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DEVELOPMENT PROGRAM

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ADVANCED TECHNOLOGY LABORATORIES

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CONTENTS

Foreword	1
Objectives of Current Work	2
Status of Program	2
A. Hydrodynamics	2
B. Kinetics	2
C. Physics	3
1. "Simplified" Analysis	3
2. PUREE'	3
D. Critical Experiment	3
1. Fuel	3
2. Void Simulation	3
3. Possible Neutron Energy Spectrum Experiment	3
Summary of Results	4
A. Physics	4
B. Hydrodynamics	5
C. Integrated Calculations	5
D. Kinetics	6
I. Hydrodynamics	7
II. Kinetics	8
A. Objectives of Program	8
B. Present Status	8
C. Thermal Analysis of UO_2 Fuel Pins	9
1. Summary	9
2. Discussion	9
3. The Analog	10
4. Evaluation of Thermal Conductivity	13
5. Analog Results	14

6. Transfer Function	15
III. Physics	17
A. PUREE' Analysis	17
1. Constants of Groups 1, 2, and 3	18
2. Constants of Group 4	23
3. Examples of the Equations to be Solved by the Computational Scheme	24
B. "Simplified" Physics Analysis	29
1. Method of Approach	29
2. Results	30
3. Status of the Program	31
IV. Critical Experiment	32
A. Fuel Procurement	32
B. Void Simulation	32
C. Possible Neutron Energy Spectrum Experiment	32

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FOREWORD

Development of the Variable Moderator Reactor (VMR) is conducted under Contract No. AT(04-3)-250, Project Agreement No. 3, by Advanced Technology Laboratories, a Division of American-Standard, for the U. S. Atomic Energy Commission. This first quarterly technical progress report covers the initiation and progress of work under Phase I of the contract, "Physics and Kinetics Analysis and Initial Evaluation," and the preparation for Phase II, "Critical Experiment and Analysis of Results."

The information contained in this progress report is preliminary and subject to change as the program evolves.

OBJECTIVES OF CURRENT WORK

The current work being carried out in the development of the VMR and as defined in the proposal ¹ consists of the following tasks:

1. To carry forward the development of the boiling core physics model, PUREE', and the hydrodynamics model, BOCH, for the VMR and determine the best method of adapting them to high-speed computers.
2. To expand the existing analog representation of VMR core kinetics to include variables which may be significant.
3. To complete coding and testing of these models.
4. To establish certain parameters with sufficient accuracy to permit design of the critical assembly to commence.
5. To prepare a fuel element fabrication specification and to order the fuel for the critical assembly.

STATUS OF PROGRAM

The following sections describe the progress in each of the above areas of the initial phase of the VMR program.

A. Hydrodynamics

A flow sheet representing the sequence of calculations for the entire BOCH program has been prepared. Coding of the program has been completed, and portions of the code have been checked against hand calculations. The hydrodynamics of a single channel have been investigated, using a portion of the code.

B. Kinetics

A preliminary block diagram of the kinetics model of the VMR has been prepared, and the detailed evaluation of the transfer functions for the "Pin Heat Transfer" block have been completed.

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1. "Program for Evaluation of the Variable Moderator Reactor under the New Reactor Concepts Program of the Atomic Energy Commission," Atomic Energy Division of American-Standard, P-470A, December 17, 1958.

C. Physics

1. "Simplified" Analysis

A "simplified" physics analysis is nearly complete. It defines certain parameters in sufficient detail to permit the critical experiment design to commence. This analysis, based on simple diffusion theory, is only approximate for the clumped-type fuel assemblies in the VMR.

2. PUREE'

The PUREE' code is designed to give a much more accurate representation of the physics of the VMR core than the simplified analysis.

Flow sheets representing the sequence of calculations for the first three energy groups and for the fourth group of the four-group PUREE' model have been prepared. Certain improvements to the original PUREE' analysis have been made to account for the heterogeneous make-up of the fuel cells and to account for the velocity-dependent neutron current hardening in the fuel element. Coding is nearly completed. Portions of the code are being checked against hand calculations.

D. Critical Experiment

1. Fuel

A fuel element fabrication specification has been prepared and released to bidders for quotation.

2. Void Simulation

A study has been made to select the most appropriate material for void simulation throughout the range of interest in the VMR. Furfural, furfuryl-alcohol, and water combinations were determined to be the most suitable for this purpose. The study has been completed.

3. Possible Neutron Energy Spectrum Experiment

As one of the series of critical experiments of Battelle, an experiment to measure the neutron velocity spectrum as a function of radial distance from the center of the fuel cell is being considered. The necessity of such an experiment will be determined in the next quarter.

SUMMARY OF RESULTS

A. Physics

The concept of control by variable moderator level as presented in the VMR has many advantages, but some areas require special design. The area of most immediate importance is in the separation of the moderator from the coolant. This separation requires that the fuel pins be arranged in clumped bundles rather than in the more homogeneous distribution of water and fuel normally found in water reactors. With this arrangement of clumped fuel elements, the physics procedures normally employed are no longer appropriate for reliable reactor performance calculations. Some work has been done on clumped fuel elements in heavy water reactors, but the results are not applicable to the light water VMR system. Therefore, special physics procedures have been developed to treat the VMR. Although these procedures are developed specifically for the evaluation of the VMR, they will also be applicable to other reactors of similar geometry.

In general, the method of treating the physics of the VMR is as follows:

- 1) Derive the neutron continuity equations for a four-lethargy-group analytical model for the clumped fuel configuration.
 - 2) Obtain values for the constants of the four-group model.
 - 3) Using the values of the constants determined in "2," calculate neutron flux distribution.
- A major portion of the development program involves obtaining constants for the physics model. The problem is separated into two parts: the first three energy groups constitute one part, and the fourth, or thermal group constitutes the other. An IBM 650 machine code called PUREE' is used to compute the constants for these two divisions. The constants of the first three groups are obtained from the machine code as follows:
- 1) Compute the effective resonance integral and normalize.
 - 2) Spread the normalized resonance capture over the three energy groups.
 - 3) Read into the code non-resonance cross section data and isotopic concentrations.
 - 4) Make a 19-group calculation of neutron slowing down for each region, as if materials in a region were homogenized.

- 5) Determine the constants from the 19-group results and correct for heterogeneity of fuel cells.

The constants of the thermal group are also obtained from the PUREE' code as follows:

- 1) Compute the flux incident upon a fuel pin for 15 to 20 energy groups, and compute blackness by group.
- 2) Solve the neutron-balance integral equation for the neutron spectrum.
- 3) Adjust for those neutrons which diffuse into the fuel clump from the moderator region.
- 4) Using 1, 2, and 3, compute the flux in the fuel clump relative to the moderator flux with a P_3 calculation.
- 5) Using the computed flux, obtain weighted constants for the fourth group.

In order to verify that the physics methods developed in the PUREE' give accurate results, the code will be compared with known reactor systems, and the calculations will be checked by the VMR critical experiments. In this manner, the critical experiments will be used to verify the analytical procedures throughout the required range of VMR parameters.

B. Hydrodynamics

To obtain overall reactor performance of the VMR, it is necessary that the physics calculations be integrated with the hydrodynamic calculations of the reactor. For this purpose, a hydrodynamic IBM 650 code, called BOCH, has been developed. As with the physics code, PUREE', BOCH will be applicable to other boiling water reactors.

C. Integrated Calculations

It is planned that the various codes representing the VMR will be used in a procedure such as the following:

- 1) Assume a radial and axial neutron flux distribution in the VMR core.
- 2) Using the assumed flux distribution as input to the BOCH hydrodynamic code, compute the radial and axial void distribution.
- 3) Adjust the core orifice coefficients so the radial void distribution approaches a constant.
- 4) Compute the homogenized physics constants from the non-dimensional PUREE' code.

- 5) Using the homogenized constants and the axial void distribution as input to the one-dimensional physics VAL PROD² code, compute the axial neutron flux distribution.
- 6) Based upon the calculated axial flux distribution and the calculated void distribution, review the originally assumed radial flux distribution and revise.
- 7) Using the calculated axial flux distribution and the revised assumed radial flux distribution as input to BOCH, iterate "1" through "7".

The assumed radial neutron flux will be based upon plots of radial flux from actual boiling water reactors. An attempt will be made to ascertain the limits of variation of this radial flux distribution so that upper and lower limits can be established.

Based upon the results of "1" through "7", $k_{\text{effective}}$ versus average void fraction and the calculated void distribution can be established. The foregoing discussion pertains to the problems involved in the steady-state analysis of the VMR.

D. Kinetics

Early analysis of VMR kinetics indicated that the thermal time response of the fuel pins is an important parameter in the kinetic behavior of the reactor. The time constant of a fuel pin of specified materials is proportional to the square of the diameter; therefore, stable operation with a positive void coefficient of reactivity may require fairly small pin diameters.

In view of the economic and technical importance of the transient response of the reactor, the kinetics analysis is proceeding. This analysis consists of a model of the reactor system which will be represented on an electronic analog or will be coded for a digital computer. To facilitate computation, certain simplifications to the system have been made, such as subjecting the nonlinear behavior of the reactor to "small-signal" analysis, and expressing the reactivity in voids in the reactor in terms of a mean void variation for the entire core. These simplifying techniques have been employed by Argonne National Laboratory and other reactor design groups to represent operating reactor systems.

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2. R. H. Stark and C. H. White, "VAL PROD, a Revision of the PROD II 630 Multigroup" General Electric, Atomic Power Equipment Division, GEAP 0952, January 9, 1957.

I. HYDRODYNAMICS

The BOCH hydrodynamic code has been prepared for use on an IBM 650 computer. The complete code is capable of predicting the hydrodynamic performance of the VMR and other boiling-water reactors. Input data for such performance calculations consist essentially of the following information.

1. Reactor geometry.
2. Reactor pressure.
3. Heat input level and distribution throughout the core volume.
4. Feedwater temperature.

The output information consists essentially of the following items:

1. Coolant density as a function of position in the core.
2. Static pressure changes at selected locations around the flow circuit.
3. Mass rate of coolant through each of the fuel elements and recirculation mass-rate.

Because heat input distribution is determined by physics codes which require coolant density as input information, it is possible to reiterate between the physics codes and BOCH to obtain a solution of reactor behavior which is consistent with both the hydrodynamics and physics of the reactor system.

The BOCH code, or parts of it, will be used in the VMR analysis to determine the following:

1. Performance of the reactor as a function of pressure, feedwater temperature, heat input, and heat input distribution.
2. Pin spacing, orifice coefficients, riser height, and other variables required to specify geometry of the reactor.
3. Steady-state operating data which can be used in the kinetics analysis of the reactor.

The BOCH program has been coded and is presently in the process of being checked out. Single-channel computations using BOCH have been checked by hand calculations. The results of a single-channel machine computation are summarized in Figure 1. Figure 2 shows a detailed flow chart for the program. The chart serves to indicate the equations used in the machine calculations. In general, most of the equations involving two-phase flow phenomena are based on Argonne National Laboratory data.

TYPICAL SINGLE-CHANNEL OUTPUT FROM BOCH CODE

FIGURE 1

BOCH FLOW CHART
(Page 1)

FIGURE 2

BOCH FLOW CHART
(Page 2)

FIGURE 2

II. KINETICS

A. Objectives of Program

The immediate objective of the kinetics program is to formulate, for a natural-circulation VMR, a mathematical model that will give an adequate representation of the kinetic aspects of the reactor behavior. The model representation will be confirmed by using the model to predict the kinetic behavior of the EBWR, or a similar existing boiling water reactor, for which measurements of kinetic behavior are available.

The ultimate objective is to use the model in an economic, stable VMR reactor design. Determination of the kinetics effect of positive and negative reactivity-void coefficients will be of particular interest. Preliminary kinetics analysis³ of the VMR has indicated that providing a positive void coefficient in the operating range will yield a reactor which is inherently load-following for moderate variations in load. If this preliminary finding is confirmed, it is expected that the kinetics model will be capable of defining the required reactor parameters in sufficient detail to enable an economic comparison of reactors designed with positive and negative void coefficient.

B. Present Status

Figure 3 is a block diagram of the kinetics model as presently conceived. The more important relationships are indicated, but further development of the model may alter parts of the diagram. In order to reduce the kinetics analysis to a tractable form, several simplifications have been made in the representation of the system. First, the essential nonlinear behavior of the reactor, when subjected to large disturbances, leads to the selection of "small-signal" analysis and the consequent elimination of the need to represent the system behavior over wide variations about the nominal operating condition. The second major simplification assumes that dependence of the reactivity on voids (i.e., coolant density) can be expressed in terms of a mean void variation for the entire core. As a consequence, the spatially distributed nature of voids in the reactor is considered only in evaluating coefficients for the kinetics analysis, and the reactor can otherwise be

3. "Analog Computer Study of the VMR Kinetics," Atomic Energy Division of American-Standard, ASAE-29, November 21, 1957.

KINETICS BLOCK DIAGRAM

FIGURE 3

considered as a point; that is, the spatial variation of conditions in the core are taken into account by the coefficient in the differential equations representing the system kinetics.

The general methods for evaluating the transfer functions indicated by the block diagram have been determined approximately, and the present emphasis of the program is on more detailed evaluation of these functions. The first detailed evaluation is given in section C below, which presents the transfer functions for the "Pin Heat Transfer" block. Transfer functions for the "Coolant Density" and "Core Hydrodynamics" blocks will be largely dependent on information supplied by the BOCH hydrodynamics code for the numerical constants.

C. Thermal Analysis of UO_2 Fuel Pins

1. Summary

The temperature dependence of the thermal conductivity of UO_2 has been considered in obtaining the transient characteristics of typical UO_2 fuel pins. Sufficient information is presented to enable the determination of the transfer functions relating changes in surface heat flux to variations in heat generation and surface temperature over the following ranges of variables:

- a) UO_2 pellet diameter (in.): 0.30; 0.40; 0.50.
- b) Heat flux level about which variations in flux are assumed to occur (Btu/hr-ft^2): 100,000; 200,000; 400,000.
- c) Thermal resistances between UO_2 surface and ambient corresponding to:
0; 0.025-in. zircaloy cladding; clad plus 0.0005, 0.0010, and 0.0015 inch of air (radial clearance).

2. Discussion

In boiling heat transfer, the temperature of the solid-liquid interface is only a few degrees above the saturation temperature of the liquid, and this temperature difference varies little with heat flux. At 600-psia pressure, the temperature difference is of the order of 20°F and varies approximately in proportion to the one-fourth root of the surface heat flux.

Thus, a 100% increase in heat flux corresponds to an increase in surface temperature of less than 4°F. A suitable approximation with boiling heat transfer is to consider the surface temperature as existing at the saturation temperature plus a constant ΔT . The time response of the heat flux from a pin is then determined by the responses to two independent excitations: a) a change in saturation temperature (i.e., a change in pin surface temperature at constant heat generation); b) a change in heat generation within the pin (no change in pin surface temperature).

The two responses are different, but closely related, because the surface heat flux response to a step change in heat generation is simply the time integral of the surface heat flux response to a step change in surface temperature (as long as the thermal system is linear). Only the response to changes in pin heat generation is considered in any detail here because of the close relation between the two responses, and because the pin response to surface temperature changes appears relatively unimportant in the reactor kinetics.

Determination of the heat flux response of a fuel pin is, in general, a nonlinear problem, because the thermal conductivity of UO_2 is a function of temperature. The problem has been linearized, however, by restricting the investigation to an evaluation of the response to small changes in heat generation. With this restriction, the temperature changes in the pin are small, and the thermal conductivity can be determined as a function of radius rather than temperature. This permits the selection of constant values of thermal conductivity for small annular sections of the pin. This procedure changes the differential equation describing the UO_2 temperature from a nonlinear to a linear equation with non-constant coefficients. This equation, although linear, cannot be solved by use of any convenient analytic method; the solution giving the pin response was therefore obtained by use of an electronic analog.

3. The Analog

The lumped thermal circuit representing the distributed system is shown in Figure 4. The capacitors represent the thermal capacitance of successive equal-area annuli

FIGURE 4

of the UO_2 cylinder. The radii of the circles bounding the equal-area annuli are denoted as r_b in Table I. The value of each thermal capacitance is the same and is given by the equation

$$C_t = \frac{\pi r_o^2}{6} \rho c \quad (\text{Btu/ft}^3\text{-}^\circ\text{F}), \quad (\text{II-1})$$

in which r_o is the radius of the UO_2 cylinder. Since the volumetric thermal capacity, ρc , of UO_2 does not vary greatly with temperature, the value for ρc was taken to be uniformly $50 \text{ Btu/ft}^3\text{-}^\circ\text{F}$.

The thermal resistances interconnecting the capacitors are calculated on the basis that the capacitor is lumped at the center of each annulus (i. e., at a radius equal to the root mean square of the radii of the circles bounding the annulus,

$$r_c = \left[\frac{r_{b_n}^2 + r_{b_{n+1}}^2}{2} \right]^{\frac{1}{2}}).$$

Denoting the radii of the lumped capacitors by r_c , the equation giving the values of the thermal resistors is

$$R_{t_{n,n+1}} = \frac{1}{2\pi k} \ln \frac{r_{c_{n+1}}}{r_{c_n}} \quad (\text{II-2})$$

Table I lists both r_c and $R_t k$ for the six-lump analog.

TABLE I
THERMAL ANALOG PARAMETERS

$\frac{r_b}{r_o}$	$\frac{r_c}{r_o}$	$R_t k$	Resistance Between $\left(\frac{r_c}{r_o}\right)_n$ and $\left(\frac{r_c}{r_o}\right)_{n+1}$
0.408	0.2886	0.141	0.28 - 0.50
0.577	0.500	0.0425	0.50 - 0.64
0.707	0.6454	0.0271	0.64 - 0.76
0.816	0.7637	0.0204	0.76 - 0.86
0.915	0.8660	0.0162	0.86 - 0.95
1.000	0.9574	0.00701	0.95 - 1.0

Evaluation of the thermal conductivity is required to determine R_t and is discussed in section 4 below.

One of the two remaining thermal resistances shown in Figure 4 represents the resistance of the cladding, R_c , which was taken to be 0.025-inch-thick zircaloy with a thermal conductivity of 8.17 Btu/hr-ft² (°F/ft). The other resistance represents that of the thermal bond R_b , between the UO_2 and the cladding. Bond resistances corresponding to air-gap thicknesses (equivalent to the radial clearance between UO_2 and clad) of 0, 0.0005, 0.001, and 0.0015 inch were used in the analog solutions. The conductivity of air was taken to be 0.027 Btu/hr-ft² (°F/ft), corresponding to an air temperature of 600°F.

The heat sources, q_s , shown in Figure 4 represent the increment (above the initial, steady-state condition) in heat generation in the UO_2 . The analog solutions presented represent only the case of uniform heat generation throughout the volume of the UO_2 . Thus,

because the volumes represented by the capacitor annuli are all equal, the output of all heat sources is the same. In the next quarter, it will be determined whether further non-uniform heat generation analysis is required.

4. Evaluation of Thermal Conductivity

As previously mentioned, the thermal conductivity of UO_2 in the pin varies with radius in the analog model. This thermal conductivity depends on temperature, porosity (or density), composition, the presence of fractures in the sample used in measuring conductivity, its crystalline state, and the integrated irradiation of the UO_2 . The status of measurements of the conductivity of UO_2 is discussed in several recent sources, the most readily available probably being the May 1959 issue of Nucleonics. For the present work, the data of Hedge and Fieldhouse,⁴ corrected to 95% of theoretical density, are selected for use. Over the temperature range covered by their studies (200 to 1700°C), the density-corrected value of thermal conductivity is closely represented by the relation

$$k = \frac{460}{T^{0.75}}, \quad (\text{II-3})$$

where k is in $\text{Btu/hr-ft}^2 (^\circ\text{F/ft})$ and T is in degrees Rankine. This equation, plotted in Figure 5, will be presumed to apply to the entire temperature range covered in the analog studies.

For evaluation of the radial distribution of thermal conductivity of the UO_2 pin, it is convenient to define a new variable,

$$\phi = \int^T k(t)dt, \quad (\text{II-4})$$

which, using relation (III-3), gives

$$\phi = 1840T^{\frac{1}{4}}, \quad (\text{II-5})$$

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4. J. C. Hedge and I. B. Fieldhouse, "Measurements of Thermal Conductivity of Uranium Dioxide," Armour Research Foundation, Final Report, September 1956.

also shown on Figure 5. In terms of this variable, the steady-state diffusion equation for heat transfer becomes

$$\frac{1}{r} \frac{d}{dr} r \frac{d\varphi}{dr} = -W(r) \quad , \quad (\text{II-6})$$

in which W is the heat generation rate per unit volume. For the case of uniform heat generation, the solution can be presented in the form

$$\varphi - \varphi_0 = \frac{r_0^2}{2} q/A \left[1 - \left(\frac{r}{r_0} \right)^2 \right] \quad , \quad (\text{II-7})$$

in which q/A is the steady-state heat flux at the surface of the UO_2 cylinder and φ_0 corresponds to the surface temperature of the cylinder. In evaluating the thermal conductivity distribution, a fixed UO_2 surface temperature of 600°F was postulated. The thermal conductivity at each annulus-bounding radius, r_b , was determined by using equation (II-7), and Figure 5.

Figure 6 presents, as a function of heat flux, the steady-state centerline temperatures of the three UO_2 pin diameters considered in the analog calculations: 0.30, 0.40, and 0.50 inch. These curves were obtained using equation (II-7) and Figure 5. It is to be noted that the heat flux is evaluated at the UO_2 surface and that the surface temperature of the UO_2 cylinder is specified to be 600°F .

5. Analog Results

Figures 7 through 15 present the time-varying surface heat flux (q/A) in response to a step increment in uniform heat generation. This surface heat flux increment approaches a value denoted as $(q/A)_s$. The quantity $[1 - (q/A)/(q/A)_s]$ is plotted on these graphs in order to show the straightline character of the response curves when plotted in semi-log coordinates. This procedure facilitates the analytic representation of the curves.

The initial, steady-state heat flux indicated on each graph serves to define, in accordance with the preceding paragraphs, the radial distribution of thermal conductivity used in the analog studies. The effect on the time response of the temperature dependence

THERMAL CONDUCTIVITY AND POTENTIAL FUNCTION, ϕ , FOR UO_2

FIGURE 5

CENTERLINE TEMPERATURE AS A FUNCTION OF
HEAT FLUX FOR UO₂ CYLINDERS WITH SURFACE TEMPERATURES OF 600°F

FIGURE 6

HEAT FLUX CHANGE AT THE SURFACE OF A UO_2 CYLINDER IN RESPONSE TO
A STEP CHANGE IN UNIFORM HEAT GENERATION

FIGURE 7

HEAT FLUX CHANGE AT THE SURFACE OF A UO_2 CYLINDER IN RESPONSE TO
A STEP CHANGE IN UNIFORM HEAT GENERATION

FIGURE 8

HEAT FLUX CHANGE AT THE SURFACE OF A UO_2 CYLINDER IN RESPONSE
 A STEP CHANGE IN UNIFORM HEAT GENERATION

FIGURE 9

HEAT FLUX CHANGE AT THE SURFACE OF A UO_2 CYLINDER IN RESPONSE TO
 A STEP CHANGE IN UNIFORM HEAT GENERATION

FIGURE 10

HEAT FLUX CHANGE AT THE SURFACE OF A UO_2 CYLINDER IN RESPONSE TO
A STEP CHANGE IN UNIFORM HEAT GENERATION

FIGURE 11

HEAT FLUX CHANGE AT THE SURFACE OF A UO_2 CYLINDER IN RESPONSE TO
 A STEP CHANGE IN UNIFORM HEAT GENERATION

FIGURE 12

HEAT FLUX CHANGE AT THE SURFACE OF A UO_2 CYLINDER IN RESPONSE TO
A STEP CHANGE IN UNIFORM HEAT GENERATION

FIGURE 13

HEAT FLUX CHANGE AT THE SURFACE OF A UO_2 CYLINDER IN RESPONSE TO
 A STEP CHANGE IN UNIFORM HEAT GENERATION

FIGURE 14

HEAT FLUX CHANGE AT THE SURFACE OF A UO_2 CYLINDER IN RESPONSE TO
A STEP CHANGE IN UNIFORM HEAT GENERATION

FIGURE 15

of thermal conductivity is illustrated by Figures 10 and 12. If the time constant is defined as the time required for the response $[1 - (q/A)/(q/A)_s]$ to attain a value of $1/e = 0.37$, an initial flux of $100,000 \text{ Btu/hr-ft}^2$ gives a time constant of 2.5 seconds for a zircaloy-clad UO_2 pin of 0.40-inch diameter (Figure 10). With an initial steady-state flux of $400,000 \text{ Btu/hr-ft}^2$, the time constant for the same pin increases to about 3.4 seconds (Figure 12), corresponding to a 36% increase.

6. Transfer Function

For use in the kinetics analysis of reactors, it is convenient to express the fuel element heat transfer characteristics in terms of a transfer function, relating variations in the surface heat flux to variations in the rate of heat generation. For this purpose, the pin can be represented, with an accuracy consistent with that to which the effective thermal conductivity of UO_2 is known, by a second-order approximation. The response to a step change in heat generation can be deduced, from Figures 7 through 15, to be of the second-order form

$$\frac{q/A}{(q/A)_s} = 1 - a_1 e^{-\alpha_1 t} - a_2 e^{-\alpha_2 t} \quad (\text{II-8})$$

For example, by curve fitting on Figure 11, it can be found, for a zircaloy-clad UO_2 pin 0.40-inch in diameter operating at a flux level of $200,000 \text{ Btu/hr-ft}^2$, that equation (II-8) takes the approximate numerical form

$$\frac{q/A}{(q/A)_s} = 1 - 0.63e^{-0.209t} - 0.37e^{-1.26t} \quad (\text{II-9})$$

which gives, for a transfer function,

$$\frac{q/A(s)}{(q/A)_s(s)} = \frac{0.209 \times 0.63}{s + 0.209} + \frac{1.26 \times 0.37}{s + 1.26} \quad (\text{II-10})$$

where s is the LaPlace transform variable.

The change with time in surface heat flux in response to a step decrease in saturation temperature (i. e., a step decrease in temperature of the outer surface of the cladding) can be deduced from equation (II-8) by making use of the linearity of the system

equations. To this end, it may be noted that the heat flux response to a step decrease in surface temperature, ΔT , is identical with the heat flux response to an impulse of heat, $\Delta T \rho c \pi r_0^2$. By using the fact that the time derivative of the response to a step change in heat generation is the response to an impulse of heat and thus is also the response to a step decrease in surface temperature, the following is obtained:

$$\frac{q/L}{\pi r_0^2 \rho c \Delta T} = a_1 \alpha_1 e^{-\alpha_1 t} + a_2 \alpha_2 e^{-\alpha_2 t} \quad (\text{II-11})$$

where q/L is the heat transfer per unit length of the fuel element. Inserting the numerical values previously derived gives

$$\frac{q/A}{\Delta T} = -198 e^{-0.209t} - 700 e^{-1.26t}, \quad (\text{II-12})$$

in which t is in seconds, q/A (Btu/hr-ft²) is the heat flux at the UO_2 surface, and ΔT , in contrast to the previous equations, is positive for an increase in surface temperature.

The transfer function specifying the variation in heat flux in response to changes in saturation temperature is derived from equation (II-12):

$$\frac{q/A(s)}{\Delta T(s)} = \frac{0.209 \times 198}{s + 0.209} + \frac{700 \times 1.26}{s + 1.26} - 898 \quad (\text{II-13})$$

This formula will be used in subsequent total reactor system kinetics.

III. PHYSICS

A. PUREE' Analysis

The procedure that is being completed for analysis of the VMR experiments involves a division of the neutron spectrum into four parts, i. e. , a four-group model. The differential equations of neutron continuity take the form:

$$-D_1 \nabla^2 \phi_1 + \Sigma_{a1} \phi_1 + \Sigma_{r1} \phi_1 - f_1 \sum_i \nu_i \Sigma_{fi} \phi_i = 0 ; \quad (\text{III-1})$$

$$-D_2 \nabla^2 \phi_2 + \Sigma_{a2} \phi_2 + \Sigma_{r2} \phi_2 - \Sigma_{r1} \phi_1 - f_2 \sum_i \nu_i \Sigma_{fi} \phi_i = 0 ; \quad (\text{III-2})$$

$$-D_3 \nabla^2 \phi_3 + \Sigma_{a3} \phi_3 + \Sigma_{r3} \phi_3 - \Sigma_{r2} \phi_2 = 0 ; \quad (\text{III-3})$$

$$-D_4 \nabla^2 \phi_4 + \Sigma_{a4} \phi_4 - \Sigma_{r3} \phi_3 = 0 ; \quad (\text{III-4})$$

where $D_i \equiv$ diffusion coefficient for i^{th} group,

$\Sigma_{ai} \equiv$ absorption cross section for i^{th} group,

$\Sigma_{ri} \equiv$ removal cross section, i. e. , the probability per cm of neutron travel that a neutron will be degraded into the next lowest group (group skipping is not allowed in the four-group model, but neutron energy loss is treated accurately in arriving at good four-group constants),

$f_i \equiv$ fraction of fission spectrum in the energy range of the i^{th} group,

$\nu_i \equiv$ neutrons per fission due to i^{th} group neutrons,

$\Sigma_{fi} \equiv$ fission cross section for i^{th} group,

$\phi_i \equiv$ flux in i^{th} group.

The use of the four-group model for H_2O reactors originated at Westinghouse Atomic Power Division (WAPD), and it is generally agreed that a four-group structure is best suited to H_2O power reactor calculations.⁵ Fewer groups cannot adequately represent the

5. H. Kouts, et al, "Physics of Slightly Enriched, Normal Water Lattices," P/1841 Second Geneva Conference.

non-thermal aspects of this reactor type, and the use of more groups becomes unnecessarily complicated.

A discussion of the method of obtaining the various constants for the four-group model falls, rather naturally, into a discussion pertaining to the constants for the first three groups (where neutrons are slowing down) on one hand, and the constants of the fourth (lowest energy) group on the other.

1. Constants of Groups 1, 2, and 3

The energy limits of the groups are chosen approximately the same as those at WAPD, in order to utilize their work where desirable and to compare results. The limits are:

<u>Group No.</u>	<u>Energy Limits</u>	<u>Remarks</u>
1	1 mev to 10 mev	Fast fission of U 238
2	530 ev to 1 mev	Unresolved U 238 resonances
3	0. 625 ev to 530 ev	Resolved U 238 resonances
4	0 to 0. 625 ev	Thermal neutrons

Certain improvements to the PUREE'⁶ analysis, previously developed by ATL, have been made, principally in the treatment of Group 1 and in the procedure for fine structure corrections to account for the heterogeneous makeup of the cells of the lattice.

The procedure in the first three groups of PUREE' is to compute, first, the effective resonance integral for U 238 capture by the method of L. Dresner.⁷ This method is based on the Wigner formulation of resonance capture, in which the capture is viewed as composed of surface capture and that which is spread uniformly through the fuel rod (volume capture). The effective resonance integral is given by:

$$\int \sigma_{a_{28}} \frac{dE}{E} = \int \left\{ a(E) + \frac{S}{M} b(E) \right\} \frac{dE}{E} \quad , \quad \text{(III-5)}$$

6. "PUREE', A Four-Group Theory for Calculating Effective Homogeneous Cross Sections," Atomic Energy Division of American Standard, ASAE-41.

7. L. Dresner, "The Effective Resonance Integrals of U 238 and Th 232," 1, 1956, p 68. Also "Effect," Nuclear Science and Engineering, 1, 1956, p 501.

$$\text{where } a(E) = \frac{\sigma_a}{1 + \frac{\sigma_a + \sigma_r}{\sigma_p}},$$

$$b(E) = \frac{1}{4} \frac{M}{N_{28} V_F} \frac{\sigma_a (\sigma_r + \sigma_a) P_c}{(\sigma_r + \sigma_p + \sigma_a)^2},$$

and $\sigma_a(E)$ = resonance absorption,

$\sigma_r(E)$ = resonance scattering,

σ_p = potential scattering,

$P_c(E)$ = probability of a neutron suffering a collision when it enters a fuel rod,

V_F = an arbitrary volume (slice) of the fuel rod,

N_{28} = atoms of U 238 in V_F ,

M = mass of V_F ,

S = rod surface associated with V_F .

The resonance absorption and resonance scattering are given for each resonance by

$$\sigma_a(E_{\text{eff}}) = \frac{\sigma_o \frac{\Gamma_\gamma}{\Gamma}}{1 + \left[\frac{E_{\text{eff}} - E_o}{\Gamma/2} \right]^2} \quad \text{(III-6)}$$

$$\text{and } \sigma_r(E_{\text{eff}}) = \frac{\sigma_o \frac{\Gamma_n}{\Gamma}}{1 + \left[\frac{E_{\text{eff}} - E_o}{\Gamma/2} \right]^2}, \quad \text{(III-7)}$$

$$\text{where } \sigma_o = 4 \pi \lambda^2 \frac{\Gamma_n}{\Gamma},$$

Γ_γ = radiation capture width,

Γ_n = neutron width,

Γ = total width,

E_o = resonance energy,

λ = the reduced wavelength = $\frac{h}{2\pi} \times \frac{1}{\sqrt{2\mu E_o}}$,

μ = reduced mass of the neutron,

h = Planck's constant.

The E_{eff} is the relative energy, considering both the motion of the neutron and the motion of the nucleus (Doppler effect). It is because of the temperature motion of the U-238 nucleus that the effective resonance integral becomes a function of the fuel temperature.

The integral indicated in equation (III-5) is carried out over all resonances, using the data on Γ_γ , Γ_n , and E_o given in BNL-325.⁸ In the unresolved (unmeasured) resonance range, the resonance structure is estimated from the data on the resolved resonances.

The result obtained in this way for the total effective resonance integral is normalized to the result given by integral measurement, as quoted in standard references, i. e., values given by an expression of the type:

$$\int \sigma_{a_{28}} \frac{dE}{E} = A(1 + \mu \frac{S}{M}) \quad (\text{III-8})$$

A correction factor is established in this way for the Dresner-type calculation.

Next, a Dancoff correction is applied to account for the decrease in surface capture which results from the close presence of neighboring fuel rods.⁹ In the clustered-fuel-pin geometry of the VMR, however, the Dancoff correction is in a range not evaluated by Dancoff and Ginzberg; it was necessary, therefore, to extend their work. A recent paper by J. A. Thie¹⁰ was very helpful in this regard for computing numerical values.

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8. Donald J. Hughes and R. B. Schwartz, "Neutron Cross Sections," Brookhaven National Laboratory, BNL-325, July 1, 1958 (2nd edition).
 9. S. M. Dancoff and M. Ginzberg, "Surface Resonance Absorption in a Close-Packed Lattice," CP-2157, October 21, 1944.
 10. J. A. Thie, "A Simple Analytical Formulation of the Dancoff Correction," Nuclear Science and Engineering, 5, 1959, p 75.

The normalized Dresner method is then used to distribute the effective resonance capture over energy. Aside from flux-fine-structure corrections, this effective capture represents the correct cross sections to use in a computational model that considers the neutrons to slow down in a homogenized mixture of fuel and moderator; i. e. , it gives the amount of capture that would take place in the actual lumped geometry when the cell materials are considered homogenized for computational purposes.

Using this effective resonance capture, together with the non-resonance cross section data, a 19-group analysis is made of the neutron slowing down behavior, treating the reactor regions (core, reflector, etc.) separately as single-region problems, as if the materials in a lattice cell were homogenized. The IBM 650 code known as VAL-PROD is used for this.

"Uncorrected" group constants for the first three groups of the four-group model are then determined from these 19-group results through formulas of the type:

$$\Sigma_{a_i} = \frac{\sum_{j=N_{i-1}}^{N_i} \Sigma_{a_j} \psi_j}{\sum_{j=N_{i-1}}^{N_i} \psi_j} , \quad (\text{III-9})$$

and similarly for Σ_{f_i} and D_i ; and

$$\Sigma_{r_i} = \left\{ \sum_{j=1}^{N_i} f_j - \sum_{j=1}^{N_i} [\Sigma_{a_j} + B^2 D_j] \psi_j \right\} / \sum_{j=N_{i-1}}^{N_i} \psi_j , \quad (\text{III-10})$$

where j refers to the groups of the 19-group calculation and i to the four-group calculation, and where ψ_j = flux in j^{th} group of the 19-group computation. Group i of the four-group model is made up of groups N_{i-1} to N_i of the 19-group model in the following way:

The final step is to find, for these "uncorrected" group constants, correction factors that account for the fact that the heterogeneous construction of the cells of the lattice leads to the flux distribution having a fine structure within each cell, which is superimposed on the smoother gross shape of the flux over the reactor. These correction factors are arrived at primarily through one-group theory applied to each group, i. e. , 1, 2, and 3. In Group 1, the procedure is based on work of F. L. Clark¹¹ in which, starting neutrons out in the fuel, the preferential probability of fuel interactions, such as fission and inelastic degradation, is computed as compared to the probabilities that would result from neutrons being born uniformly over a homogenized mixture of the cell contents. This leads to correction factors for the absorption, fission, and removal terms in Group 1. The corrections for Groups 2 and 3 are made by computing the fine structures of the spatial flux distribution, using mono-energetic diffusion theory, and weighting the different materials in a manner similar to that used to compute thermal utilization in cylindrical cells.¹² Figure 16 is a schematic flow sheet which summarizes the method.

The above procedure, together with that for the fourth group, provides the four differential neutron-continuity equations for the four-group model. The multiregion criticality (and reactivity) problem for the complete reactor is then solved, using the one-dimensional VAL-PROD code for IBM 650. The identical procedure can be used to obtain good constants for a two-dimensional code, if the use of two-dimensional codes is ever deemed necessary.

PUREE', the coding for the above procedure, is nearly completed and will soon be ready to test on some experimental assemblies, such as those constructed at Brookhaven National Laboratory and Westinghouse Atomic Power Division.⁵ The code will then be ready for use in analysis of the VMR experiments.

11. F. L. Clark, "Variation of Fast Fission Effect with Homogeneity in Infinite Slab Reactor," Knowles Atomic Power Laboratories, KAPL-743.

12. See, e. g. , S. Glasstone and M. Edlund, The Elements of Nuclear Reactor Theory, New York, D. Van Nostrand Co. , Inc. (1952), pp 264-272.

FLOW SHEET FOR
CALCULATION OF CONSTANTS OF FIRST THREE GROUPS OF FOUR-GROUP PUREE' MODEL

FIGURE 16

2. Constants of Group 4

As an alternative method of analysis to the customary one-velocity group diffusion and transport calculations, a formulation of the problem for handling the thermal neutrons has been developed. This formulation avoids several of the simplifying assumptions that are usually made for thermal utilization calculations, and it is expected to yield improved accuracy.

The characteristic features of this method are:

- a) The velocity-dependent current hardening in the fuel element is taken into consideration.
- b) The Wigner-Wilkins spectrum is computed without the simplifying assumptions of a homogeneous mixture of fuel and moderator.
- c) The spatial variation of the flux in the fuel region is described without the necessity to assume a Wigner-Seitz equivalent cell.¹³
- d) Removing these restrictions from the treatment of closely packed light water lattices necessitates assuming a uniform flux in the moderator.

The six nearest and the six next nearest neighboring fuel rods essentially shield a fuel rod from the remainder of the closely packed fuel rod cluster characteristic of the VMR. The formulation computes the vector flux, $\psi(\vec{r}, \vec{\Omega})$, incident upon a fuel pin for each of 15 to 20 energy groups.

Using the incident flux, $\psi(\vec{r}, \vec{\Omega})$, arising from sources in the water and emitted by the 12 neighbors, the blackness of the fuel rod is computed by a spherical harmonics expansion of the transport equation. Blackness values and the flux obtained for each energy group are used to set up a neutron-balance integral equation, which is solved for the neutron-velocity spectrum. The solution immediately yields the fuel disadvantage factor. The spectrum computed in this manner is characteristic of those neutrons which slow down, diffuse, and are absorbed in the fuel-bearing region only.

13. Applied to lattice calculations, the Wigner-Seitz equivalent cell requires that the flux be a function of r only and the current be zero on the periphery when applied to the diffusion equation. When applied to the harmonic solution of the transport equation, this same peripheral line of constant $\psi_{0,0}$ is required to exist with the odd moments set equal to zero upon it.

The treatment of the spatially dependent energy spectrum of those neutrons which slow down outside the fuel region, then diffuse into the clump, remains to be formulated for the fourth-group portion of the code. Work on this portion is scheduled to begin during the next quarter.

Figure 17 is a schematic flow sheet which summarizes the computational method. Examples of the equations to be solved by the computational scheme are given in section 3 below.

The computation of the flux incident upon the fuel rod employs integrals similar to those used to compute the Dancoff effect.⁹ The coding and error checking of this step is about three-fourths completed. The remainder of the computational procedure is being coded for machine calculation and will be completed in the next quarter.

3. Examples of the Equations to be Solved by the Computational Scheme

a. Analytic Form of the Current Incident on the Fuel Rod (ψ_1) of the Expansion

of $\psi(\vec{r}, \vec{\Omega})$

Define the blackness β by $J^{\text{in}} = \frac{J^{\text{out}}}{1 - \beta}$. Also define the following quantities:

$K(\nu, \nu')$ = probability of a neutron of velocity ν' scattering to velocity ν ; $S(\nu)$ = sources due to neutron slowing down, with a dE/E dependence assumed for the slowing down distribution. Then $\int_0^{\nu^*} K(\nu, \nu') N(\nu') d\nu'$ is the contribution to $N(\nu)$ by scattering in the water, $N(\nu)$ is the ν -dependent neutron density, and ν^* is an arbitrarily chosen upper bound for the thermal neutron spectrum. Then it is easily shown that the current incident upon a fuel rod is

$$J^{\text{in}} = \frac{[\int_0^{\nu^*} K(\nu, \nu') N(\nu') d\nu' + S(\nu)] \frac{\lambda \Sigma_m}{4} [1 - 6 C_1 - 6 C_2]}{1 - 2(1 - \beta) [6 C_1 + 6 C_2]}, \quad (\text{III-11})$$

where C_1 is the well-known Dancoff integral⁹ for the near neighbors,

$$C_1 = \frac{1}{\pi \Sigma_m} \iint d\Sigma^1 d\Sigma \cos \alpha \cos \alpha' \frac{e^{-|\vec{r} - \vec{r}'|/\lambda}}{|\vec{r} - \vec{r}'|^2},$$

of which there are six; and C_2 represents the same integrals for the six next nearest neighbors.

FLOW SHEET FOR
CALCULATION OF FOURTH GROUP OF FOUR-GROUP PUREE' MODEL

FIGURE 17

The above expression assumes a hemispherically isotropic distribution for the neutrons emitted by the fuel rods. The removal of this restriction is exhibited later.

The programming and error checking of these C_1 and C_2 functions is three-fourths completed. An adequate table of the $K_{i,n}(x)$ functions required for the numerical integration of the C functions is being computed from existing sources¹⁴ and by calculation of values from the asymptotic expansion. The program to compute the C_1 functions is complete and free of errors. The subroutine to compute the limits of integration for the calculation of the C_2 functions, a subroutine which simply adds to the C_1 program already completed, has been flow charted and is being programmed.

b. The Neutron-Balance Integral Equation

Using the expression for the incoming current, and the expressions not shown, which are its constituent parts, the neutron-balance equation becomes:

$$\begin{aligned} & A \left\{ S(\nu) + \int_0^{\nu^*} K(\nu, \nu') N(\nu') d\nu' \right\} - \left\{ S(\nu) + \int_0^{\nu^*} \right\} \frac{\lambda \Sigma_m}{4} [1 - 6 C_1 - 6 C_2] \\ & + \frac{[\int_0^{\nu^*} + S(\nu)] \frac{\lambda \Sigma_m}{4} [1 - 6 C_1 - 6 C_2] (1 - \beta) [1 - 2(6 C_1 + 6 C_2)]}{1 - 2(1 - \beta) [6 C_1 + 6 C_2]} \\ & = A \left\{ V(\nu) + \gamma(\nu) \right\} N(\nu) \end{aligned} \quad \text{(III-12)}$$

where A is the area of water associated with each fuel rod,

$V(\nu)$ is the probability/unit time of a neutron of velocity ν scattering,

$\gamma(\nu)$ is the probability/unit time of a neutron of velocity ν undergoing a capture collision.

This integral equation is broken into groups and solved by iteration.

The above approach is quite similar to that used by Takahashi,¹⁵ except for the following: 1) the assumption of a flat flux in the fuel is avoided, 2) slab geometry is not used, 3) the use of an average f as employed in Takahashi's "approximate" calculations is not necessary.

14. G. M. Muller, "Table of the $K_{ij}(x)$ Function," General Electric Co., Hanford Works Project, HW-30323.

15. Hiroshi Takahashi, "Thermal Neutron Spectra in Heterogeneous Reactors," Nuclear Science and Engineering, 5, 1959, p 338.

c. Calculation of the Blackness by Energy Group

Blackness by group is computed in a manner used in the successive generations method.^{16,17} The approximation used is to compute the blackness, β , for small rod diameters from the expression

$$\beta = \frac{(\sigma_a/\sigma_t)P_o}{1 - (\sigma_s/\sigma_t)P_c}, \quad (\text{III-13})$$

where P_o is the first collision probability density characteristic of a current derived from an isotropic source on the fuel rod surface, and P_c is the modal collision probability as tabulated by Case, et al.¹⁸

The assumption of a current that is equivalent to an isotropic source on the surface of the fuel rod is rather seriously violated in a closely packed lattice. If one computes the Dancoff integrals to obtain the current magnitude and then employs the blackness as computed above, the effect of the angular dependence of $\psi(\vec{r}, \vec{\Omega})$ on blackness is wholly ignored. The proper consideration of the angular dependence of $\psi(\vec{r}, \vec{\Omega})$ is treated below.

To compute blackness from a proper consideration of the angular dependence of $\psi(\vec{r}, \vec{\Omega})$, the incident current is analyzed in terms of a spherical harmonic series. This series is then employed as a boundary condition for the spherical harmonics solution of the Boltzmann equation interior to the fuel rod. The P_3 expansion yields a series of the form¹⁹

$$\begin{aligned} \psi(\vec{r}, \vec{\Omega}) = & A_o \psi_{o,o}(r) + A_1 Y_1^1(\vec{\Omega}) \psi_{1,1}(r) + A_2 \left\{ Y_2^0(\vec{\Omega}) \psi_{2,0}(r) \right. \\ & \left. + Y_2^2(\vec{\Omega}) \psi_{2,2}(r) \right\} + A_3 \left\{ Y_3^1(\vec{\Omega}) \psi_{3,1}(r) + Y_3^3(\vec{\Omega}) \psi_{3,3}(r) \right\}, \quad (\text{III-14}) \end{aligned}$$

where $Y_n^m(\vec{\Omega}) = P_n^m(\Theta) \cos m(\varphi' - \varphi)$.

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16. G. W. Stuart and R. W. Woodruff, "Method of Successive Generations," Nuclear Science and Engineering, 3, 1958, p 339.
 17. G. W. Stuart, "Multiple Scattering of Neutrons," Nuclear Science and Engineering, 2, 1957, p 617.
 18. K. M. Case, et al, "Introduction to the Theory of Neutron Diffusion," Vol. I, U. S. Government Printing Office.
 19. B. Davison, Neutron Transport Theory, Oxford, England, Oxford University Press, (1957) (e. g., 12.46).

The solution for the vector flux interior to the cylinder pictured is: ²⁰

$$\psi_{0,0}(r) = \sum_{i=1}^2 C_i I_0(\nu_i r)$$

$$\psi_{1,1}(r) = \sum_{i=1}^2 G_1(\nu_i) C_i I_1(\nu_i r)$$

$$\psi_{2,0}(r) = -\frac{1}{2} \sum_{i=1}^2 G_2(\nu_i) C_i I_0(\nu_i r) + D I_0(\beta r)$$

$$\psi_{2,2}(r) = 3 \sum_{i=1}^2 G_2(\nu_i) C_i I_2(\nu_i r) + 2 D I_2(\beta r)$$

$$\psi_{3,1}(r) = -\frac{3}{2} \sum_{i=1}^2 G_3(\nu_i) C_i I_1(\nu_i r) - \frac{5}{\beta} D I_1(\beta r)$$

$$\psi_{3,3}(r) = 15 \sum_{i=1}^2 G_3(\nu_i) C_i I_3(\nu_i r) - \frac{30}{\beta} D I_3(\beta r) \quad (\text{III-15})$$

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20. J. H. Tait, "Fine Structure of Thermal Flux," Proceedings of First Geneva Conference, 5, P/433.

where the ν_i are the roots of the determinantal equation.

$$\frac{3}{8} \nu^4 - \left(\frac{35 + 55(1 - C)}{24} \right) \nu^2 + \frac{35(1 - C)}{8} = 0. \quad (\text{III-16})$$

$$G_n(\nu) = (-1)^n \left\{ P_n\left(\frac{1}{\nu}\right) - \frac{C}{\nu} \left[Q_0\left(\frac{1}{\nu}\right) P_n\left(\frac{1}{\nu}\right) - Q_n\left(\frac{1}{\nu}\right) \right] \right\} \quad {}^{21} \quad (\text{III-17})$$

$$\beta = \sqrt{7}. \quad (\text{III-18})$$

The interior solution consists of six harmonic terms with only three undetermined constants; $\psi_{0,0}(r)$ is uniquely determined by $\psi_{1,1}(r)$ as $\psi_{2,0}(r)$ and $\psi_{2,2}(r)$ are determined by $\psi_{3,1}(r)$ and $\psi_{3,3}(r)$.

To solve this problem of an incident flux on an exposed surface, Marshak's boundary conditions are used. In the representation employed, these boundary conditions appear as:²²

$$\int \int_{\text{Interior solution}} \psi(\vec{r} = \vec{a}, \vec{\Omega}) Y_n^m(\vec{\Omega}) d\vec{\Omega} = \int \int_{\text{Incident flux}} \psi(\vec{\Omega}) Y_n^m(\vec{\Omega}) d\vec{\Omega} \quad (\text{III-19})$$

for all $\vec{\Omega}$ inward, all m, n odd. $\psi(\vec{\Omega})$ is expressed by⁹

$$\psi(\vec{\Omega}) d\vec{\Omega} = q \frac{\int d\Sigma d\vec{\Omega} \int_0^{\bar{s}} ds e^{-s/\lambda}}{4\pi \Sigma_m}, \quad (\text{III-20})$$

which gives the value of $\psi(\vec{\Omega}) d\vec{\Omega}$ averaged over the surface of the recipient rod. Thus,

$$\begin{aligned} & \int \int \psi(\vec{\Omega}) P_n^m(\Theta) \cos m(\varphi' - \varphi) d\vec{\Omega} \\ &= \frac{q}{4\pi \Sigma_m} \int \int d\vec{\Omega} \int d\Sigma P_n^m(\Theta) \cos m(\varphi' - \varphi) \int_0^{\bar{s}} ds e^{-s/\lambda} \end{aligned} \quad (\text{III-21})$$

For $P_1^1(\Theta) \cos(\varphi' - \varphi)$, the right hand integral is simply the C function or Dancoff integral.

21. Davison, loc. cit. (e. g. , 10. 9).

22. Davison, loc. cit. (e. g. , 10. 55).

For $Y_3^3(\vec{\Omega}) = P_3^3(\Theta) \cos 3(\varphi' - \varphi)$, two terms result which are variations of the Dancoff integrals already programmed:

$$\frac{-15q\rho^2}{\pi\Sigma_m} \iint d\varphi d\varphi' \frac{\vec{X}^3 \cdot \vec{X}'}{|\vec{\rho} - \vec{\rho}'|^5} K_{i,5}(|\vec{\rho} - \vec{\rho}'|/\lambda) \quad ; \quad (\text{III-22})$$

and

$$\frac{15q\rho^2}{4\pi\Sigma_m} \iint d\varphi d\varphi' \frac{\vec{X}^3 \cdot \vec{X}' K_{i,5}(|\vec{\rho} - \vec{\rho}'|/\lambda)}{|\vec{\rho} - \vec{\rho}'|^5 \cos^2(\varphi' - \varphi)} \quad (\text{III-23})$$

For $Y_3^1(\vec{\Omega}) = P_3^1(\Theta) \cos(\varphi' - \varphi)$, two terms result. The first is equal to the term from $Y_1^1(\vec{\Omega})$ to within a multiplicative constant; the second equals the second term from $Y_3^3(\vec{\Omega})$ to within a multiplicative constant.

To obtain the blackness appropriate to $\psi(\vec{r}, \vec{\Omega})$ for each energy group, the intention is to obtain J^{in} from the incident $\psi(\vec{r}, \vec{\Omega})$, and to obtain J^{out} from $J^{\text{out}} = J^{\text{in}} - \text{number of neutrons absorbed}$, this last quantity being obtained by integrating the scalar flux, $\psi_{0,0}$, over the fuel rod.

It is indicated in the integrals presented above, by using g , that the fuel rod exit flux is hemispherically isotropic. To avoid this, the angular expansion obtained from $\psi_{1,1}$; $\psi_{3,1}$; and $\psi_{3,3}$ may be used, with the magnitude of the current adjusted to agree with the J^{out} computed from $J^{\text{out}} = J^{\text{in}} - \text{number of neutrons absorbed}$.

B. "Simplified" Physics Analysis

1. Method of Approach

The familiar four-factor critical equation $K_{\text{eff}} = \frac{\eta \epsilon f p e^{-\tau B^2}}{1 + L^2 B^2}$ is being used as an approximate short-cut method to determine the enrichment and amount of fuel required for the critical experiments. Values for ϵ , the fast effect, are determined from the experimental values of the ratio of the fission rate in U 238 to that in U 235 as published by H. Kouts, et al.²³ Thermal utilization and resonance escape probability are computed, using diffusion theory calculations for a complex cell of cylindrical geometry. The method

23. H. Kouts, et al, "Physics of Slightly Enriched, Normal Water Lattices," Peaceful Uses of Atomic Energy, Volume 12, p 446 (1958).

was checked against values of f and p measured by Kouts for 1.3% enriched, 0.383-inch diameter, UO_2 fuel pins. The calculated values of f were about 1.5% too high, and those of p were high by approximately 2.5%.

In addition to determining the enrichment and quantity of fuel required for the critical experiments, the objectives of the calculations are to study, with a simple method, the effects on neutron multiplication of fuel pin diameter, fuel enrichment, ratio of moderator to fuel, and clustering of fuel rods, the last two being of particular interest. It is convenient to interpret the last two effects in terms of two "volume" ratios, $W_{\text{eff}}/\text{UO}_2$ and C/UO_2 . The ratio C/UO_2 is the volume ratio of coolant (see Figure 18) to UO_2 . $W_{\text{eff}}/\text{UO}_2$ is the "effective" ratio of coolant and moderator volume to UO_2 volume. Here, the "effective" volume of coolant and moderator is the ratio of the volumes occupied by the coolant and moderator to the volume of UO_2 , multiplied by the ratio of slowing down strength of the coolant and moderator to that of water alone:

$$W_{\text{eff}}/\text{UO}_2 = \frac{\text{Vol. coolant} + \text{Vol. moderator}}{\text{Vol. UO}_2} \times \frac{\xi \Sigma_s \text{ coolant and moderator}}{\xi \Sigma_s \text{ H}_2\text{O}} \quad (\text{III-24})$$

2. Results

Investigations have been made of a fuel element composed of 61 fuel rods, 1.0 cm in diameter and clad with 0.068 cm of aluminum, encased in a steel shroud 0.152 cm thick. An enrichment of 2.2% has been used throughout. $W_{\text{eff}}/\text{UO}_2$ ratios from 0.622 to 3.5, and C/UO_2 ratios from 0.5 to 2.5 have been studied. Since the critical experiment will contain furfuryl alcohol and furfural to simulate rods, in the calculations the mixture of steam and water in the coolant region has also been simulated by furfuryl alcohol (roughly 30% voids) and furfural (roughly 50% voids). Figures 19 and 20 show K_∞ plotted against $W_{\text{eff}}/\text{UO}_2$. The solid lines indicate the behavior of K_∞ for a fixed coolant material and C/UO_2 ratio as the volume of moderator (in all cases water) is varied. Dashed lines indicate the behavior of K_∞ as the coolant material is varied and the volume ratio is held constant.

The conclusions to be drawn from the results obtained to date are:

FUEL ELEMENT

FIGURE 18

FIGURE 19

FIGURE 20

a) In order to design a critical experiment that has an increase in reactivity as furfuryl alcohol and furfural are added as void-simulating materials, it is necessary for the ratio of coolant-plus-moderator to UO_2 volume to exceed 2.5 for the small cores being considered. Larger cores for actual reactor systems will have a smaller ratio.

b) As the fuel rods are more tightly clustered (decreasing C/UO_2), the reactivity decreases.

c) The minimum critical masses calculated for cylindrical critical assemblies range from 300 kg UO_2 (5.8 kg of U 235) for a loosely clustered fuel element with near optimum moderation, to 2500 kg UO_2 (48 kg U 235) for a more tightly clustered ($C/\text{UO}_2 = 1.0$) over-moderated assembly ($W_{\text{eff}}/\text{UO}_2 = 3.5$).

3. Status of the Program

The investigation of K_∞ versus C/UO_2 and $W_{\text{eff}}/\text{UO}_2$ ratios will be extended for the present pin size and enrichment to $W_{\text{eff}}/\text{UO}_2$ ratios of 4. Additional investigations will be made of the effects of pin diameter, fuel and coolant region size, and fuel enrichment.

IV. CRITICAL EXPERIMENT

A. Fuel Procurement

Specification RED-160, "Aluminum-Clad Uranium Oxide Fuel Pins," dated August 17, 1959, covering the fabrication of fuel for the critical experiment has been released to manufacturers for quotation. The specification called for the fabrication of 2,000 kg of 2% enriched UO_2 . Figure 21 shows a typical fuel pin to be used in the critical experiment.

The time schedule for fabrication and delivery of the fuel is as follows:

September 25, 1959	Fuel order placed with Fabricator.
November 15, 1959	UO_2 powder delivered to Fabricator.
January 1, 1960	Fuel pins delivered to Battelle Memorial Institute.

B. Void Simulation

A study was made to determine the most suitable material for void simulation in the critical experiment. The ideal material is one which has the same slowing down characteristics and thermal neutron diffusion and absorption characteristics as water. Polyethylene meets these requirements, but is expensive to fabricate and does not lend itself to changes in void simulation or changes in reactor geometry during the testing period.

Furfural, furfuryl alcohol, and combinations of these substances with water permit a wide variation of void fraction and reactor geometry to be simulated. Based on hydrogen density, combinations of the above liquids can be used to simulate void fractions in an operating reactor from 0 to about 0.5. Since the purpose of the critical experiment is to verify the analytical physics methods rather than to represent a prototype reactor, the furfural and furfuryl alcohol mixtures are better suited than polyethylene as void simulators and will therefore be used in the critical experiment.

C. Possible Neutron Energy Spectrum Experiment

As a check against the analytical procedures being developed to account for the spatial variation in the neutron energy spectrum, certain experimental techniques to measure this property are being considered. The desirability of including such an experiment will be determined in the next quarter.

FIGURE 21

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