved merging the special communications software² into the released version of the monitor. The actual number of lines of code was relatively small, but a considerable amount of time had to be spent in determining where all the necessary changes had to be made.

Local modifications were made to improve interactive time sharing and remote display use while at the same time discouraging "number crunching" (compute-bound jobs). Various disk file manipulation routines have been written for the convenience both of the systems group and of users.

The new release (505) of the monitor has several beneficial features. There is support for experimental system libraries as well as the current system library. The disk file service routines will now support extra large file generation (ORELA data)³ for easier data management.

The monitor now supports the ASCII (American National Standard Code for Information Interchange) compatible CRT terminals. This type of interactive terminal operates at a higher data transmission speed and has the ability to stop and continue the display of information at any time.

The special heavy-duty paper tape reader has been put into production. The monitor service program for the device was implemented by modifying a regular paper tape reader service program.

JUGGLE, the IACC/PDP-10 communication subsystem,² has been modified slightly to correct errors that occurred while logically connecting and disconnecting a line. The current version of JUGGLE now supports three additional communications lines: the IBM 360/91, Thermonuclear Division's PDP-11/45 remote access terminal, and the Naval Research Laboratory's dial-up line, bringing the total number of lines in use to 11 of a possible 12. Approximately 150 jobs are processed daily through the network.

1. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 114.

2. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, pp. 114-15.

3. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 116.

A system to permit time-sharing users of the PDP-10 to generate pen-and-ink plots has been implemented. The user's plot commands are stored in a temporary disk file during the plot generation. The data file is later transferred to an IBM 360, where the plotter commands are written onto magnetic tape.

PDP-10 User Support

R. K. Gryder J. E. Jansen J. A. Watts

Program libraries. *BASIC.* A collection of 140 BASIC programs from DECUS (Digital Equipment Computer User's Society) and local users has been made available to users.

JCL. A library of JCL (job control language) statements for commonly used programs on the IBM 360 computers at ORNL has been collected and made available to users of the DECsystem-10 computer.

CTC-39. The Computing Technology Center Numerical Analysis Library has been made available to users for the debugging of programs to be run on the IBM 360s.

TMPLIB. A temporary library of FORTRAN-callable subroutines has been created on the DECsystem-10. These routines include many special-purpose programs designed to give the FORTRAN user control over such things as his paper tape reader and terminal echo. This library also contains many routines which are available on the IBM 360s, such as string manipulation routines for compatibility with that system. We are testing a version of the permanent FORTRAN library which includes the more important of these routines.

Plot. A Czicomp pen-and-ink plotter package has been developed for the DECsystem-10. Most standard FORTRAN/Calcomp subroutine calls are accepted by this package.

SSP. The Scientific Subroutine Package, a collection of over 250 FORTRAN mathematical and statistical programs, has been adapted for use on the DECsystem 10.

Computer-assisted preparation of reports. Facilities have been developed for computer-assisted production of reports. A program (RUNOFF), distributed by Digital Equipment Corporation, formats text files into a format suitable for publication. This format is not compatible with the standards established for ORNL reports. The program was modified locally to enable users to prepare reports compatible with local standards. The output of RUNOFF is routed to the IBM 360 1403 printer with the special text character train. At this point, it can be printed on mats for photographic reproduction or printed on blank paper.

FGCAL. FOCAL, an interactive language commonly used on small computers, has been implemented on the DECsystem-10. This version of FOCAL was jointly written by Digital Communications Associates, Inc., and the Emory University Chemistry Department. It is extremely core efficient and remarkably compatible with the small-computer version. It also contains extensions to make use of powerful system-provided functions of the DECsystem-10.

CSMP10. A block-oriented continuous dynamic system modeling program, CSMP10, has been implemented on the ORNL PDP-10. This program simulates dynamic systems modeled by ordinary differential and difference equations. CSMP10 has been modified to be compatible with the ORNL device designations.

Other Activities

The ORNL DECsystem-10 computer now has over 300 users. To provide statistics on their usage for billing and managerial information, several programs have been implemented.

Two programs have been written to aid users in the submission of programs from the PDP-10 to the IBM/360s.

Several DECtape handling routines have been written.

A user's handbook for the ORNL DECsystem-10 will be distributed in January 1973. This handbook contains information on the DECsystem-10 and local additions or extensions to the system. This manual contains user information which may otherwise be undocumented and allows one to use the system without benefit of other published documentation.

Several introductory time-sharing seminars were held during the year for ORNL staff members who were interested in learning how to use the PDP-10. One advanced seminar was held and a special one-week seminar covering user problems was conducted for Programming Assistance.

DATA ACQUISITION AND ANALYSIS SYSTEMS

N. A. Betz R. L. Goodman
J. G. Craven S. M. Kaplan
J. K. Dyer C. H. Ferritt
C. L. Thompson

ORELA

We made many improvements to the ORELA data acquisition systems. Malfunctions of the experimental equipment can no longer crash ODAR (ORELA data acquisition routines), the maximum update rate was increased to 5400 events per second, an improved method of writing crash routines was standardized, and the ability to operate the data acquisition portion of an experiment completely under program control was implemented. We provided routines to display raw data in either semilog or linear mode, with the gamma-ray or neutron energy at a given point printed out upon request, to acquire data from newly designed experiments, and to allow anyone to inquire into the status of all operating experiments.

The peripheral equipment controller (PEC), a System Engineering Laboratories (SEL) 810B, was delivered, checked out, and put into normal use. The peripheral and computer links were transferred from DAC-2 to the PEC. The five computers, including the IACC system, which are directly connected to the PEC can transfer programs and data to each other via their link to the PEC and can use any of the peripherals connected to the PEC as if the peripherals were directly connected to the requesting computer. The PEC has no program storage facilities of its own and calls upon DAC-1 or DAC-2 whenever it requires the use of a routine not currently residing in its core memory.

We wrote new communications routines to provide cleanup and recovery procedures in the event of software or hardware malfunctions during data transfers. When the operating system on one of the computers is reloaded, all of the other computers are notified. Any computer which was in the process of communicating with the reloaded computer will inform all of its routines which were concerned with the reload, and the incomplete transmission will be ignored. These new recovery procedures prevent software or hardware malfunctions in one computer from adversely affecting the operation of another computer in the system.

We wrote an assembler and loader for the SEL 810B's to run on the IACC system. The program produces an assembly listing with a cross-reference table, a relocatable object output file, and a core image file. The listings can be sent to the PEC for listing, and the files can be sent to any of the SEL disks for storage and execution. Using the IACC to develop SEL programs has cut in half the time required to write and debug SEL programs.

SEL's bid on the specifications for DAC-3 was accepted. The DAC-3 system is similar to the DAC-1 system except for an improved disk design which will allow for increased data rates. A copy of the ORELA

data acquisition system, modified to reflect the new disk design was sent to SEL for check-out of the DAC-3 computer system. DAC-3 is scheduled for delivery in the first quarter of 1973 and will be interfaced to the PEC.

We have written various IACC programs to process and display ORELA data. These include programs to correct for dead time; correct for detector response; subtract backgrounds; compute transmissions, cross sections, and associated errors; interactively display and fit resonances in transmission data using the Harvey-Atta area analysis method; output data in CSISRS format for transmission to other laboratories; and convert results from IBM 360 data analysis programs into a format suitable for displaying the data. Many of the display programs allow the user to obtain a Calcomp plot of the picture he has displayed. We have provided user-callable display subroutines such as PLOT, PLOTS, SYMBOL, NUMBER, and INTRIGUE which are compatible with their Calcomp counterparts, along with Greek letters and centered symbols.

We modified the PDP-10 and PDP-15 graphics primitives to more closely fit ORELA's requirements and to increase the reliability of transmissions between the PDP-10 and the PDP-15 display stations.

We established a library of subroutines which handle and display ORELA data. The library facilitates the use, distribution, and documentation of the subroutines in it.

Thermonuclear Division's Data Acquisition System

Specifications for the Thermonuclear Division's data acquisition system⁴ were completed and placed out on bid, and the award was made to Digital Equipment Corporation. The system has been delivered and is currently undergoing acceptance tests. The usual problems encountered in checking out a system of this complexity (five new interlinked computers plus a link to the IACC system) have occurred.

A job control language for the remote entry station (RES) which will allow the user to easily transfer files among all of the computers in the system, list files at the RES, and submit jobs to the computers at the ORNL central computer facility, with output returned to the RES for listing, has been designed and is being implemented. Routines to list IACC files at the RES's line printer have been written and are in use.

Environmental Sciences Division Remote Batch Station

The Environmental Sciences Division is in the process of procuring a remote batch station (RBS) to be used in the reduction and analysis of data generated in the various programs within the division.

The functions of the RBS will include submission of batch jobs to the central computer facility, with output returned to the RBS, and utility operations such as listing cards, editing magnetic tapes, and creating and editing files on the disk storage. We have been involved in planning the system and writing the specifications for it.

The RBS computer will include a fixed-head disk, a seven-track magnetic tape unit, card reader, line printer, paper tape reader and punch, and interface to a 9600-baud binary synchronous data set. The interface will be used to link the RBS to the IACC system.

The detailed specifications for the system were placed out for bid in December 1972. Bid responses are due in January, with system delivery in June 1973. We are responsible for developing a job control language (similar to the one being developed for the Thermonuclear Division's remote entry station), communication routines, and utility packages for the RBS.

4. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 117.

Computer Services

Pearl N. Coffey	T. A. Gardner, Jr.	S. O. Smith
L. S. Finch	L. G. Hodge	C. S. Williams
R. L. Finch	J. E. Parham	

EQUIPMENT

The DEC Computer

The initial installation of the Digital Equipment Corporation PDP-10 computer system has been described previously.¹ The system was well into the extended test period at that time and successfully passed the acceptance test on January 19, 1972. Various problems in the software (support programs) were solved during the software warranty period, and by mid-March, operation and use of the system were in production mode.

Many staff members of the Laboratory had heretofore subscribed to commercially available time-sharing service in order to perform small, quick computations. With the acceptance of the PDP-10 systems, however, more and more of these users began to avail themselves of the time-sharing capabilities of this machine. The time-sharing load grew rapidly to the point where the number of lines into the system became inadequate and users were unable to sign on the system for long periods of time. To remedy this situation, additional lines were added in midyear, together with an additional disk unit to provide storage space for the increased number of users. This acquisition brought the number of dial-up lines to 14, the number of hard-wired lines to 10, and the number of user-oriented disk units to 5.

A new data line was added to the system which permits communication between the 360/91 and the PDP-10; thus it is now possible for the PDP-10 to transmit data to and from both IBM computer systems. With appropriate additions to the PDP-10 operating software (see also the section on Systems Programming), it became possible for users at remote terminals to gain access to any of the three computer systems.

During the early part of 1972, it became apparent that the paper-tape reader, which is an integral part of the console of the PDP-10, was not adequate to perform the volume of paper-tape work routinely processed at the computing center. Therefore, a heavy-duty, high-speed paper-tape reader was procured from the Talley Corporation and interfaced into the PDP-10 system by DEC. This device has proved to be fast, reliable, and capable of handling the paper-tape work load.

Additional core memory was also added to the system during the year to avoid degradation of system performance due to the increased work load.

The total memory capacity of the PDP-10 was increased to 114,688 36-bit words.

1. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, pp. 118-19.

Figure 16 is a schematic diagram of the PDP-10 computer system and reflects the changes to the system which have just been described.

The IBM Computers

No major pieces of equipment were added to either IBM computer system during the report period; however, some changes were made, primarily in the area of remote data transmission. With the acceptance of the PDP-10 computer and the development of appropriate software, remote job entry (RJE) equipment at ORIC and at the Reactor Division at Y-12 was permanently connected to the PDP-10. The data transmission lines from these two stations to the 360/75 were therefore removed. During the report period, the Naval Research Laboratory, which had maintained a remote line to both IBM computer systems, discontinued the line to the 360/75 and upgraded their line to the 360/91. This permitted removal of a piece of leased equipment from the 360/75.

Additional low-speed (voice-grade) telephone lines were added to the 360/75 in order to cope with increased demands on the CRBE and ATS terminal systems, as well as to permit evaluation of IBM's time-sharing option terminal system. There are now 31 low-speed lines to the 360/75; this represents the maximum number possible with existing equipment.

Although no equipment changes were required locally, it is of interest to report that the number of terminals on the RECON system² doubled during the year. Twelve terminals are operational as of this writing, with three more pending.

Figure 17 depicts the current status of the ORNL computer network and includes the changes described above.

The CDC Computer

Use of the CDC 160-A computer system decreased during the year, and plans were finalized to surplus the system at the end of February 1973. This was made possible primarily by the addition of a heavy-duty paper-tape reader to the PDP-10, so that by the end of the report period essentially all CDC 160-A work has been successfully transferred to the PDP-10.

Work Load and Performance

Figure 18 shows the average number of jobs processed per scheduled work day at the ORNL computing center, and the upward growth of this work load over the past three years is clearly indicated. During this report period, over 235,000 jobs were processed. Once again, this number reflects an increase over last year. By the end of this period, approximately half the number of jobs submitted to the center come in via remote terminals.

Other figures follow which reflect the performance of the equipment and the use made of it during the period. Figures 19 and 20 show the hours in use and downtime experienced by the IBM 360/91 and the IBM 360/75 respectively. Figures 21, 22, and 23 show the use by various divisions of the IBM 360/91, IBM 360/75, and DEC PDP-10 computer systems respectively.

The computing center is scheduled to operate 24 hr a day, Monday through Friday; however, the size of the work load requires additional shifts to be worked during the weekends. In addition, the center now has at least one operator on duty in the machine rooms at all times, weekends and holidays included. The Computer Services staff increased slightly during the period and now totals 48 people.

2. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 97.

Fig. 16. The DEC PDP-10 computer system.

Fig. 17. The ORNL computer network.

Fig. 18. Average number of jobs processed per scheduled work day.

Fig. 19. Hours in use and downtime, IBM 360/91 computer system.

Fig. 20. Hours in use and downtime, IBM 360/75 computer system.

Fig. 21. Divisional use of the IBM 360/91 computer system.

ORNL-DWG 73-1536

Fig. 22. Divisional use of the IBM 360/75 computer system.

ORNL-DWG 73-1537

Fig. 23. Divisional use of the DEC PDP-10 computer system.

Mathematical Statistics

Introduction

D. A. Gardiner

Despite the retrenching the Laboratory has had to undergo in the face of reduced support and increasing costs, the Statistics Department has continued to be active in contributing to the advancement of statistical theory in particular and to the welfare of science in general. Contributions have been made in the areas of experimental design, tests of hypotheses, estimation, and probability theory. As in the past, our statisticians have been busy in developing new techniques and adapting old ones to applications in diverse fields such as biology, medicine, chemistry, ecology, safety, materials, and engineering, as the following pages will attest.

Statistical Research

CONSTRUCTION OF "D-OPTIMAL" EXPERIMENTAL DESIGNS

Toby J. Mitchell

A previous report¹ described an algorithm which has been written for the purpose of constructing "D-optimal" experimental designs, that is, designs that maximize $|X'X|$ for a specified linear model $E(y) = X\beta$. At that time, the algorithm (now called DETMAX) had been applied to the construction of designs for the first-order model $E(y) = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$ over a cubic region of interest $-1 \leq x_i \leq 1, i = 1, 2, \dots, p$. In various test cases, the value of n (the number of runs) was chosen to be some multiple of 4, since the optimal design is then known to be orthogonal. Since that time, DETMAX has been applied to the construction of designs of the following types:

1. *First-order two-level designs.* This is an extension of the work described previously.¹ Designs were constructed for values of p and n shown in Table 4, where p is the number of variables and n is the number of runs.

Although DETMAX does not guarantee D-optimality (principally because the objective function has many local maxima), an investigation of the properties of the best designs constructed by the algorithm suggests some "rules" for constructing D-optimal designs for first-order models. These "rules" are given below, where it is assumed that t is the largest integer such that $n \geq 4t \geq p + 1$. (If no such t exists, these "rules" do not apply, and the corresponding cases must be considered separately. For $p \leq 9$, there are 12 such cases.) All runs are to be taken at the corners of the region of interest, namely, $x_i = \pm 1$.

- (i) If $n = 4t$, use an orthogonal design in p variables and n runs.
- (ii) If $n = 4t + 1$, add any run to an orthogonal design in p variables and $n - 1$ runs.

1. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971, ORNL-4761, p. 125.*

- (iii) If $n = 4t + 2$, add two runs to an orthogonal design in p variables and $n - 2$ runs. These two runs should be chosen so that the corresponding two rows in X will be as nearly orthogonal to each other as possible.
- (iv) If $n = 4t + 3$, remove any run from an orthogonal design in p variables and $n + 1$ runs.

Many of the best designs found by DETMAX for the values of p and n shown in Table 4 have now been cataloged.² In addition to the design matrix, this report also gives in each case the variance of the fitted response at the design points, the maximum variance of the fitted response over the cubic region of interest, the covariance matrix of the coefficients, the average variance of the coefficients, the determinant of $X'X$, and two measures of efficiency. The alias matrix is also given to indicate the nature of the confounding that occurs if a second-order model, rather than the assumed first-order model, is correct.

These designs can all be "folded over"³ to give resolution IV designs in $p + 1$ variables and $2n$ runs. Resolution IV designs are useful for detecting departures from the assumed first-order model, even though it will not, in general, be possible to estimate the coefficients of all the second-order terms. The efficiencies of the foldover designs based on the first-order designs constructed by DETMAX compare favorably with those given by Srivastava and Anderson⁴ for their "balanced resolution IV*" designs.

2. *Second-order two-level designs.* When the model includes not only the linear terms in the x_i but also all second-order (cross-product) terms, it has the form:

$$E(y) = b_0 + \sum_i b_i x_i + \sum_i \sum_{j>i} b_{ij} x_i x_j.$$

For this model, orthogonal designs can exist only when n is a multiple of 16, so a set of good nonorthogonal designs is required to fill in the gaps.

The algorithm DETMAX has been applied to construct D -optimal second-order two-level designs for the values of n and p shown in Table 5. These designs are currently being studied and compiled for inclusion in an ORNL report. The efficiencies of these designs compare favorably with those given by Srivastava and Chopra,⁵ whose "balanced" designs now form the most comprehensive set of second-order two-level designs appearing in the literature.

3. *Incomplete block designs.* A vast literature exists on the subject of balanced and partially balanced incomplete block designs. The motivation comes from experimental situations in which the effects of v

2. T. J. Mitchell, *An Algorithm for the Construction of "D-Optimal" Experimental Designs, Applied to First-Order Models*, ORNL-4777 (1972).

3. S. R. Webb, *Technometrics* 10, 291-99 (1968).

4. J. N. Srivastava and D. A. Anderson, *J. Amer. Statist. Ass.* 65, 828-43 (1970).

5. J. N. Srivastava and D. V. Chopra, *Technometrics* 13, 257-69 (1971).

Table 4. Cases in which DETMAX was applied to construct first-order designs

p	n
≤ 6	$p + 1$ through 20
7	8 through 16
8, 9	$p + 1$ through 12

Table 5. Cases in which DETMAX was applied to construct second-order two-level designs

p	n
3	7 through 14
4	11 through 22
5	16 through 32 in steps of 2
6	22, 24, 28, 32, 36, 40, 44
7	29, 32, 40, 48, 56

treatments are to be compared on experimental units that have been grouped into blocks. In the usual notation, v is the number of treatments, b is the number of blocks, k is the number of units in each block, and r is the total number of units receiving any treatment. Ideally, one would like to apply each treatment at least once within every block, but frequently the number of experimental units per block is less than the number of treatments. Most of the literature is concerned with the combinatorial problems that arise. For example, the construction of a balanced incomplete block design requires that every pair of treatments appear together in exactly the same number of blocks as any other pair of treatments.

Although DETMAX was not set up to handle problems of this kind directly, it can be applied if we consider the model

$$E(y) = \mu + v_i + b_j, i = 1, 2, \dots, v; j = 1, 2, \dots, b, \quad (1)$$

subject to the restriction that $\sum_i v_i = \sum_j b_j = 0$. This is the usual model for a fixed effects two-way analysis of variance, where one factor corresponds to treatments and the other corresponds to blocks.

It is beyond the ability of DETMAX to require that every treatment appear in r runs and that every block appear in k runs, but initial trials have indicated that if n is chosen to be a multiple of both v and b , this "requirement" is a natural property of the D -optimal design.

The systematic construction of D -optimal designs for the model (1) for values of n that are multiples of both b and v is now under way. It will be of interest to compare these designs with the incomplete block designs now in the literature and to determine the potential of DETMAX for constructing new incomplete block designs.

LOG-NORMAL REGRESSION

J. J. Beauchamp Norma C. Hull J. S. Olson⁶

In a previous report,⁷ approximations through terms of $1/n^2$, where n is equal to the sample size, were given for the mean, $E(z)$, and variance, $\text{Var}(z)$, of the log-normally distributed random variable z . It was assumed that

$$E(\ln z) = \beta_0 + \beta_1 x, \quad (1)$$

where x is an independent nonrandom variable. As shown in the earlier report,⁷ the unbiased estimator of $E(z)$ for $x = w$ was given by

$$a_1(\hat{y}, \hat{\sigma}^2) = \psi(\hat{\sigma}^2/2) \exp(\beta_0 + \beta_1 w). \quad (2)$$

The approximations to the mean and variance of z were obtained by expanding $\psi(\hat{\sigma}^2/2)$ in powers of $1/n$. However, it was later found that

$$\psi(t) = \frac{\Gamma[(n-2)/2]}{[(1-\phi/n)(n-2)t/2]^{(n-4)/4}} I_{(n-4)/2} \left[\sqrt{2 \left(1 - \frac{\phi}{n}\right) (n-2)t} \right], \quad (3)$$

6. Environmental Sciences Division.

7. Math. Div. Annu. Progr. Rep. Dec. 31, 1971, ORNL-4761, pp. 137-38.

where $\Gamma[(n-2)/2]$ is the usual gamma function,

$$\phi = \left[\sum_{i=1}^n (x_i - w)^2 \right] / \left[\sum_{i=1}^n (x_i - \bar{x})^2 \right], \quad (4)$$

and the generalized expression for the last term in (3),

$$I_\nu(u) = \sum_{r=0}^{\infty} \frac{1}{r! \Gamma(\nu + r + 1)} \left(\frac{u}{2} \right)^{\nu + 2r}, \quad (5)$$

is a modified Bessel function. Since the unbiased estimator of $\text{Var}(z)$ was found to be

$$\left[\psi(2\hat{\sigma}^2) - \psi\left(\frac{1 - 2\phi/n}{1 - \phi/n} \hat{\sigma}^2\right) \right] \exp(2\hat{\beta}_0 + 2\hat{\beta}_1 w), \quad (6)$$

the expression in Eq. (3) may be substituted into (2) and (6) to give an expression in closed form for the unbiased estimators of $E(z)$ and $\text{Var}(z)$. It has also been possible to obtain the following closed form for the variance of the predicted value $a_1(\hat{y}, \hat{\sigma}^2)$:

$$\begin{aligned} \text{Var}[a_1(\hat{y}, \hat{\sigma}^2)] &= [\exp(2\hat{\beta}_0 + 2\hat{\beta}_1 w + 2\sigma^2 \phi/n)] \\ &\times \left\{ \frac{2^{3/2} \Gamma(n-2) \Gamma[(n-3)/2]}{\Gamma[(n-1)/2] \Gamma(n-3)} {}_2F_2 \left[\frac{n-3}{2}, \frac{n-2}{2}; \frac{n-2}{2}, n-3; 2 \left(1 - \frac{\phi}{n}\right) \sigma^2 \right] - e^{(1-\phi/n)\sigma^2} \right\} \\ &+ \exp \left[2\hat{\beta}_0 + 2\hat{\beta}_1 w + \left(1 - \frac{\phi}{n}\right) \sigma^2 \right] (e^{2\sigma^2 \phi/n} - e^{\sigma^2 \phi/n}), \quad (7) \end{aligned}$$

where

$${}_pF_q(\alpha_1, \dots, \alpha_p; \nu_1, \dots, \nu_q; u) = \sum_{R=0}^{\infty} \frac{(\alpha_1)_R (\alpha_2)_R \dots (\alpha_p)_R}{(\nu_1)_R (\nu_2)_R \dots (\nu_q)_R} \frac{u^R}{R!} \quad (8)$$

is a generalized hypergeometric series as defined in Gradshteyn and Ryzhik⁸ with

$$(\alpha_i)_R = \Gamma(\alpha_i + R) / \Gamma(\alpha_i). \quad (9)$$

The log-normal regression computer program⁹ has been modified to incorporate the new Bessel function expressions to be used in Eq. (2).

8. I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products*, p. 1095, Academic Press, New York, 1965.

9. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 177.

CONDITIONAL PROBABILITY INTEGRAL TRANSFORMATION

F. L. Miller, Jr.

The conditional probability integral transformation¹⁰ can be used to test assumptions about the distribution of random variables. The joint distribution of the random variables is conditioned on the sufficient statistics for the parameters to be estimated. In this manner the original set of random variables can be transformed to a smaller set of random variables uniformly distributed on the unit interval. Thus, the problem of testing the distributional assumptions can be reduced to testing uniformity on (0, 1). One candidate for a test statistic, the sum of squares of distances between the ordered random variables, was suggested by Greenwood.¹¹ Moran¹² showed that the Greenwood statistic is asymptotically normally distributed. It approaches normality slowly, however, and tables of empirically obtained critical values have been prepared for samples of size 3(1)50 and 55(5)100. The study used 27,000 replications for each sample size in order to be 99% sure that the empirical distribution function would be within 1% of the true distribution function.¹³

KOLMOGOROV-SMIRNOV TEST FOR UNKNOWN PARAMETER GAMMA DISTRIBUTIONS

F. L. Miller, Jr. J. J. Beauchamp Norma C. Hull

The Kolmogorov-Smirnov statistic provides a means of testing whether a set of observations come from a specified distribution. In many cases it is not possible to completely specify the distribution of interest; for example, it may be known that the distribution is normal, but exact values of the mean and variance may be unknown. Lilliefors¹⁴ has provided tables which may be used to apply a Kolmogorov-Smirnov-type test for normality with mean and variance unknown. A simulation study is in progress to provide the tables needed to apply a test of this type to a gamma distribution in which the sample estimates of the parameters are used instead of hypothesized values. The tables will be prepared by drawing 1000 or more samples of a specified size from a gamma distribution and investigating the distribution of this statistic when the sample parameter estimates are used. The estimates will be found by a method due to Thom, which is simple and has been found to have many desirable properties.¹⁵ This work is motivated by the problem of testing distributional assumptions about pollution data.

AIR QUALITY INDICES

J. J. Beauchamp W. D. Shults¹⁶

Since the development of the air quality indices presented in an earlier report,¹⁷ there have been modifications which will hopefully result in an improved air quality index. Two of the problems associated with the index were:

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10. F. J. O'Reilly and C. P. Quesenberry, *Ann. Math. Statist.* **44** (1973).
 11. M. Greenwood, *J. Roy. Statist. Soc.* **109**, 85-110 (1946).
 12. P. A. P. Moran, *J. Roy. Statist. Soc. B* **9**, 92-98 (1947).
 13. F. J. Massey, *J. Amer. Statist. Ass.* **46**, 68-78 (1951).
 14. H. W. Lilliefors, *J. Amer. Statist. Ass.* **62**, 359-402 (1967).
 15. L. R. Shenton and K. O. Bowman, *Mon. Weather Rev.* **98**, 154-60 (1970).
 16. Analytical Chemistry Division and Environmental Indices Team.
 17. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971, ORNL-4761*, pp. 133-37.

1. If an extremely low concentration happened to be observed for a particular pollutant, this could excessively influence the value of the index.
2. The second problem dealt with the ambiguity of the weighting factor for each pollutant. In addition, it was difficult to associate any particular physical meaning to a numerical value of the weighting factors.

As an alternative to the index, the following modified index is proposed:

$$I'(t) = 1 - \left\{ \prod_{i=1}^{k(t)} [1 - P_i(t)] w_i^* \right\}^{1/k(t)}, \quad (1)$$

where

t = particular time of observation,

$k(t)$ = number of pollutants observed at time t ,

$$w_i^* = 1 + \exp \left(\frac{\mu_i - S_i}{\sigma_i} \right),$$

σ_i = standard deviation of the assumed distribution of the observed concentrations for the i th pollutant,

μ_i = mean or average value of the assumed distribution of the observed concentrations for the i th pollutant,

S_i = standard value associated with the distribution of the i th pollutant, and

$P_i(t)$ = estimated probability that the i th pollutant concentration will be less than or equal to the observed value.

The following properties and improvements over the original index have been observed:

1. When the value of $P_i(t)$ is quite small (which would be the case when low concentration levels of the i th pollutant are observed), this will have very little influence on the final value of I' . For example, if $k = 2$, $P_1(t) \approx 0$ and $P_2(t) \approx 1$, then $I' \approx 1$, which would be a more realistic description of the actual conditions.
2. When the average pollutant concentration, μ_i , is equal to the standard concentration, S_i , then the weight w_i^* is equal to 2. For the case when $\mu_i < S_i$, then $w_i^* < 2$. However, w_i^* is always greater than 1.

During the past year, a new air quality index has been proposed which has the following two components: (1) a type of extreme value component which could be used as a short-term description of the air quality and (2) a long-term component which averages out the extreme values so that certain long-term trends may be more readily seen. In addition to the notation associated with Eq. (1), the following notation is needed:

$C_i(t)$ = observed concentration of i th pollutant at time t ,

S_i = primary standard for i th pollutant,

S_i^* = secondary standard for i th pollutant,

B_i = background value for i th pollutant,

w_i^* = weight for i th pollutant,

for $i = 1, 2, \dots, k(t)$. Define

$$I_i^*(t) = A_i[(C_i - B_i)/S_i] ,$$

where

$$A_i = 100[S_i/(S_i - B_i)] ,$$

and let

$$SS_i = A_i[(S_i^* - B_i)/S_i] .$$

The long-term component of the index, termed TRENDX, is given by

$$\text{TRENDX} = \left[\sum_{i=1}^{k(t)} w_i^* I_i^*(t) \right] / \left(\sum_{i=1}^{k(t)} w_i^* \right) .$$

On any particular day if $I_i^*(t) < SS_i$ for all $i = 1, 2, \dots, k(t)$, then the short-term (daily index) value is equal to TRENDX, and the day's condition is said to be good. If all $I_i^*(t) < 100$ but at least one $I_i^*(t) > SS_i$ for $i = 1, 2, \dots, k(t)$, then the daily index value is equal to the maximum of the $I_i^*(t)$'s which are greater than their corresponding SS_i 's. In this case, the day's condition is termed undesirable. If any $I_i^*(t)$ is greater than 100, then the daily index value is $\max_i [I_i^*(t)]$, and the day's condition is termed unhealthy. One of the obvious advantages of this two-component air quality index is the association of certain adjectives with the index values for a particular day. This attempt should make such an air quality index more palatable to the general public. The adjectives were determined as follows:

1. If all of the pollutant concentrations are below their secondary standard values, then the day's condition is considered good.
2. If all of the pollutant concentrations are below their primary standard value but at least one concentration is above its secondary standard value, then the day's condition is considered undesirable.
3. If any pollutant concentration is above its primary standard value, then the day's condition is considered unhealthy.

In addition to the above air quality index work, a procedure for predicting air quality indices is being investigated. This procedure operates under the assumption that one of the primary factors affecting air quality is wind velocity and attempts to use the predicted wind velocity to predict the air quality index.

TEST OF DEPARTURE FROM NORMALITY

Kimiko O. Bowman

The problem of finding the distribution of skewness statistic $\sqrt{b_1}$ from nonnormal distribution was introduced previously.¹⁸⁻²⁰ Studies were continued to find the percentage points of these statistics using

18. K. O. Bowman and L. R. Shenton, *Bull. Inst. Int. Statist.*, pp. 115-21.

19. K. O. Bowman and L. R. Shenton, *Biometrika* 60.

20. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, pp. 143-44.

Cornish-Fisher expansions based on the normal and Johnson's S_u as kernel. For selected sample size contours of the power of test for $\sqrt{b_1}$ ($\alpha = 0.05$, $\beta = 0.10$) sampling from normal is given for the three alternative distributions, namely, Pearson type 1, mixture of two normals, and Gram-Charlier type A distributions.

Also, the study of kurtosis statistics b_2 , the ratio of the fourth central moment to the square of the second central moment, is carried out in identical manner to $\sqrt{b_1}$ statistic. The use of those two statistics will make a powerful tool for the testing of departure from normality.

PERCENTAGE POINTS OF THE MOMENT ESTIMATOR FOR THE SHAPE PARAMETER OF THE GAMMA DISTRIBUTION²¹

W. E. Dusenberry K. O. Bowman

Bowman and Shenton²² carried out an extensive study of the distributional properties of the maximum likelihood estimator for the shape parameter, ρ , of the gamma distribution with probability density function (p.d.f.) given by

$$f(x) = \frac{e^{-x/a} (x/a)^{\rho-1}}{a \Gamma(\rho)}, \quad x > 0, a, \rho > 0.$$

The maximum likelihood estimators, $\hat{a}$ and $\hat{\rho}$, of a and ρ for a random sample $x_1, x_2, \dots, x_n$ from $f(x)$ are not simple and require an iterative solution. An estimator of ρ that is much simpler and easier to compute than $\hat{\rho}$ is the moment estimator ρ^* given by $\rho^* = m'_1{}^2/m_2 = \bar{x}^2/s^2$, where $\bar{x}$ and s^2 are the sample arithmetic mean and sample variance.

In studying the distributional properties of $\hat{\rho}$, Bowman and Shenton used Taylor-series moment expansions to find the sampling moments of $\hat{\rho}$ and thereby to determine some of the important finite-sample distributional properties of $\hat{\rho}$. It is of interest to know similar distributional properties for ρ^* , since it is much easier to compute. One would want to know if cases exist where ρ^* could be used instead of resorting to the more complicated $\hat{\rho}$. However, when Bowman and Shenton tried to find the sampling moments of ρ^* by methods similar to those used for $\hat{\rho}$, the resulting ρ^* -moment expansions in terms of Taylor series looked to be very divergent and led one to believe that the moments of ρ^* were large or infinite. By contrast, Monte Carlo results indicated that this divergency was not the case. Thus, to determine the distributional properties of ρ^* it was necessary to consider some new approach other than Taylor-series expansions.

The percentage points of the sampling distribution of an estimator contain considerable information about the distributional properties of that estimator and are also very useful and necessary in practical applications. Since it was not possible to find the sampling moments of ρ^* , it was decided to try and find some method by which the percentage points of ρ^* could be determined, without knowing its sampling moments. The 100α percent point, τ , of ρ^* is defined by the probability statement $\Pr(\rho^* < \tau) = \alpha$. The method used to find these τ values was to linearize the ratio statistic ρ^* as follows:

$$\Pr(\rho^* < \tau) = \Pr(m'_1{}^2/m_2 < \tau) = \Pr(m'_1{}^2 - \tau m_2 < 0) = \Pr(y < 0) = \alpha.$$

21. This research will constitute a portion of W. E. Dusenberry's doctoral dissertation at Virginia Polytechnic Institute and State University. Mr. Dusenberry's research is being supported by an Oak Ridge Associated Universities Graduate Fellowship at Oak Ridge National Laboratory.

22. K. O. Bowman and L. R. Shenton, *Small Sample Properties of Estimators for the Gamma Distribution*, CTC-28, UCCND (1970).

Now, the problem of finding the percentage point τ in the sampling distribution of ρ^* is changed to a problem concerning the percentage point of the linearized statistic y , which does not suffer from the disadvantage of being a difficult-to-work-with ratio like ρ^* . The sampling moments of y are then used in conjunction with percentage point methods discussed below to find the percentage points of y and, subsequently, those of ρ^* , which is the final result we are looking for.

The linearized statistic y can be written in terms of orthogonal Q statistics²³ as:

$$y = m'_1{}^2 - \tau m_2 = a^2 \rho(\rho - \tau) + 2a(\rho - \tau)Q_1 - \tau Q_2 - (1 + \tau)Q_1{}^2.$$

The Q_i 's are defined in terms of the central moments, μ_i , of the parent gamma distribution and the sample size n . Thus, y is a function of the μ_i 's and the parameters a , ρ , τ , and n . A general computerized scheme has been developed which works with an estimator which is a linear function of the first two sample moments, such as y above. The output of the program is the central moments of the linearized statistic expressed as a series in powers of n^{-1} . For example, taking $a = 1$, $\rho = 1$, $\tau = 2$, the exact third central moment of y would be given as

$$\mu_3(y) = \frac{-1064}{n^2} + \frac{4464}{n^3} - \frac{6048}{n^4} + \frac{3240}{n^5}.$$

The program can be used to find up to the 15th or higher central moment and up to the n^{-15} or higher-order term in each moment, depending on computer storage available.

Now it is necessary to find the percentage points of the sampling distribution of y , where the exact p.d.f. of y is not known but where the first 10 or 15 or higher moments of y are known. A study of several possible methods including fitting normal curves, fitting Pearson curves, and three different series expansion approximations to the unknown p.d.f. — Gram-Charlier type A, Edgeworth type A, and Cornish-Fisher series expansion — showed that the Cornish-Fisher expansion with normal kernel was the most accurate and fastest computing method for our purposes. The final results, using the Cornish-Fisher expansion with normal kernel, are graphs of the cumulative distribution function (c.d.f.) of ρ^* for given values of ρ and n ($a = 1$). Graphs of the c.d.f., from which any percentage point of the distribution of ρ^* can be determined, have been computed for the following combinations of ρ and n :

$$\rho = 1.0, 1.5, 2.0, 2.5, 3.0, 4.0, 5.0, 10.0, 15.0, 20.0;$$

$$n = 50, 75, 100, 150, 200, 300, 500, 750, 1000.$$

These graphs of the c.d.f. of ρ^* can be of use in problems concerning inferences about the shape parameter, ρ , of the gamma distribution, either for finding confidence intervals for ρ or alternatively for testing hypotheses concerning ρ .

SYSTEMATIC POISSON SAMPLING

D. A. Gardiner K. O. Bowman

This problem was suggested by a sampling process from a supposedly Poisson distribution in which an automatic device, such as a Geiger counter, registers only every k th impulse received. At the end of a

23. L. R. Shenton, K. O. Bowman, and D. Sheehan, *J. Roy. Statist. Soc. B* 33, 444–57 (1971).

counting interval, then, there remains a number $0, 1, 2, \dots, k - 1$ of impulses which have been received but ignored. Common practice has been to multiply the count in the register by k and to treat the product as an observation from a Poisson distribution. The degree of approximation inherent in such practice was investigated.²⁴

Let $F(x)$ be the distribution function of a random variable X from a Poisson distribution with parameter λ . Let Y be the random variable corresponding to the observation obtained through a systematic sampling scheme such as that described above. Then the probability density function of Y is

$$g(y) = F[k(y + 1) - 1] - F(ky - 1), y = 0, 1, 2, \dots,$$

for k a positive integer. Let $M(\theta)$ represent the factorial moment generating function of Y . Then it can be shown that

$$M(\theta) = \frac{1}{k} \sum_{j=0}^{k-1} \frac{(1 - 1/\theta) \exp\{\lambda(\omega_j \theta^{1/k}) - 1\}}{1 - 1/(\omega_j \theta^{1/k})},$$

where

$$\omega_j = \exp\{i 2\pi j/k\},$$

where

$$i^2 = -1.$$

Using this moment generating function and the FORMAC computing language, the first four moments of the random variable kY were examined for values of $k = 1(1)8$ and for several values of λ . It was discovered that for $\lambda \geq 100$ the mean (μ_1), variance (μ_2), third moment (μ_3), and fourth moment (μ_4) of kY had reached their asymptotic values to four decimal places. These are shown below.

Moment	Asymptotic value
μ_1	$\lambda - (k - 1)/2$
μ_2	$\lambda + (k^2 - 1)/12$
μ_3	λ
μ_4	$3\lambda^2 + \lambda(k^2 + 1)/2 + (3k^2 - 7)(k^2 - 1)/240$

The mean and variance had reached their asymptotic values for $\lambda \geq 50$, but for smaller λ , the asymptotic values are good approximations only at the smaller values of k .

SPARSE CELLS, CROWDED CELLS, AND DIRICHLET INTEGRALS

Milton Sobel²⁵ V. R. R. Uppuluri

Suppose n balls are dropped independently into c cells. A cell is said to be u -sparse if the number of balls in it is less than or equal to u . Let b ($\leq c$) of the cells be colored blue, and let p be the probability that

24. The assistance of Professors A. C. Cohen and L. R. Shenton of the University of Georgia is appreciated.

25. Consultant.

a ball may fall in a blue cell. The probability distribution of the number of u -sparse blue cells is obtained in terms of incomplete Dirichlet integrals. This distribution is used in the sparse cell test, which is an extension of the empty cell test.²⁶ As a dual concept, a cell is said to be t -crowded if it has at least t balls in it. We obtained the distribution of t -crowded blue cells and the joint distribution of t -crowded and u -sparse blue cells, and studied some properties of the moments

A METHOD OF GENERATING PERMUTATIONS

V. R. R. Uppuluri J. A. Carpenter

Some usual methods of generating permutations of n distinct elements are summarized by Lehmer²⁷ in Chap. I of the book *Applied Combinatorial Mathematics*, edited by Beckenbach. Some other methods are described in an earlier paper also by Lehmer.²⁸ It may be worth noting that in some problems, all the $n!$ permutations may not be of interest, and special methods like rosary methods are developed applicable to the scheduling problem.²⁹ We developed a method of generating all the $n!$ permutations, based on an idea in the folklore of mathematical games, and use the factorial representation theorem to identify the permutations. The method has the feature that after generation of the first block of $(n-1)!$ permutations, the remaining $n-1$ blocks can be generated independently by cyclic permutations on the first block. In fact, any block of $(n-1)!$ consecutive permutations generated by this method constitutes a set of cyclic generators for the group of all the $n!$ permutations.

EXTENSION OF GRIFFITHS' INEQUALITIES TO GAUSSIAN SPIN CONFIGURATION MODELS. II

V. R. R. Uppuluri J. M. Dolan

In the previous annual report,³⁰ we proved the validity of Griffiths' inequalities when the Hamiltonian is given by

$$H = -J_0 \sum_{1 \leq u < v \leq n} \sigma_u \sigma_v$$

and the random vector $(\sigma_1, \sigma_2, \dots, \sigma_n)$ has the equicorrelated multivariate Gaussian distribution $N(0, A)$, with

$$A = (\lambda a_{ij}), \lambda > 0, a_{ii} = 1, a_{ij} = \rho \text{ for } i \neq j.$$

26. F. N. David, *Biometrika* 37, 97-110 (1950).

27. D. H. Lehmer, "The Machine Tools of Combinatorics," chap. I of *Applied Combinatorial Mathematics*, ed. by E. F. Beckenbach, Wiley, New York, 1964, pp. 5-31.

28. D. H. Lehmer, "Teaching Combinatorial Tricks to a Computer," in *Combinatorial Analysis*, ed. by R. Bellman and M. Hall, Jr., Proceedings of Symposia in Applied Mathematics, vol. 10, American Mathematical Society, Providence, R.I., 1960, pp. 179-93.

29. K. Harada, "Generation of Rosary Permutations Expressed in Hamiltonian Circuits," *Commun. ACM* 14, 373-79 (1971).

30. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, pp. 139-42.

We extend this result and consider more general Hamiltonians given by

$$J = - \sum_{1 \leq u < v \leq n} J_{uv} \sigma_u \sigma_v$$

and prove the following:

Theorem. In the case of an equicorrelated Gaussian "spin" configuration model, with the conditions

$$(i) \quad -1/(2n-3) < \rho < 1,$$

$$(ii) \quad -\rho / \{(1-\rho)[1+(n-1)\rho]\} < \lambda \beta J_{kl}$$

for

$$k, l = 1, 2, \dots, n,$$

and

$$(iii) \quad \text{for } k \neq l,$$

$$\lambda \beta \sum_{l=1}^n J_{kl} < \frac{1 - \rho + (n-1)(\rho - |\rho|)}{(1-\rho)[1+(n-1)\rho]}$$

for

$$k = 1, 2, \dots, n,$$

we have Griffiths' inequalities

$$\langle \sigma_k \sigma_l \rangle \geq 0 \tag{a}$$

and

$$\langle \sigma_k \sigma_l \sigma_u \sigma_v \rangle - \langle \sigma_k \sigma_l \rangle \langle \sigma_u \sigma_v \rangle \geq 0 \tag{b}$$

for

$$k, l, u, v = 1, 2, \dots, n.$$

GROUP TESTING TO IDENTIFY SETS WITH DEFECTIVE OBJECTS

W. E. Lever V. R. R. Uppuluri

Sobel and Groll³¹ introduced sequential decision procedures which would enable one to classify each member of a set of n independent objects as being either good or defective, given that the probability that

31. M. Sobel and P. A. Groll, "Group Testing to Eliminate Efficiently All Defectives in a Binomial Sample," *Bell System Tech. J.* 18, 1179 (September 1959).

an object is good is q . At any given time the procedure required only the separation of the unclassified objects into two sets: (1) the defective set, that is, a set of which it is known at least one object in the set is defective, and (2) the binomial set, that is, the set for which no additional information has been learned about the state of these objects. The procedures permitted variable-size groups to be tested and allowed for the recombination of subsets of the groups.

Sobel proposed several methods of selection of the optimum group size to be tested in a given situation; two of these were (1) the R_1 procedure, which minimized the expected number of group tests at any stage in the decision process, and (2) the R_2 procedure, which maximized the "amount of information" the next test would yield.

Sobel's procedures classify every element in the set of objects. However, it is reasonable to consider situations where one would not need to classify every element but only to classify subsets as good or defective. A subset would be called defective if it contained at least one defective object. As in the case when every element is classified, the subsets will be classified into two groups: (1) the defective group, D , that is, the group of sets for which it is known there is at least one defective object in at least one set in the group, and (2) the binomial group, B , that is, the group of sets for which no additional information is known.

For the procedure to be proposed here, subgroups of either the defective group or the binomial group will be chosen to maximize the "amount of information" the next test will yield. For example, let q be the probability that any element of the total set is good, let $C(D)$ be the cardinality of the defective group, D , let $C(S_D)$ be the cardinality of a nonempty proper subgroup S_D of D , let $C(B)$ be the cardinality of the binomial group, and let $C(S_B)$ be the cardinality of a nonempty subgroup S_B of B . Then the "amount of information" $I(D)$ gained by testing a nonempty proper subgroup of S_D of D is given by

$$I_1(D) = \max_{S_D \subset D} \{-Q_1(D, S_D) \cdot \log[Q_1(D, S_D)] - [1 - Q_1(D, S_D)] \cdot \log[1 - Q_1(D, S_D)]\},$$

where

$$Q_1(D, S_D) = [q^{C(S_D)} - q^{C(D)}] / [1 - q^{C(D)}]$$

is the probability that S_D does not contain any defective sets.

Similarly, the "amount of information," $I(B)$ gained by testing a nonempty subgroup S_B of B is given by

$$I_2(B) = \max_{S_B \subseteq B} \{-Q_2(B, S_B) \cdot \log[Q_2(B, S_B)] - (1 - Q_2(B, S_B)) \cdot \log[1 - Q_2(B, S_B)]\},$$

where

$$Q_2(B, S_B) = q^{C(S_B)}$$

is the probability that S_B does not contain any defective sets.

Tables have been computed which will yield the optimum choices of S_D and S_B for $C(D)$ and $C(B)$ up to 30 and for q equal to 0.5(0.05)0.90 and 0.92(0.02)0.98.

Let $G(D|B)$ be the expected number of tests required to classify the defective and binomial groups and let $H(B)$ be the number of tests required to classify a binomial group solely. Then given S_D and S_B as optimum choices,

$$G(D|B) = 1 + Q_1(D, S_D) \cdot G(D - S_D|B) + [(1 - Q_1(D, S_D))] \cdot G(S_D|B + D - S_D)$$

and

$$H(B) = 1 + Q_2(B, S_B) \cdot H(B - S_B) + [(1 - Q_2(B, S_B))] \cdot G(S_B | B - S_B),$$

where

$$G(D - S_B | B) = H(B)$$

if $D - S_B$ contains only one set, $H(B) = 1$ if B contains only one set, and $H(B) = 0$ if B is the empty set.

Statistical Applications

ANALYTICAL CHEMISTRY DIVISION

ANALYSIS OF ERROR IN THE DETERMINATION OF THE ABUNDANCE OF KRYPTON

T. L. Hebble J. R. Walton¹ A. E. Cameron¹ R. L. Walker¹

An error analysis was conducted for an experimental program which determined the natural abundance of krypton by mass spectrometry using isotope dilution with highly enriched ^{86}Kr . Surface air was collected in evacuated tanks of calibrated volume and spiked with a known amount of krypton isotope for determination of isotopic composition in a static mass spectrometer. Seven determinations were made over a period of three months.

The error analysis was composed of three parts: (1) a measure of the precision obtained from repeated runs, (2) an expression for estimating the precision, and (3) estimates of the effects of small departures from the observed value of the input variables on the calculated value of krypton. The first part provides a measure of the reproducibility of the experimental procedure. The second gives an equation to estimate this variability in terms of the variability of ten input variables. The third part provides a measure of the effect of small systematic errors and also may be used to rank the input variables according to their contribution to overall variability.

The precision, or measure of reproducibility, of the method for determining the abundance of krypton as expressed by the standard deviation for each of the seven repeated experiments is 0.00801 ppm krypton. Under reasonable assumptions, this may be rewritten in terms of the 95% confidence interval about the mean of seven observations:

$$1.1019 \text{ ppm} \pm 0.0074 \text{ ppm.}$$

An expression for estimating the variance was derived from the equation used to calculate the abundance of krypton from measured input quantities. Using the experimenter's estimate of variability of input variables, this expression yielded a value which was in good agreement with the above measure of precision.

The third part of the analysis consisted of determining the effects of small changes in ten input variables on the abundance of krypton. Each variable (U_i , $i = 1, 2, \dots, 10$) was treated as though it had two levels:

1. Analytical Chemistry Division.

$(U_i + \text{standard error unit})$ and $(U_i - \text{standard error unit})$, where the standard error is based on the experimenter's estimate of variability. The abundance of krypton was calculated for the $2^{10} = 1024$ possible combinations of levels. An effect is then found by taking one-half the difference between the average of $2^9 = 512$ values at the upper level and the average of 512 values at the lower level of an input variable. A positive effect means the abundance of krypton (ppm) increases by an amount equal to the effect for each standard error unit that is added to the input variable.

The input variables may be ranked according to their contribution to the overall variability by ordering the magnitudes of their effects. This indicates where greater emphasis should be placed when attempting to improve overall precision of the experimental technique. From these ranks, tracer ratio has the largest effect and sample volume has the smallest effect on the variability of krypton. Thus, greater precision in future experiments can be achieved by improving the measurement of tracer ratio, while less effort is needed in measuring sample volume. It is important to note that these rankings are a function of error estimates given by the experimenter and can change with a different set of estimates.

BIOLOGY DIVISION

RBE MEASUREMENT FROM NEUTRON-X-RAY LENS OPACITY DATA

J. J. Beauchamp E. B. Darden, Jr.¹

Neutron and x-ray radiation have been used to investigate the effect of these types of radiation on the induction of lens opacities in mice. The experiment was designed so that animals in cages, each containing approximately eight animals, received a designated type and dose of radiation. In addition, there was a control group of mice which received no irradiation. For a particular type and dose of irradiation, the observations were $[t, Y(t)]$ where

t = time after treatment

and

$Y(t)$ = average percent lens opacity of the animals observed at time t .

In an earlier report,² an exponential expression was used to express the relation between t and $Y(t)$. The present experiment covers a much wider dose range than the experiment mentioned above, and for each dose group and type of radiation, $Y(t)$ is closely related to the reciprocal of t , that is, $Y(t) = A + B/t$, where A and B are parameters to be estimated.

From observed values of $Y(t)$ and t , least-squares estimates of A and B were found for each type and dose of radiation. For the control group and each dose of a given type of radiation, the "total response" is defined as

$$R = \int_{t_1}^{T_{\max}} (A + B/t) dt,$$

which is the area under the time-percent-opacity curve from the end of the latent period ($t_1 = -B/A$) to the end of the experiment ($T_{\max}$). Let R_0 represent the "total response" for the control group. If R represents the "total response" for a particular x-ray or neutron dose group, then $\Delta = R - R_0$ is the increase in the "total response" over and above the spontaneous or control response.

1. Biology Division.

2. Math. Div. Annu. Progr. Rep. Dec. 31, 1967, ORNL-4236, pp. 73-75.

From an investigation of the average ages of the animals in the control and irradiated groups, it was found that these ages differed by as much as 17 days. To account for this difference in ages, the "total response" for the control group was adjusted. The amount of change in the "total response" which may be attributed to a particular type and dose of radiation, after correcting for the age difference, is $\Delta^{(c)} = R - R_0^{(c)}$, where $R_0^{(c)}$ is the adjusted "total response" for the control group. From an investigation of a semi-logarithmic plot of doses vs estimates of $\Delta^{(c)}$,

$$\Delta_X^{(c)} = \beta_0 + \beta_1 \ln D_X + \beta_2 (\ln D_X)^2$$

for x-ray radiation and

$$\Delta_N^{(c)} = \alpha_0 + \alpha_1 \ln D_N + \alpha_2 (\ln D_N)^2$$

for neutron radiation were used to approximate the relationship between dose and $\Delta^{(c)}$. Least-squares estimates of the coefficients α and β were obtained.

The RBE is defined as the ratio D_X/D_N for the case when $\Delta_X^{(c)} = \Delta_N^{(c)}$. By equating $\Delta_X^{(c)}$ and $\Delta_N^{(c)}$ and solving a quadratic equation, the RBE is the following function of D_N :

$$\text{RBE} = \exp[f(D_N)]/D_N,$$

where

$$f(D_N) = \frac{1}{2\beta_2} \left[-\beta_1 + \sqrt{\beta_1^2 - 4\beta_2(\beta_0 - \alpha_0) + 4\beta_2\alpha_1 \ln D_N + 4\beta_2\alpha_2 (\ln D_N)^2} \right].$$

Similarly, an expression for RBE in terms of D_X may be found. The solution to the quadratic equation given above uses only the positive root, since the negative root yields a solution outside the range of definition.

CHROMOSOME ABERRATION MODELS

D. G. Gosslee

The fitting of dose-response models to observed numbers of aberrations induced by irradiation for each of seven species³ was generalized. When the chromosome arm number was included as a new variable, a great majority of the interspecific variation was accounted for by the new model.⁴ Man was included as one of the species from which leukocytes were sampled, cultured, irradiated, and analyzed for aberrations. Thus, some extrapolations of genetic hazards to man could be made.⁴

SEQUENTIAL TESTS FOR MUTAGENIC EFFECTS

D. G. Gosslee

Improved procedures for testing chemicals for mutagenic effects in mice were developed using statistical concepts.^{5,6} The mutagenic effect of chemicals can be tested through their ability to induce heritable

3. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971*, ORNL-4761, p. 147.

4. *Biol. Div. Annu. Progr. Rep. June 30, 1972*, ORNL-4817, pp. 70-73.

5. *Biol. Div. Annu. Progr. Rep. June 30, 1971*, ORNL-4740, pp. 96-97.

6. *Biol. Div. Annu. Progr. Rep. June 30, 1972*, ORNL-4817, pp. 122-23.

translocations which cause sterility and semisterility. A simple procedure based on litter size is used to screen a large proportion of fertile mice from a second test which is more accurate and expensive. The litter sizes are examined sequentially in order to minimize the number of litters required in the screening procedure. Statistical methods are used to control the chances of misclassifying nonfertile animals as fertile.

BIOMETRY NOTES

D. G. Gosslee T. J. Mitchell

A series of short informal notes on biometry are being written and distributed to approximately 275 ORNL investigators about twice a month. The topics of the notes are intended to be of interest to research biologists. Topics for the 20 notes written to date included general concepts of statistical methods, design of experiments, analysis of data, and interpretation of experimental results. Numerical examples based on biological experiments are frequently included to illustrate the statistical procedures.

MISCLASSIFICATION IN CELL FUSION EXPERIMENTS

T. J. Mitchell

In an experiment to study the fate of Moloney leukemia virus in fused cells, mouse cells (M) were fused with labeled human cells (H^*) prior to the introduction of the virus. If the uptake of label were complete, there would be three types of fused cells: H^*H^* , H^*M , and MM , and the number of labels could be used to classify them. The types cannot be distinguished otherwise. Since only about 82% of the human cells could be successfully labeled, the presence of unlabeled human cells introduces the possibility of misclassification. It was of interest to the experimenter to estimate the expected number of misclassified cells of each type. Although he was willing to assume that the probabilities of fusion for any two cells are the same, be they mouse or human, it was possible to use his data to estimate these probabilities as well.

A mathematical model was set up to express the expected number of cells of each type as a function of the original number of single human cells (n_H), the original number of single mouse cells (n_M), and "fusion factors" ρ_{MM} , ρ_{MH} , and ρ_{HH} . The labeling factor p was also incorporated into the model by assuming that pn_H human cells are labeled and $(1 - p)n_H$ are unlabeled. It was also assumed that the labeling has no effect on the fusion factors.

Because the expected number of cells in any observational category is a linear combination of the fusion factors ρ_{MM} , ρ_{MH} , and ρ_{HH} , it was possible to set up a system of simultaneous linear equations, which were then solved for these parameters. Using the model, the expected number of misclassified cells of each type was also determined.

Data from this and related experiments are still being collected. It is anticipated that this model will eventually be applied to the construction of statistical tests of various hypotheses regarding the mechanism of the resistance of human cells to Moloney leukemia virus.

CLASSIFICATION OF INDUCED TRANSLOCATIONS

T. J. Mitchell

When a translocation is induced in a germ cell from a male mouse by some mutagenic agent, the offspring will carry that translocation in every cell. These cells can be classified according to the form in which the translocation is expressed at diakinesis of spermatogenesis (e.g., "rings," "chain type A," "chain type B"). It is assumed that, if n cells from the offspring are examined, the vector of class frequencies (x_1 ,

$x_2, \dots, x_k$) follows a multinomial distribution with parameters $(n; \theta_1, \theta_2, \dots, \theta_k)$, where k is the number of classes and θ_i is the probability that a cell falls in class i .

The classification of any cell is determined by the presence or absence of a chiasma (fusion) at each of four different locations. There are $2^4 = 16$ basic events, subsets of which correspond to "rings," "chains," etc. By letting p_1, p_2, p_3 , and p_4 represent the probabilities of chiasma at locations 1, 2, 3, and 4, and assuming independence among locations, a probability model was constructed for the probabilities $\{\theta_i\}$ of each type of cell observed.

Given a sample classification vector $(x_1, x_2, \dots, x_k)$, the log likelihood L is:

$$L = \text{constant} + \sum_{i=1}^k x_i \log \theta_i. \quad (1)$$

Noting that each θ_i is a known function of the basic $\{p_j\}$ in the model, the estimates $\hat{p}_1, \hat{p}_2, \hat{p}_3$, and $\hat{p}_4$ are obtained by maximizing L with respect to the p 's. To test the model, the maximum L under the model can then be subtracted from the maximum L obtained when no restrictions are placed on the θ 's. By constructing Wilks' statistic, which is twice this difference, and comparing with a chi-square distribution, a lack-of-fit test for the model can be made. This has been done for five different translocations in an experiment with $k = 6$ classifications. Some of these indicated a very good fit for the model; others indicated a poor fit. More data are currently being taken, and it is expected that new models will be developed. Once a satisfactory model is determined, the dependence of its parameters on the type of mutagenic agent will be investigated.

CONSTRUCTION OF A "STANDARD" DOSE-RESPONSE CURVE FOR THE SIMONSEN ASSAY

T. J. Mitchell

In the Simonsen spleen weight assay, spleen cells from a donor mouse are injected into a recipient, causing an increase in the size of the recipient's spleen, presumably in proportion to the "immunocompetence" of the dose of donor cells. In order to use this as an assay for immunocompetence in spleens taken from experimental animals, it was necessary to construct a "standard" dose-response curve. A large experiment was conducted for this purpose, in which mice from 254 litters were injected with cells from 34 donor pools at four different cell doses. Because of the presence of several different types of random variation and the possibility of a nonlinear dose-response curve, a rather complicated statistical analysis was undertaken.

Since the weighing of the spleen necessitates the killing of the animal, the increase in spleen weight cannot be measured for a single mouse. Instead, litters of mice are divided randomly into two approximately equal groups. One group, injected with Tyrode's solution, serves as the control for the other group, which is injected with spleen cells. It is observed that the greater the dose of cells, the greater is the discrepancy between the spleen weights of the "cells group" and the "Tyrode's group."

Since the spleen weight is directly related to the body weight, the basic measurement for each mouse was taken to be $r = \log (\text{spleen weight/body weight})$. Within each litter, the mean response $\bar{r}$ and the logarithm of the estimated variance s^2 were calculated for the cells group. These were plotted against all variables thought to be capable of influence, namely, pool, sex of donor, dose, age of recipient, and litter number. (The "litter number" refers to the order of birth of that litter relative to all other litters born of the same mother.) Plots of the mean response $\bar{r}$ did, of course, show the effect of dose, but no influence of the other variables was apparent. The within-group variance, as measured by $\log s^2$, showed a dependence

on $\bar{r}$, different at every dose. In the subsequent analysis, therefore, the true within-group variance was estimated by a quadratic fit of $\log s^2$ to $\bar{r}$ within each dose.

For each litter, the index of response W was calculated, where $W = \bar{r}_C - \bar{r}_T$. The subscripts C and T refer to the cells group and the Tyrode's group respectively. In addition to the variation among animals within a group, W is also subject to random variation due to differences among litters at a given dose from a given pool of donors and to differences among pools. All three sources of random variation were incorporated into a statistical model, which was then used as a basis for estimating μ_j , the "standard" index at dose j , for $j = 1, 2, 3$, and 4. The standard is defined to be the mean true index for the hypothetical population of pools from which the experimental set of 34 is assumed to be a representative sample. Responses from different pools were assumed to be independent, but responses within a single pool were not. At this point, no special relationship to dose was postulated; the emphasis was entirely on calculating the estimates $\hat{\mu}_1, \hat{\mu}_2, \hat{\mu}_3, \hat{\mu}_4$ and their estimated covariance matrix.

Assuming that the vector $\hat{\mu}$ is normally distributed with true mean μ and covariance matrix U , the quantity

$$S(\mu) = \sum_{i=1}^4 \sum_{j=1}^4 C_{ij} (\hat{\mu}_i - \mu_i) (\mu_j - \mu_j) \quad (1)$$

has a chi-square distribution with four degrees of freedom, χ_4^2 , where $C = U^{-1}$. (This is only an approximation, since U is not known exactly but was estimated using the data.) If μ is determined by a dose-response model that depends on k parameters, which are estimated in such a way as to minimize $S(\mu)$, then the resulting minimum value of $S(\mu)$ is distributed approximately as χ_{4-k}^2 . This fact was used to test several proposed forms for the standard dose-response curve.

The following logistic model was found to give an excellent fit:

$$\mu = \log \left[\frac{1 + ce^{a+bx}}{1 + e^{-bx}} \right], \quad (2)$$

where μ is the standard index at dose x and a , b , and c were estimated by minimizing $S(\mu)$ in (1). Upper and lower bounds for the curve (2) were constructed by defining as "acceptable" any values for a , b , and c in (2) that gave a value of $S(\mu)$ less than the upper 5% point of the χ_4^2 distribution. The upper and lower boundary curves contain all curves (2) corresponding to acceptable values of a , b , and c .

For the standard curve to be useful in an assay, it is desirable to express variation among donors in terms of a relative potency ρ . Thus, for the i th donor pool, we consider the model

$$\mu = \log \left[\frac{1 + ce^{a+b\rho_i x}}{1 + e^{a+b\rho_i x}} \right], \quad (3)$$

where a , b , and c are the parameters previously estimated for the standard curve. It was found that the relative potency model (3) fitted the data well. Moreover, the hypothesis that $\rho_i = 1$ for all i was rejected, indicating the existence of variation among donor pools beyond that which can be explained by variation among recipient litters. The distribution of the relative potencies for the 34 donor pools was also examined.

As a final check on the influence of other experimental variables, the residuals from the model (3) were calculated. These residuals are primarily an expression of variation among litters, with some effect of variation within litters as well. They were plotted against age of recipient, litter number, and sex of donor. Analysis of variance methods showed no influence of these variables on the residuals. However, the estimated variance of the residuals does increase with dose, nearly sixfold over the range of doses covered in

this experiment. Because of this, it may be difficult, when using the standard curve, to determine the precision of a potency estimate based on the injection of a single dose into a single litter.

ENVIRONMENTAL SCIENCES DIVISION

EFFECT OF NITROGEN, PHOSPHORUS, AND POTASSIUM ON CROP UPTAKE OF CESIUM AND COBALT

J. J. Beauchamp J. A. Adepetu¹

Members of the Environmental Sciences Division have been conducting an experiment to study the effect of nitrogen (N), phosphorus (P), and potassium (K) fertilization on the crop uptake of radioactive cesium (Cs) and cobalt (Co) from a contaminated soil. The experiment was set up and analyzed as a 3 X 3 X 3 factorial design with the factors at the following levels:

1. N was at 0, 50, and 100 lb/acre.
2. P was at 0, 25, and 50 lb/acre.
3. K was at 0, 75, and 150 lb/acre.

Each of the 27 combinations of N, P, and K was replicated three times, where each replicate represented an individual plant pot. The observation for each of the elements of interest represented the activity in picocuries per gram weight of harvested material.

An equal number of Japanese millet seeds were planted in each pot and allowed to mature, and the crop from each pot was harvested. The results from these plant tissues represent crop 1. From the remaining stalk and roots in each pot, the plant was allowed to mature, at which time it was harvested again. This crop had results from seeds as well as plant tissue material and represents crop 2. The soil in each pot was mixed again, and new seeds were planted. The results from the plant tissue material of the harvest of these seeds represent crop 3.

From the observed concentrations of Cs and Co, an analysis of variance was performed on the results from each of the three crops. At the 1% level of significance, the linear nitrogen effect on the cobalt concentration in plant tissue of crops 1 and 2 and the quadratic nitrogen effect in the cesium concentration of crop 1 were significant. Phosphorus did not have a significant effect in any of the crops or element concentrations observed. For the cesium concentration from the plant tissue of crop 2, the quadratic potassium effect was found to be significant at the 1% level of significance. The linear potassium effect was significant at the 1% level of significance for the cesium concentration in crop 1, for the cobalt concentration in the plant tissue of crop 2, and for the cesium concentration in the seeds of crop 2. None of the three-factor interactions between N, P, and K was found to be significant. Only the following two-factor interactions were found to be significant at the 1% level of significance:

1. the linear X linear and quadratic interaction between P and K for the cesium concentration of crop 1
2. the quadratic X quadratic interaction between N and P for the cobalt concentration of crop 1

It was interesting to note that none of the main effects or interactions were significant for crop 3, possibly indicating a depletion of the elements from the soil by this time.

1. IAEA Fellow, Environmental Sciences Division.

IRRADIATION OF SEEDS - 1971 DATA

J. J. Beauchamp Linda K. Mann²

An earlier report² described a study initiated by members of the Environmental Sciences Division to investigate the effect of chronic irradiation on production and germination of tall fescue (*Festuca arundinacea*) seeds, and described the results from the analysis of seeds collected during the summers of 1969 and 1970. During the summer of 1971, standing panicles were again gathered from the same eight plots that were in the original experiment started in 1968. These were also the same eight plots from which the data were collected for the 1969 and 1970 analysis. No new treatments had been administered to these plots, so the purpose of the 1971 study was to determine whether the factors (grazing cotton rats and irradiation) considered in the earlier analyses still had any significant effect upon the responses to be mentioned. By using the same experimental design as was used for the 1970 data, the same analysis of variance may be used to test for significant factors. In this 1971 study, approximately 16 standing panicles were collected from each subplot, and the following quantities for each panicle were observed: (1) total number of seeds, (2) proportion of seeds that germinate, and (3) proportion of seeds that are empty. Because of physical limitations, it was not possible to use all of the seeds produced for the estimation of the proportion germinated and empty seeds. Therefore, a random sample containing approximately 50% of the total seeds produced was used in order to estimate these proportions.

A first investigation of the data from the 1971 study tested whether the factors of grazing and irradiation had significant effects upon the total seed production. Since the observations of total seed production represent a count, the square root transformation was employed in order to more nearly satisfy the distributional assumptions of the analysis of variance. From the results of the analysis, the only nonsignificant factor at the 5% level of significance was the plot-effect factor.

Although there was an unequal number of observations from each subplot, it was possible to obtain a pooled estimate of the basic variability between the observations within a subplot. This variance estimate was used to determine whether there was a significant difference in the subplot effect from one subplot to another within a plot. At the 1% level of significance, the subplot effect was found to be significant in three of the four plots which received no irradiation.

An analysis was also performed on the proportion of sampled seeds that germinated. Before analyzing the proportion of germinated seeds, this observed random variable was transformed by the arc sine transformation. This transformation was used in order to more nearly satisfy the assumptions in the analysis of variance. From the results of this analysis, the interaction between the grazing and irradiation factors was found to be significant at the 5% level of significance.

The arc sine transformation was used on the proportion of empty seeds in the sample, and analysis of variance was performed on these random variables. From the results of this analysis, the irradiation effect was found to be significant at the 5% level of significance.

ANALYSIS OF LITTER STUDY DATA

J. J. Beauchamp Tom Grizzard²

Recent work in the Environmental Sciences Division gave information on major nutrients in overstory vegetation of different forest types within the Walker Branch Watershed. The quantities observed in this

2. Environmental Sciences Division.

3. Math. Div. Annu. Prog. Rep. Dec. 31, 1970, ORNL-4661, p. 164.

study were (1) total litter production and (2) total content of nutrients in the three following components of litter: leaves, limbs, and reproductive parts.

In order to estimate the necessary litter fall information, 80 litter traps were distributed throughout 300 $\frac{1}{2}$ -acre plots proportional to the presence of four forest types in the watershed; that is, if 60% of the watershed were made up of pine, then 60% of the 80 litter traps were randomly placed in those $\frac{1}{2}$ -acre plots of pine. The four basic forest types were determined on the basis of species-density-height classes within the 241-acre watershed and were (1) pine, (2) pine-oak-hickory, (3) oak-hickory, and (4) mesophytic hardwood. The location of the litter trap in each plot was randomly chosen by distance from the center of the plot and by degrees from grid north.

The litter collected was separated into the three components: (1) leaves and needles, (2) limbs and bark, and (3) reproductive parts. At the end of the experimental period the following quantities were observed for each litter box: (1) total dry weight (DW) of litter measured in grams and (2) total content of the following elements in litter measured in milligrams: calcium (Ca), magnesium (Mg), potassium (K), sodium (Na), nitrogen (N), and phosphorus (P).

Therefore, from each litter box there were three 7×1 observation vectors which contained the total dry weight of litter and the total amount of the six elements of interest for the entire experimental period. One of the observation vectors was for leaves, one for limbs, and the third one for reproductive components. For these three litter components, and also for the total litter collected in the 80 boxes, it was desired to determine if there were significant differences among the four forest types. By using the multivariate technique, canonical analysis, it was possible to make inferences about the different forest types.

In Fig. 24a, a plot of the first two canonical variates for the mean vectors of the leaf litter components from each forest type is given along with 95% confidence circles. From this figure, the pine and pine-oak-hickory forest types do not appear to differ significantly. However, the oak-hickory and mesophytic hardwood types appear to differ significantly from each other and also from both pine and pine-oak-hickory. In Fig. 24b, a similar plot is given for the limb litter component. From this figure, pine,

Fig. 24. Mean canonical points with 95% confidence circles.

pine-oak-hickory, and oak-hickory do not appear to differ significantly, but there is a slight indication that mesophytic hardwood differs from pine-oak-hickory and oak-hickory. In Fig. 24c, where the reproductive litter component is considered, pine appears to differ significantly from the other three forest types. However, the general overlapping of the confidence circles for pine-oak-hickory, oak-hickory, and mesophytic hardwood indicates no essential difference among these three forest types. As a final consideration, the total litter from leaves, limbs, and reproductive components was combined, and the first two canonical variates from the mean vectors for each forest type were plotted along with the associated 95% confidence circles (Fig. 24d). From this figure, pine and pine-oak-hickory appear to differ significantly from oak-hickory and mesophytic hardwood, but pine and pine-oak-hickory do not appear to differ significantly from each other. Again there is a slight indication that oak-hickory and mesophytic hardwood differ significantly from each other.

EFFECT OF RADIATION-INDUCED MUTATIONS ON THE FITNESS OF *DROSOPHILA* POPULATIONS

J. J. Beauchamp H. H. Shugart²

A study has been conducted by members of the Environmental Sciences Division to study the effect of radiation on the rate of change in the frequencies of *Drosophila melanogaster* and *Drosophila simulans* when the two populations are in competition. Equal numbers of *D. melanogaster* and *D. simulans* were placed in the same environment, and the male *D. simulans* were treated with a fixed dose of radiation (0, 250, 500, or 1000 rads) at the start of the experiment and every 21 days for 147 days. Equal numbers of males and females at the same stage of development were utilized. Except for one dose (1000 rads), there were replicate cages at each dose.

At 21-day intervals after the initial radiation was administered, the total number of *D. melanogaster* and *D. simulans* was recorded for each cage. The number of *D. melanogaster* and *D. simulans* at different times after irradiation for a particular cage constitutes a vector of observations. All of the *Drosophila* used in this experiment came from two basic highly inbred lines, denoted as stock type 1 or 2. From these data the following questions were considered:

1. By using the percentage of *D. simulans*, total population size, number of *D. simulans*, and percentage of *D. melanogaster*, is there a significant treatment effect?
2. By using the same observation vectors mentioned in question 1, is there a significant stock difference within a treatment group?

The statistical technique used to answer the above questions was canonical analysis. The first and second canonical variates for the mean vector of each treatment group with an associated 95% confidence circle of uncertainty are used to infer treatment differences. By considering only the observation vectors within a treatment group (e.g., the control group) and partitioning these vectors into two groups, one for stock type 1 and the other for stock type 2, a significant stock type difference was found for each of the responses mentioned in question 1. Therefore, the observation vectors from each stock type were considered separately for the canonical analyses used in answering the question 1.

In Fig. 25, the results of the canonical analysis, omitting the observation vectors from stock type 2, are shown. Because of the small number of observation vectors and the constraints of canonical analysis, only five of the observation times could be used. Therefore, since the main interest was in the later periods of observation, the last five observation times were used in the analysis for stock type 1. From this figure the following conclusions may be made:

Fig. 25. Mean canonical points with 95% confidence circles.

1. In Fig. 25a, where the observation vectors consist of the total population size at the specified times, the treatment groups fall into two clusters that differ significantly from each other. The first cluster consists of the control and 1000-rad treatment groups, which do not differ significantly. The second cluster consists of the 250-rad and 500-rad treatment groups, which again do not differ significantly.
2. In Fig. 25b, where the observation vectors consist of the percentage *D. melanogaster* in the population at the specified times, the conclusions are not quite as obvious because of the general overlapping of the confidence circles. The only clear-cut conclusion from this figure is that the 250-rad treatment group differs significantly from both the control and 500-rad treatment groups.
3. In Figs. 25c and 25d, where the observation vectors consist of the percentage *D. simulans* and total number of *D. simulans* in the population at the specified times, respectively, the four treatment groups each differ significantly from each other. It is interesting to note in Fig. 23d that the control and 1000-rad treatment groups appear to be concentrated in one region of the graph, and the 250-rad and 500-rad treatment groups are concentrated in another region of the graph. This conclusion may be compared with the partitioning that was observed in Fig. 25a.

A similar canonical analysis was performed on the four responses of interest by using the observation vectors from stock type 2. In this analysis there were only two treatment groups (control group and the 500-rad group). Again it was necessary to limit consideration in this analysis to the last four times of observation because of the constraints of canonical analysis. Although not shown here, the mean canonical points with the associated 95% confidence limits were disjoint for the two treatment groups, except for the response of percentage *D. simulans* in the population. Therefore, by considering the four responses mentioned earlier, a significant treatment effect is present in stock type 2 except for the response of percentage *D. simulans* in the population.

CHYDORID ECOLOGY

J. J. Beauchamp M. C. Whiteside⁴

A study carried out in Elk Lake, Minnesota, was conducted by Whiteside to test methods of collecting chydorid populations which live in the littoral muds, the submerged vegetation, and the open water. Two quadrates were constructed over an offshore shoal in Elk Lake. Forty numbered stakes, spaced approximately 1 m apart, were placed in each quadrate, and a weighted Tuffy ball was placed next to each stake. The Tuffy balls were used in order to provide an area readily inhabited by chydorids. Approximately ten days after the Tuffy balls were submerged, all odd-numbered stations were sampled. The following week, even-numbered stations were sampled, and the routine continued for 25 weeks. A total of 40 stations were sampled each week, and the counts of animals for each date and station were recorded.

For any fixed date, the variance of the observed counts was always greater than the mean number of counts observed, which implied the possibility of a patchy pattern to the distribution of the chydorids. It has been suggested that the negative binomial distribution is the appropriate distribution for such data. Therefore, a negative binomial distribution was fitted, using the method of moments, to the observed counts for each of the 25 sampling dates. In addition, a chi-square goodness-of-fit test was performed to test the fit of the chydorid data to the negative binomial distribution. At the 1% level of significance the data from one date were found to differ significantly from the negative binomial distribution. This date was during a peak in numbers for the population. Since the patchy pattern for the distribution of the chydorids may not be evident during peak population numbers, this may explain the reason for the significance at this date. Therefore, from these data the null hypothesis that the distribution of chydorid populations follows the negative binomial distribution would not be rejected.

4. Department of Zoology, University of Tennessee, and Environmental Sciences Division.

METALS AND CERAMICS DIVISION

FREQUENCY DISTRIBUTION PLOTTING POSITIONS

D. G. Gosslee

When observed frequency distributions are analyzed, a plot of the cumulative distribution is often made. An easy, and perhaps common, procedure is to plot pairs of values, x_j and $j/(N+1)$, where $j = 1, 2, \dots, N$ and the x_j 's are ordered so that $x_1 \leq x_2 \leq \dots \leq x_N$. A plotting procedure may be used to test the assumption that the frequency distribution is Gaussian, or assuming a Gaussian distribution, it may be desired to estimate certain percentiles. In either case, the ratio $j/(N+1)$ is a good approximation only for large N .¹ The ratio $(j - 3/8)/(N + 1/4)$ is nearly exact for small samples, is good for large N , and is easy to use. However, this ratio is not necessarily good for non-Gaussian distributions. Kimball¹ and Gumbel² have compared approximations for other distributions. For example, the ratio $j/(N+1)$ has advantages for extreme value data, especially in estimating the return period.²

1. B. F. Kimball, *J. Amer. Statist. Ass.* 55, 546-60 (1960).

2. E. J. Gumbel, *Statistics of Extremes*, Columbia University Press, New York, 1958.

VARIABILITY OF SS308 WELDING RODS

T. L. Hebble G. M. Goodwin³

The Welding Research Council is conducting a study of the variability of SS308 welding rod composition. Four major weld rod producers submitted analytical data consisting of their own chemical analysis and a corresponding analysis from the mill which supplied the stainless steel. Tolerance limits were determined for all components from each producer. In several cases, the producer's analysis differed significantly from the mill analysis. For example, some mills tended to submit higher nickel and lower carbon analyses than those determined by the producers. Identification of mill is being sought so that problems common with certain mills can be detected.

A tolerance ellipse ($P = 0.90$, $\lambda = 0.95$) based on estimates of errors in analytical technique covered a 3% ferrite range in the Schaeffler diagram for stainless steel welds. Thus, from a single measure of nickel and chromium equivalents, the uncertainty in ferrite composition due to component chemistry is 3% ferrite. The error in the analytical technique to determine composition was estimated from the differences between mill and producer analysis and included a bias correction. This error was then used to estimate the variability of chromium and nickel equivalents applicable to the Schaeffler diagram. Ferrite measurement error and variability of ferrite composition within a single weld pad were not included. An experimental program has been proposed to complement an existing ferrite measurement study so that a complete statistical analysis of the Schaeffler diagram can be made.

ANALYSIS OF FAST FLUX TEST FACILITY WELD DATA

T. L. Hebble R. T. King³

Multiple comparison and analysis of variance techniques were applied to tensile property data from Fast Flux Test Facility vessel test welds prepared by joining 2 $\frac{3}{8}$ -in.-thick type 304 stainless steel plates with type 308 rods. Longitudinal specimens taken close to the surface of the weld tended to have significantly lower strength and greater strain properties than those specimens taken from locations deeper into the weld. As expected, test temperature significantly affected most of the 18 responses, the magnitude of the effect diminishing with increasing temperature. Virtually all two-factor interactions were nonsignificant. The complete statistical analysis will include results of specimens now being tested.

EXPERIMENTAL PROGRAM FOR PRESSURIZED WATER REACTOR AND BOILING WATER REACTOR FUEL CLADDING EMBRITTLEMENT STUDIES

T. L. Hebble J. R. Weir, Jr.³

An experimental program is proposed to study the effects of transient temperature, cladding configuration, quench temperature, and fuel sensible heat on pressurized water reactor fuel cladding embrittlement. A summary of the statistical design for a set of 12 experiments is shown in Fig. 26 for one of seven transients. A similar set exists for each transient temperature. Seven sets of 12 experiments plus 30 replications to measure experimental error require a total of 114 quenches for the PWR case. A similar experimental design can be constructed for boiling water reactor tubes; however, much of the information from the above experiments will be representative of the BWR tubing behavior, and fewer experiments will be necessary.

Fig. 26. Revised experiment design for cladding embrittlement study.

A binary response such as the fracture–no-fracture response to be used in this program presents difficulties in statistical analysis. For example, the calculated effect due to quench temperature is the difference between the fraction of failures on immersion at 2200°F and the fraction of failures on immersion at 900°F. Statistical tests on these differences are not very sensitive. That is, when the response is binary, such tests are less likely to detect a significant difference (and, hence, a significant effect) when, in fact, one exists. This difficulty may dictate the need for more experiments to improve sensitivity.

MIXED OXIDE REACTOR FUELS

F. L. Miller, Jr. R. B. Fitts³

The analysis of data from the SG-3 test capsule reported earlier⁴ has been completed.⁵ The use of low-order polynomial regression of one thermocouple on another combined with probability plots and plots of the residuals vs time enabled us to detect anomalous behavior in the data recording equipment, eliminate nonsteady-state data, and detect changes in the conditions of the reactor environment. Figures 27 and 28 show the effect of eliminating aberrant and nonsteady-state data on the relationship between average heat generation rate and center-line temperature. We were able to conclude at the 99% confidence level that for a given fuel center temperature, the Sphere-Pac fuel produces $11.7 \pm 1.2\%$ more heat than the pellet fuel.

4. Math. Div. Annu. Progr. Rep. Dec. 31, 1971, ORNL-4761, p. 169.

5. R. B. Fitts and F. L. Miller, Jr., *Trans. Amer. Nucl. Soc.* 15, 180 (1972).

Fig. 27. Sphere-Pac fuel central temperature in SG-3 as a function of heat generation rate. All steady-state data included.

Fig. 28. Sphere-Pac fuel central temperature in SG-3 as a function of measured heat generation rate. Refined data.

NUCLEAR SAFETY PROGRAM

THERMOCOUPLE DETERIORATION IN LIQUID METAL FAST BREEDER REACTOR FUEL FAILURE MOCKUP STUDY

T. L. Hebble L. F. Parsly¹

Using nonparametric techniques, thermocouple deterioration as measured by a linear time effect was not detected in readings from five repeated experiments in the liquid metal fast breeder reactor Fuel Failure Mockup study. Although average reading tended to decrease with time, the negative slopes were not statistically significant. Three thermocouple types were included in the study: (1) channel exit, (2) ungrounded junction wire wrap, and (3) grounded junction wire wrap.

EFFECT OF CHANNEL BLOCKAGE AND COOLANT FLOW RATE ON DIMENSIONLESS TEMPERATURE

T. L. Hebble L. F. Parsly¹

A statistical analysis was performed on two sets of dimensionless temperature data from thermocouples in liquid metal fast breeder reactor Fuel Failure Mockup (FFM) bundle 2B. Each data set consisted of thermocouple readings from six channels taken 3 in. into the bundle. One set included data from experiments when all fuel rods were heated and the other from experiments in which one rod was not heated.

By regression analysis methods, a strong quadratic effect due to channel blockage was detected for most channels. It is believed that the mechanical structure which generated the 24-channel blockage created a substantially different coolant flow pattern within the bundle. As expected, the linear effect due to coolant flow was significant. Reactor power level exhibited little or no effect on dimensionless temperature.

1. Nuclear Safety Program.

OAK RIDGE ASSOCIATED UNIVERSITIES MEDICAL DIVISION

AN ANALYSIS PROPOSAL FOR A BIRTH CONTROL PILL STUDY

W. E. Lever L. B. Littlefield¹
F. L. Miller, Jr. J. B. Mailhes¹

A proposal has been submitted for the analysis of data collected over a period of three years on a group of people to study possible effects of birth control pills on rate of occurrence of chromosomal aberrations. Blood samples were taken from each subject on a somewhat periodic basis during the three years. From each blood sample a culture was formed; and if the culture was successful, 100 metaphases were scored for chromosomal aberrations.

Initially, the group was divided into three classes: men, women who had never used birth control pills, and women who were using birth control pills. However, during the course of the study, several of the women stopped using birth control pills for a period of time. Some of these women became pregnant and

1. Medical Division, Oak Ridge Associated Universities.

returned to the use of birth control pills at the end of their pregnancy; some women did not use birth control pills for the remainder of the study. In addition to the above changes, several women left the study.

Since a preliminary analysis of the data indicates that analysis of variance techniques would not be appropriate, rank tests have been proposed as a method of comparing the responses of the various groups.

REACTOR DIVISION

CONFIDENCE STATEMENTS FOR CRACK LENGTHS OF REACTOR BOLTS

W. E. Lever J. J. Beauchamp

During a periodic inspection in late 1971, three closure bolts were removed from the upper lead flange of the High Flux Isotope Reactor pressure vessel for examination. Dye-penetrant testing revealed several small cracks.

By using the observed crack lengths of the 3 available bolts from a total population of 44, confidence statements were made concerning the crack lengths. These statements were based on the following assumptions:

1. the observed crack lengths were a random sample from an infinite population of crack lengths,
2. the probability distribution of crack lengths is the normal probability distribution.

The validity of the second assumption was almost impossible to verify, since only a few data points were available. The necessary information for the calculation of upper tolerance and confidence limits was made available. In addition, tolerance statements for the probability that 2 or fewer and 5 or fewer of the remaining 41 bolts have crack lengths greater than a specified value were also calculated from the observed data.

SAMPLING FROM A FINITE POPULATION

T. L. Hebble V. R. R. Uppuluri
W. E. Lever

A request was made to determine the number of welds to be inspected in a buried stainless steel pipeline so there is some degree of assurance that no defectives would remain in the uninspected portion. Prior to use as a waste pipe, excessive corrosion was detected in welds connecting several lengths of pipe. In one section of pipe there were a large number of defective welds, while in another section, on the opposite side of the hill, there were virtually no defective welds. A third stretch of pipeline containing 56 welds remains to be inspected. The question arose as to how many welds should be inspected so there is a probability of 0.99 that there are no defective welds in the uninspected section. Assuming that the number of defective welds followed a binomial distribution, finding no defects in a sample size of 55 (out of 56) would not be sufficient to generate a probability of 0.99 that the last weld is not defective. Other distributions for the number of defective welds were considered, each yielding similar results. The reasons for such a high proportion of the population to be sampled are that the population is finite and that the probability level and number of acceptable defectives in the remaining sample are too restrictive.

Y-12 PLANT

STATISTICAL ANALYSIS OF LATHE MAINTENANCE DATA

T. L. Hebble D. R. Passons¹

Mechanical and electrical maintenance data on 226 lathes from seven shops over a two-year period (1969–1971) were analyzed by multiple comparison techniques. Hours of total utilization per maintenance hour were compared in several partitions of the data, including a comparison of all lathes from seven shops and a comparison of manufacturers of numerical control, straight, and tracer lathes. Although several shops and lathe types exhibited significantly lower lathe utilization per maintenance hour, in most cases these shops and lathes also performed the more complex and exacting work.

EVALUATION OF SOME OF THE MECHANICAL PROPERTIES OF A TUNGSTEN, NICKEL, AND IRON ALLOY

W. E. Lever

A series of eight experiments was set up and analyzed to investigate mechanical properties of a tungsten, nickel, and iron alloy.

The properties were measured on tensile bars cut from hollow cylinders in both the vertical and horizontal directions. Since it is known that the top, middle, and bottom of the cylinders produce slightly different results, all cylinders were sampled in each of these three regions.

In order to evaluate methods of forming the cylinders, they were subjected to various conditions during their formation, such as prestraining, thermal aging, different types of tooling, and various furnace heat cycles. The mechanical properties were then measured on the tensile bar under the influence of several temperatures.

In addition to the comparison of the effects of the various factors, tolerance limits and prediction equations were computed for some of the property levels for several of the experiments.

Further consideration of the mechanical properties of this alloy is expected in the future.

1. Fabrication Division, Y-12.

Statistical Programming

A USE OF THE FORMAC SYMBOLIC MANIPULATION LANGUAGE

T. C. Tucker J. J. Beauchamp

Work has continued in the application of the FORMAC symbolic manipulation language, described in a previous report.¹ A program has been written to produce the necessary partial derivatives which may be used in certain nonlinear regression codes. The program allows the function and coefficients to be specified as symbolic data and, in addition, if the function of interest is too large to be written in one expression, to be broken into pieces. The output of the program, which gives the partial derivatives of the input function with respect to specified parameters, is given both in common algebraic form and in a form similar to that

1. *Math. Div. Annu. Progr. Rep. Dec. 31, 1971, ORNL-4761, pp. 175–76.*

used in FORTRAN coding. Numerical values may be substituted for any of the quantities in the input function to obtain numerical function or partial derivative values. In addition to ordinary batch operation, this code can be submitted directly from CRBE.

DATANAL

Norma Hull

A computer program, DATANAL, has been written to present a graphical and basic statistical analysis of data. Data sets may be read in, transformed, and plotted in pairs at the user's option. The elementary statistics which are printed out are means, standard deviations, and correlation coefficients.

CANONICAL ANALYSIS PROGRAM

Norma Hull J. J. Beauchamp

The canonical analysis program RELSIM² has been updated to permit internal scaling on the two plots produced by the program. One plot is of the raw data. The other is a plot of the means of the groups and the associated confidence circles at a chosen level of significance.

TAT DATA

Norma Hull E. Leach
J. J. Beauchamp F. L. Miller, Jr.

A series of computer programs are being written to analyze data obtained from a sample of 400 students who have completed the Training and Technology (TAT) program at the Y-12 Plant. The data cover personal and community history in addition to job evaluation records. At this initial stage, preliminary analyses are being performed on such variables as job classification, job satisfaction, and student-supervisor evaluation of the TAT program. Later, more sophisticated statistical methods will be used to investigate areas of greatest interest.

FEIUDR PROGRAM

E. Leach

The FEIUDR program is a revised version of an older program written in FORTRAN 63. The revised program is written in FORTRAN IV and has been changed to enable the user to run the program through a remote terminal attached to the FDP-10 computer at the Mathematics Division of the Oak Ridge National Laboratory.

The data are automatically punched into paper tape by a counter and later read into a file to be used by the program as the input file. The counter that punches the tape has three channels and can punch data from any or all of the channels. The program will process data from a single isotope experiment or a double isotope experiment. The data tape will contain data from one channel for single isotope experiments and data from two channels for double isotope experiments. The data consist of group numbers, test tube numbers within each group, and counts taken on the test tubes in each group.

The desired statistics computed from the counts for each group consist of the mean, the variance, the standard deviation, the standard error, and the total number of counts.

2. *Math. Div. Annu. Progr. Rep. Dec. 31, 1969*, ORNL-4514, pp. 71, 125.

NEWINDEX

Norma Hull J. J. Beauchamp

A computer program, NEWINDEX, has been written to compute the daily index and the TRENDINDEX calculation from pollutant concentration data.³ The program prints a table containing the standards, background, and weight for each pollutant used in the calculation of the two indices. Also, for each day the daily index, TRENDINDEX, the condition (either good, undesirable, unhealthy, or no data), and the raw concentration for each pollutant are printed.

The program produces three plots – daily index, TRENDINDEX, and daily index and TRENDINDEX combined – to help interpret the data.

CONVERSION OF COMPUTER PROGRAMS

E. Leach

Several programs have been written in the BASIC programming language to create various combinations of pathological data files. Originally these programs were written to be used on the commercial time-sharing computers.

Many programming changes were necessary to allow the user to run the programs on the PDP-10 computer located at the Mathematics Division of the Oak Ridge National Laboratory. Most of the changes made were in reference to the naming, scratching, reading, and writing of files.

EXTENSION OF A TABLE FOR GROUP TESTING

G. Hirsch⁴ W. E. Lever

E. Leach

Sobel and Groll⁵ produced several tables which enabled one to calculate the expected number of groups required to classify each of N objects as being good or defective. One function

$$F_1^*(m) = \sum_{i=1}^m q^{i-1} + \min_{1 \leq x \leq m-1} [q^x F_1^*(m-x) + F_1^*(x)]$$

and

$$F_1^*(1) = 0,$$

which was important in calculating the expected number of tests required to classify all the objects under the R_1 procedure, was tabulated for several values of q for $m = 1$ to 16.

This table has now been extended to include values of m up to 25. This result was accomplished by the use of a program written for the IBM 360-75.

3. J. J. Beauchamp and Norma C. Hull, "Air Quality Indices," this report.

4. ORAU Fellow.

5. M. Sobel and P. A. Groll, "Group Testing to Eliminate Efficiently All Defectives in a Binomial Sample," *Bell System Tech. J.* 18(5), 1179 (September 1959).

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- Dwyer, P. S. (University of Michigan, Ann Arbor, Michigan), "The Selection of Variables in Regression," April 13, 1972.
- Funderlic, R. E. (Mathematics Division, ORNL), "Computational Aspects of Linear Least Squares," December 6, 1972.
- Gautschi, Walter (Purdue University, Lafayette, Indiana), "On Practical Fourier Analysis," April 4, 1972.
- Kaper, Hans G. (Argonne National Laboratory, Argonne, Illinois), "The Use of Interpolatory Polynomials for a Finite-Element Solution of the Multi-Group Diffusion Equation," February 14, 1972.
- Leaverton, P. (University of Iowa, Iowa City, Iowa), "Statistical Methods in Human Experiments," May 17, 1972.
- Levin, S. A. (Cornell University, Ithaca, New York), "Structural Aspects of Mathematical Modeling and Ecological Communities," January 10, 1972.
- Meyer, Gunter H. (Georgia Institute of Technology, Atlanta, Georgia), "Invariant Imbedding for Fixed and Free Boundary Value Problems," February 4, 1972.
- Mitchell, T. J. (Mathematics Division, ORNL), "A Method for Selecting Samples from a Finite Population," January 26, 1972.
- Nelson, William (University of Pittsburgh, Pittsburgh, Pennsylvania), "X and Y Functions of Chandrasekar," May 17, 1972.
- Quesenberry, C. P. (North Carolina State University, Raleigh, North Carolina), "Conditional Probability Integral Transformations," August 25, 1972.
- Rubinstein, Robert (Massachusetts Institute of Technology, Boston, Massachusetts), "Local Solvability of Partial Differential Equations with Multiple Characteristics," April 17, 1972.
- Wilson, D. G. (Virginia Commonwealth University, Richmond, Virginia), "The Time-Dependent Linear Transport Equation in a Multidimensional Parallelepiped with Partially Reflecting Walls," May 8, 1972.
- Wilson, D. G. (Mathematics Division, ORNL), "Piecewise Linear Approximations of Fewest Line Segments," September 27 and October 4, 1972.

Professional Activities

Beauchamp, J. J., Referee, *Biometrics*.

Beauchamp, J. J., Referee, *Journal of the American Statistical Association*.

Bowman, Kimiko O., Referee, *Journal of Statistical Computation and Simulation*.

Bowman, Kimiko O., Assistant Professor, University of Tennessee.

Brooks, A. A., Member, ACM SIGPLAN Committee for Symposium on Data Structures in Programming Languages.

Brooks, A. A., Member, COINS Committee, University of Florida.

Carter, H. P., Associate Professor, University of Tennessee.

Carter, H. P., Co-chairman, Computer Operations Managers Seminar, Kansas City, September 1972.

Carter, H. P., Report on Computer Operations Managers Seminar, Atomic Energy Systems, Operations, and Programming Association, Idaho Falls, October 1972.

Carter, H. P., Chairman, Working Session of Association for Scientific Computer Information Exchange, Oak Ridge, October 1972.

Chang, S. J., Lecturer, University of Tennessee.

Chang, S. J., Lecturer, Traveling Lecture Program, Oak Ridge Associated Universities.

Coleman, P. R., Instructor, University of Tennessee.

Coveyou, R. R., Lecturer, Traveling Lecture Program, Oak Ridge Associated Universities.

Crowell, J. S., Instructor, University of Tennessee.

Dolan, J. M., Lecturer, University of Tennessee, Oak Ridge Resident Graduate Program.

Dolan, J. M., Lecturer, Traveling Lecture Program, Oak Ridge Associated Universities.

Dolan, J. M., Referee, *Journal of Differential Equations*.

Funderlic, R. E., Lecturer, University of Tennessee.

Funderlic, R. E., Referee, American Mathematical Society and Society for Industrial and Applied Mathematics.

Gardiner, D. A., Associate Professor, University of Tennessee.

Gardiner, D. A., Member, Editorial Advisory Board, *Journal of Statistical Simulation and Computation*.

Gardiner, D. A., Member, Editorial Board, *Communications in Statistics*.

Gardiner, D. A., Editor, *Technometrics*.

Gardiner, D. A., Chairman, Section on Physical and Engineering Sciences, American Statistical Association.

Gardiner, D. A., Member, Council of the American Statistical Association.

Gardiner, D. A., Member, Committee on the Constitution, American Statistical Association.

Gardiner, D. A., Member, Regional Committee on Statistics, Southern Regional Education Board.

Gardiner, D. A., Consultant, Office of Director of Regulation, U.S. Atomic Energy Commission.

- Gardiner, D. A., Lecturer, Visiting Lecture Program in Statistics, Committee of Presidents of Statistical Societies.
- Gosslee, D. G., Lecturer, Oak Ridge Graduate School of Biomedical Sciences, University of Tennessee.
- Gosslee, D. G., Member, Program Committee, Biometrics Society (ENAR).
- Gosslee, D. G., Lecturer, Traveling Lecture Program, Oak Ridge Associated Universities.
- Hamilton, H. J., Publication Review, Research, and Software, The Chemical Notation Association Newsletter.
- Heath, M. T., Referee, Society for Industrial and Applied Mathematics.
- Hebble, T. L., Lecturer, Traveling Lecture Program, Oak Ridge Associated Universities.
- Hermann, O. W., Referee, *Nuclear Science and Engineering*.
- Leinius, R. P., Assistant Professor, University of Tennessee.
- McCulloch, R. D., Referee, *Atomic Energy Review*.
- Miller, F. L., Book Reviewer, *Journal of Quality Technology*.
- Mitchell, T. J., Lecturer, Oak Ridge Graduate School of Biomedical Sciences, University of Tennessee.
- Mitchell, T. J., Referee, *Technometrics*.
- Mitchell, T. J., Referee, *Sankhya*.
- Mitchell, T. J., Consultant, University of Tennessee Memorial Research Center.
- Mitchell, T. J., Short-Course Instructor, University Extension, University of California at Los Angeles.
- Nelson, Paul, Lecturer, Traveling Lecture Program, Oak Ridge Associated Universities.
- Nelson, Paul, Referee, *Nuclear Science and Engineering* and *International Journal of Systems Sciences*.
- Nelson, Paul, Reviewer, *Mathematical Reviews* and *Computing Reviews*.
- Nelson, Paul, Member, Mathematical Modeling Committee, SIMULATION Councils, Inc.
- Nestor, C. W., Reviewer, *Computing Reviews*.
- Nestor, C. W., Referee, *Nuclear Science and Engineering*.
- Perry, S. K., Member, Shielding Subcommittee, Codes and Formats Subcommittee, and Nuclear Codes Task Force of the Cross Section Evaluation Working Group, Brookhaven National Laboratory.
- Penny, S. K., Reviewer, *Nuclear Science and Engineering*.
- Raridon, R. J., Secretary-Treasurer, Association of Academies of Science.
- Textor, R. E., Reviewer, *Zentralblatt für Mathematik*.
- Textor, R. E., ORNL representative, Numerical Analysis Special Interest Groups.
- Uppuluri, V. R. R., Referee, *Sankhya*.
- Uppuluri, V. R. R., Referee, *Bulletin of the Canadian Mathematical Society*.
- Uppuluri, V. R. R., Consultant, Medical Division, Oak Ridge Associated Universities.
- Uppuluri, V. R. R., Lecturer, Traveling Lecture Program, Oak Ridge Associated Universities.
- Uppuluri, V. R. R., Co-chairman, Planning Session on Undergraduate Mathematics.
- Whitesides, G. E., Executive Committee, Criticality Safety Division, American Nuclear Society.
- Whitesides, G. E., Executive Committee, Mathematics and Computations Division, American Nuclear Society.
- Whitesides, G. E., Chairman, Finance Committee, Mathematics and Computations Section, American Nuclear Society.

Whitesides, G. E., Chairman, Committee for the Validation of Computational Methods for Nuclear Criticality Safety, American Nuclear Society.

Whitesides, G. E., Member, Committee for Nuclearly Safe Pipe Intersections for Solutions of Fissile Materials, American Nuclear Society.

Whitesides, G. E., Member, Committee to Write Guide for the Storage of Low Enriched Uranium, American Nuclear Society.

Whitesides, G. E., Reference, *Nuclear Science and Engineering*.

Williams, C. S., Session Chairman, Computer Operations Managers Seminar, Kansas City, September 1972.

Publications

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