METHOD FOR ANALYZING LOW-ENRICHMENT LIGHT-WATER CORES

Supplementary Study

Related To BONUS And Nuclear Superheat Programs

by

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Preface

As a result of the preliminary BONUS design study (subcontract NP-1 under contract AT-(40-1)-2484), it was found necessary to perform critical experiments to fully evaluate the physics problems introduced by nuclear superheat. These experiments are being performed by Combustion Engineering, Inc. under contract AT-(11-1)-795. A major goal of the critical experimental program is the development of analytical methods that can predict the results of the critical experiments as well as yield reliable answers to the complex problems usually encountered in the physics core design of a power reactor.

In order to properly plan these experiments, it was first necessary to evaluate the accuracy of the analytical methods used at GNEC by comparing the theoretical analysis with presently available critical experimental information utilizing low-enrichment oxide fuel. This report summarizes both the analytical methods and the comparison. As a consequence of these results, critical experiments have been planned which will yield information that will further test and expand the analytical methods and, in addition, can be used directly in physics core design.

Abstract

A three-group method is developed for analyzing light-water UO_2 cores of low enrichment. The method is composed of a series of subroutines that are consolidated to produce a set of self-consistent multigroup parameters. The thermal cross sections are determined by averaging the cross section over a "hardened" or shifted Maxwellian spectrum, the amount of hardening being a function of the macroscopic absorption-to-slowing-down ratio. The disadvantage factor is calculated using diffusion theory for the moderator and a transport condition at the surface of the rod, the accuracy of the calculation being comparable to a P_3 calculation. The epithermal capture cross section of U^{238} is based on the measurement of Hellstrand including a 1.1-barn $\frac{1}{v}$ absorption, and ignores epithermal self-shielding effects even for very close-packed lattices. The fast-fission factor is calculated relative to the experimental measurements for UO_2 . The diffusion coefficients are found by averaging the measured cross sections over the appropriate neutron flux in each neutron energy group. The slowing-down cross section is defined as the diffusion coefficient divided by the neutron age, the age being determined by calculating equivalent transport and slowing-down factors relative to light-water measurements.

Utilizing the two-dimensional IBM-704 PDQ digital computer code, a comparison is made with the available experimental information using oxide fuel. These experiments, which include rod-type fuel elements, use U^{235} enrichments from 1.3 to 4.0 wt. % and water-to-uranium-metal ratios from 2.2 to 4.9. The reactivity and power-distribution predictions are very good. The reactivity calculations check to within 2% Δk for all cases, most cases being within 1% Δk .

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I. INTRODUCTION

The physics information desired by the reactor designer consists mainly of the gross operating characteristics of the reactor, such as reactivity, reactivity coefficients, and power distributions. In order to obtain this information for power reactors possessing hydrogenous moderators, the physics analysis is usually based on multigroup equations whose solution requires the utilization of large digital computer machines. Although the machine with its accompanying nuclear codes has removed many of the geometrical uncertainties that were formerly associated with nuclear core design, the basic accuracy of the theoretical analysis has not been greatly increased. The fact that most light-water power reactors scheduled for construction today require prototype critical experiments or extreme conservatism in the nuclear design is indicative of the reliability attributed to theoretical analysis. Unfortunately, further improvement in computer machines will not remedy the situation. The machine is only a tool that will do the bidding of its master. If the multigroup equations with the appropriate multigroup coefficients do not describe adequately the physical system, the answers will be wrong regardless of the size of the machine.

In recent years, there has been a large accumulation of both theoretical and experimental information associated with neutron interaction in fission reactors. Therefore, it may seem surprising that the calculation of input data has not been able to keep pace with the rapid growth of the capability of digital computers. However,

a closer examination of the available physics information reveals that most of the information cannot be used directly in core analysis, but usually requires a considerable amount of interpretation. For example, most of the critical experiments usually are affected by several variables whose effects are automatically lumped together in a critical fuel loading measurement. At the other extreme, individual microscopic quantities (lattice parameters) are measured, which contribute to the understanding of physical processes, but do not yield quantities which can be used directly in a practical calculation. Therefore, although there is a wealth of information available, the amount that can be used to predict the behavior of a core design that deviates from present designs is comparatively small.

In the development of a few-group method based on present experimental information, one must necessarily make many arbitrary assumptions. These assumptions not only include the averaging of cross sections and the determination of lattice parameters but also involve the choice of multigroup equations; the number of groups, the energy interval for each group, and possible simplifications — such as the neglect of specific epithermal phenomena — are often made arbitrarily. The choice of a geometric model for the core is affected by the definition of the fuel element boundaries and by the method of treating the structural regions and water channels. In order to support a valid and systematical procedure, a comparison should be made with several critical experiments. The results of this comparison could determine directly some parameters, or they

could be fed back into the analysis to change the averaging process, the definition of equations, or the definition of geometric model. In this manner, one arrives at a complete analytical "package" in which all components are interrelated. To be worthwhile, this "package" should then be capable of calculating any similar configuration under any prescribed conditions to a known degree of accuracy without introducing any further changes in the "package."

In a previous paper, a "package" method is described for determining three-group constants for homogeneous, hydrogenous, fully enriched reactors.¹ The method, although comparatively simple, has been quite successful in predicting the nuclear characteristics of this reactor type. This paper extends the method, with some modifications, to determine three-group constants for low U^{235} enrichment, light-water-- UO_2 cores. The method of analysis is composed of a series of sub-routines that are consolidated to produce a self-consistent set of multigroup parameters. These methods can be applied in a straightforward fashion to the usual complex engineering core designs, and are in good agreement with present experimental information.

II. DESCRIPTION OF METHOD

A. Three-Group Equations

The three-group method that is used to calculate reactivity and power distributions assumes that only thermal fissions occur in U^{235} and that fast fissions and epithermal absorptions occur only in U^{238} . The three-group equations are the following:

$$\begin{aligned} -D_1 \nabla^2 \phi_1 + \sum_{sl_1} \phi_1 &= \epsilon \nu \sum_{f_3} \phi_3 \\ -D_2 \nabla^2 \phi_2 + (\sum_{a_2} + \sum_{sl_2}) \phi_2 &= \sum_{sl_1} \phi_1 \\ -D_3 \nabla^2 \phi_3 + \sum_{a_3} \phi_3 &= \sum_{sl_2} \phi_2 \end{aligned} \tag{1}$$

where D is the diffusion coefficient, $\sum_{sl}$ is the slowing-down or removal cross section, $\sum_a$ is the absorption cross section, $\sum_f$ is the fission cross section, ϵ is the fast-fission effect, ν is the number of neutrons released per fission, and the subscripts are designations of the neutron energy groups.

The three neutron energy groups can be defined as the fast, epithermal, and thermal groups. The energy interval for the first group is from 10 Mev to 180 Kev; for the epithermal group, the energy interval is from 180 Kev to a thermal cutoff; for the thermal group, the energy interval is from the thermal cutoff to zero energy.

The number of groups and their energy intervals have been chosen arbitrarily. It appears that it is necessary to have at least two groups other than the thermal group to describe adequately neutron

losses in hydrogenous reactors. One of these, the high-energy group, describes fast-neutron leakage; the other, the epithermal group, describes resonance capture in U^{238} and in control rods. For very large reactors the fast leakage becomes small, and there appears the possibility that two groups might be adequate. However, it still may be necessary to perform small reactor analyses upon sections of the core that are used in critical experiments. Thus, it is preferred to use three groups and to have a method that is independent of reactor size.

The energy interval for the first group, 10 Mev to 180 Kev, is wide enough to permit the assumption that all prompt neutrons are born within this group. The second group extends from 180 Kev to a thermal cutoff energy. This cutoff energy is lower than the cadmium cutoff energy for all systems that are considered. This definition, which is an analytical convenience, makes it difficult to compare directly thermal-flux measurements with analysis. However, the important quantity is power distribution and, here, a direct comparison is possible.

The assumption that there are no epithermal fissions and captures in U^{235} requires some explanation. Although experiments have been performed using almost pure U^{235} samples, no experiments have been reported that measure the epithermal absorption of U^{235} in the presence of 25 to 75 times greater concentrations of U^{238} . It is difficult to evolve an analytical expression for epithermal capture and fission in U^{235} in the presence of U^{238} . It was originally intended to use some critical measurements to determine this parameter. However, it has turned out that the agreement with critical experiments

in both reactivity and power distribution is achieved without inclusion of epithermal fission. These results seem to indicate that the epithermal neutron capture of U^{235} in low-enrichment lattices is relatively small and, for this particular method, is compensated by the methods used in calculating the other parameters.

B. Thermal Cross Sections

1. Neutron Temperature

In order to determine the thermal cross sections, the microscopic cross sections must be averaged over the proper thermal-neutron spectrum. The procedure that has been adopted is to assume a "hardened" or shifted Maxwellian spectrum whose most probable energy, T_n , is determined by the following expression:

$$T_n = T \left(1 + 0.75 \frac{\sum_a}{\sum_s} \right)^2 \quad (2)$$

where T is the physical temperature in electron volts and $\frac{\sum_a}{\sum_s}$ is the ratio of the absorption cross section at temperature T to the slowing-down cross section just above thermal energies. The shifted Maxwellian spectrum has a thermal cutoff at $4 T_n$. The 0.75 factor in Equation 2 has been determined by a comparison with analysis using the Wigner-Wilkins thermal spectrum for $\frac{\sum_a}{\sum_s} \leq 0.5$. This expression will yield essentially the same average thermal cross sections for U^{235} and for a $\frac{1}{v}$ absorber as the comparable Wigner-Wilkins spectrum.²

A neutron temperature, T_n , is chosen for every fuel and water channel region within the reactor. For a structural region that is adjacent to a water channel, the neutron temperature of the water channel is used.

The method of spectrum hardening has a very significant effect on the disadvantage factor calculations and, consequently, on the thermal utilization. This is particularly evident in cores utilizing stainless steel cladding and containing a relatively high U^{235} enrichment.

2. Microscopic Absorption Cross Sections

The microscopic cross sections for $\frac{1}{v}$ absorbers at a neutron velocity of 2200 meters/sec are the following:³

	<u>σ_{2200} (barns)</u>
Al	0.23
H	0.332
Cr	3.10
Fe	2.53
Ni	4.8
Mn	13.2
U^{238}	2.71
Zr	0.18

The average thermal cross sections are found by averaging over the Maxwellian spectrum determined by Equation 2 in the interval from 0 to $4 T_n$. For the $\frac{1}{v}$ absorbers, numerical factors can be simply calculated to convert from the value at 2200 meters/sec.

$$\bar{\sigma}_{\frac{1}{v}} = 0.93 \sqrt{\frac{0.0253}{T_n}} \bar{\sigma}_{2200} \quad (3)$$

For the non- $\frac{1}{v}$ absorbers, a numerical average of the cross sections is required. For U^{235} , the following average absorption microscopic cross sections have been computed:

<u>T (ev)</u>	<u>$\sigma_{U^{235}}$ (barns)</u>
0.025	633
0.040	484
0.060	387
0.080	338
0.100	303

The value of ν , neutrons released per thermal fission, for U^{235} is 2.46. The value of α , the ratio of resonance-to-fission capture for thermal neutrons, is assumed to be 0.184 for U^{235} independent of neutron energy.

3. Microscopic Thermal Transport Cross Sections

The transport cross section, σ_{tr} , of an atom is defined in the usual manner for isotropic scattering:

$$\sigma_{tr} = \sigma_s \left(1 - \frac{2}{3A}\right) \quad (4)$$

where σ_s is the scattering cross section and where A is the atomic mass. The hydrogen transport cross section is assumed to have a $\frac{1}{v}$ dependence and is averaged in a similar manner to the $\frac{1}{v}$ absorber. For all other elements, the transport cross section is assumed to be independent of temperature and spectrum.

	$\sigma_s (1 - \frac{2}{3A}) \text{ (barns)}$
Al	1.4
H	36.8 ($\frac{1}{v}$)
Cr	3.0
Fe	11.0
Ni	17.5
Mn	2.3
O	4.0
U ²³⁸	8.3
Zr	8.0

4. Macroscopic Cross Sections

The macroscopic thermal cross section for a fuel region within the core is

$$\Sigma_{a_3} = \frac{v_F \Sigma_F + \frac{\phi_M}{\phi_F} v_M \Sigma_M + \frac{\phi_{Cl}}{\phi_F} v_{Cl} \Sigma_{Cl} + \frac{\phi_{St}}{\phi_F} v_{St} \Sigma_{St}}{(1 - v_M - v_{Cl} - v_{St}) + \frac{\phi_M}{\phi_F} v_M + \frac{\phi_{Cl}}{\phi_F} v_{Cl} + \frac{\phi_{St}}{\phi_F} v_{St}} \quad (5)$$

where F, M, Cl, and St refer to the fuel, moderator, cladding, and structure, respectively; v is the volume fraction; $\frac{\phi_M}{\phi_F}$, $\frac{\phi_{Cl}}{\phi_F}$ and $\frac{\phi_{St}}{\phi_F}$ refer to the disadvantage factors for the respective regions.

Σ_{tr3} is similarly defined. The total transport cross section $\Sigma_{tr_{tot}}$ is the sum of Σ_{tr3} and Σ_{a3} . The thermal diffusion coefficient D_3 for the region is

$$D_3 = \frac{1}{3 \Sigma_{tr_{tot}}} = \frac{1}{3 (\Sigma_{tr3} + \Sigma_{a3})} \quad (6)$$

5. Thermal Constants for Water Channel Regions

The average absorption and transport cross sections for water channel regions are calculated, based on the neutron temperature determined by Equation 2. In addition, correction is made to account for discontinuity in neutron temperature between the water channel region and the fuel region. The water in the fuel region adjacent to the water channel should be slightly less hardened or have a slightly higher absorption than the remainder of the fuel region. The following formula, which assumes the channel dimensions to be increased by a transport mean free path, is applied to the absorption cross section in the water channel region to account for this increased absorption:

$$\Sigma'_{a3} = \Sigma_{a3} \left(\frac{1 + \frac{2\lambda}{t}}{1 + \frac{2\lambda}{t} \sqrt{\frac{T_C}{T_F}}} \right) \quad (7)$$

where λ is the transport mean free path in the water channel, t is the channel width, and T_C and T_F are the neutron temperatures of the channel and fuel, respectively.

C. Disadvantage Factors

The disadvantage factor can be evaluated by a P-3 calculation in which the hardened cross section prescription that has been previously described is used to calculate the input data. However, for rod-shaped

elements, an analytical expression was developed which agrees almost identically with the P-3 calculation. In this formulation, the disadvantage factor is calculated using diffusion theory in the moderator and using a transport condition at the surface of the rod. The clad is treated as a void region to calculate $\frac{\phi_M}{\phi_F}$, the relative flux in the water to that in the fuel. The disadvantage factor of the clad is then taken as $1 + \frac{\phi_M}{\phi_F}$.

$$\frac{\phi_M}{\phi_F} = \frac{3}{2} \frac{\Sigma_{R_0}}{k \lambda} \left\{ kd + \frac{I_0(kR_1) K_1(kR_2) + I_1(kR_2) K_0(kR_1)}{I_1(kR_2) K_1(kR_1) - I_1(kR_1) K_1(kR_2)} - \frac{2 k R_1}{k^2 R_2^2 - k^2 R_1^2} \right\} \quad (8)$$

d is the reciprocal of the logarithmic derivative of the flux at the surface of the rod and is defined, as follows:

$$d = \Delta \left(\frac{R_0}{\lambda} \right) + \frac{4}{3} \lambda \left(\frac{1 - 2 f \Sigma_{R_0}}{2 f \Sigma_{R_0}} \right) \quad (9)$$

R_0 = radius of fuel pellet;

R_1 = outer radius of fuel element cladding;

R_2 = outer radius of unit cylindricalized cell;

λ = neutron transport mean free path in the moderator;

k = inverse neutron thermal diffusion length;

Σ = microscopic absorption cross section of fuel;

f = self-shielding factor for a cylinder and is shown in Figure 1 and described in reference 4;

$\Delta \left(\frac{R_0}{\lambda} \right)$ = geometrical function and is shown in Figure 2 and described in reference 5.

D. Epithermal Capture in U^{238}

The macroscopic epithermal capture cross section for U^{238} within a region at room temperature is

$$\Sigma_{a2} = \frac{v_F N_F \sigma_0}{\Delta u} \quad (10)$$

where v_F is the volume fraction of the fuel, N_F is the number of fuel atoms/cm³, σ_0 is the resonance integral, and Δu is the lethargy of the epithermal group.

The resonance integral that is used in Equation 10 is

$$\sigma_0 = 5.25 + 26.6 \sqrt{\frac{S}{M}} \quad (11)$$

where $\frac{S}{M}$ is the surface-to-mass ratio of the fuel. This value is based on the single rod measurements of Hellstrand,⁶ and includes 1.1-barn $\frac{1}{v}$ absorption. This cross section is applied without any correction for epithermal self-shielding, such as the Dancoff correction. It is not clear why this simple definition should apply for very tight lattices. However, another aspect of Equation 11 is: it is the resonance integral that is consistent with the entire calculational procedure and that happens to coincide with Hellstrand's measurements.

The resonance escape probability, p , which is not explicitly used in the analysis, can be defined:

$$p = \frac{\Sigma_{sl2}}{\Sigma_{sl2} + \Sigma_{a2}} \quad (12)$$

This is the quantity that will be compared to the experimental measurement.

E. Fast Fission in U^{238}

The fast-fission factor, ϵ , is calculated relative to the experimental measurements for UO_2 .⁷ It is assumed that ϵ , which is a measure of the number of fast fissions occurring in U^{238} relative to the number occurring in U^{235} , can be calculated as though the entire fuel region were homogeneous. The calculated fast-fission factor, ϵ , for a light-water lattice relative to an experimental measurement, ϵ' , is

$$\epsilon - 1 = (\epsilon' - 1) \frac{N_0}{N'_0} \frac{(v'_{H_2O} \Sigma'_{H_2O} + v'_{U-238} \Sigma'_{U-238} + v'_{St} \Sigma'_{St})}{(v_{H_2O} \Sigma_{H_2O} + v_{U-238} \Sigma_{U-238} + v_{St} \Sigma_{St})} \quad (13)$$

where v is the volume fraction of each material; N_0 is the number of U^{238} atoms per cubic centimeter; Σ is the total slowing-down cross section; the subscript, St, refers to the structural and cladding material; the prime refers to the experimental measurement.

In using the homogeneous approximation to calculate ϵ , it is necessary to include all regions within the fuel zone to compute the composition. If the fuel element and water channels are treated as separate regions within the fuel zone, the composition used for the determination of ϵ must include both the fuel element and the water channel as though they were a homogeneous mixture.

The microscopic cross sections used in Equation 13 are the following:

	σ (barns)
Al	0.38
H ₂ O	5.20
Stainless steel (18% Cr; 8% Ni)	1.04
UO ₂	3.70
Zr	1.16

F. Diffusion Coefficients

The diffusion coefficients for the first and second groups are defined in a manner similar to that used for the thermal diffusion coefficients — with the exception that the absorption, which is relatively small, is neglected. The microscopic transport cross sections are found by averaging the measured values over appropriate neutron fluxes. The first group flux is assumed to be the flux determined by the infinite medium Boltzmann equation for a fission source in pure water. The second group is assumed to have a $\frac{1}{E}$ energy dependence. The resulting microscopic transport cross sections are the following for each group:

	σ_{tr_1} (barns)	σ_{tr_2} (barns)
Al	3.08	1.78
H ₂ O	6.03	16.44
Stainless steel (18% Cr; 8% Ni)	3.09	9.02
UO ₂	14.18	21.28
Zr	6.27	7.08

The total macroscopic transport cross section, Σ_{tr} , is the sum of the volume-weighted individual macroscopic cross sections and

$$D = \frac{1}{3 \Sigma_{tr}}.$$

G. The Slowing-Down Cross Section and The Neutron Age

The slowing-down or removal cross section, Σ_{s1} , for each group, is defined as the ratio of the diffusion coefficient to the neutron age for a nonabsorbing medium.

The neutron age is determined for the fast and epithermal groups by calculating the equivalent transport and slowing-down factors of the materials relative to those of pure water and neglecting absorption occurring within the group. The displacement of water by other materials perturbs the experimentally measured water age. The experimental age in pure water has been selected as 30.5 cm^2 to indium resonance.^{8,9} Although there is a published measurement of a smaller age value,¹⁰ for this particular method of analysis the 30.5-cm^2 value is best able to predict both the results of migration area measurements and the reactivity of small oxide-fueled cores in which the neutron leakage is high. The age is divided so that 25 cm^2 of the total is associated with the first group and the remainder with the second group. In addition, the age in the second group must be extended to the thermal cutoff. For the first group,

$$\tau_1 = \frac{25 \left(1 + \sum_{i=1}^N v_i\right)^2}{(\rho_{H_2O} + \sum_{i=1}^N v_i X_i)(\rho_{H_2O} + \sum_{i=1}^N v_i Y_i)} \quad (14)$$

where v_i is the volume ratio of i^{th} material to water, X_i and Y_i are the transport and slowing-down equivalence of the i^{th} material to water; and ρ is the density of water.

For the second group,

$$\tau_2 = \frac{5.5 \frac{\Delta u}{11.75} (1 + \sum_i v_i)^2}{(\rho_{\text{H}_2\text{O}} + \sum_i v_i X_i)(\rho_{\text{H}_2\text{O}} + \sum_i v_i Y_i)} \quad (15)$$

where v , X , and Y are defined the same as for the first group, and Δu is the lethargy interval of the epithermal group. The equivalence factors are the following for each group:

	<u>X_1</u>	<u>X_2</u>	<u>Y_1</u>	<u>Y_2</u>
Al	0.922	0.195	0.103	0.006
Stainless steel [$\rho = 7.85 \text{ g/cc}$ 18% Cr; 8% Ni]	1.30	1.39	0.189	0.021
UO_2 (10.25 g/cc)	1.61	0.885	0.445	0.019
Zr	1.33	0.547	0.107	0.005

This total age, τ , for any region, corrected for the absorption in the epithermal group is

$$\tau = \tau_1 + \frac{\sum_{s1_2}}{\sum_{s1_2} + \sum_{a_2}} \tau_2 \quad (16)$$

The migration area, M^2 , is the sum of the total age and the square of the thermal diffusion length.

H. Reflector Savings and Hand Calculations

The reflector savings of the water reflector is a function of the leakage of neutrons from the core. An expression for the reflector savings, δ , which appears to be consistent with both the machine calculations and the experimental measurement is

$$\delta \text{ (cm)} = 7.2 + 0.10 (M^2 - 40.0) \quad (17)$$

where M^2 is the migration area.

This expression may be used to calculate the geometric bucklings that enter into multigroup problems.

For uniform lattices whose outer boundaries approach simple geometric shapes, one can use the reflector savings to calculate an over-all geometric buckling, B^2 . This buckling can then be inserted into Equation 1 to yield a simple reactivity expression that will approximate the comparable machine calculation. Setting $\nabla^2 \phi = -B^2 \phi$, in Equation 1, yields

$$k = \frac{\frac{\epsilon V \Sigma_{f3}}{\Sigma a_3}}{(1 + B^2 \tau_1)(1 + B^2 \tau_2 + \frac{\Sigma a_2}{\Sigma s l_2})(1 + B^2 L^2)} \quad (18)$$

For a cylindrical geometry,

$$B^2 = \left(\frac{2.405}{R + \delta} \right)^2 + \left(\frac{\pi}{H + 2 \delta} \right)^2 \quad (19)$$

where δ is determined by Equation 17.

I. Control Rod Calculations

For core analysis in which it is desirable to treat highly absorbing materials (such as control rods) as discrete regions, it is necessary to use a transport condition at the surface of the region. This transport condition is a function of the transmission probability.^{11,12} The assumption is made that it is only necessary to consider the absorption in the thermal and epithermal groups. Since the rods are normally thermally black, the thermal transmission probability is very close to zero. On the other hand, the epithermal transmission probability will tend to be closer to unity, since the rods are normally epithermally grey. The epithermal transmission probability cannot be calculated directly with any degree of certainty because of uncertainties in both the epithermal flux and the cross sections. It is best to determine this value directly from experiment. Presently, critical experiments are being planned in which the epithermal transmission probability consistent with the entire calculational procedure will be measured for cadmium and borated stainless steel rods.*

For applications to core analysis in which it is desirable to homogenize the control rod region with the fuel region, the area absorption method can be used.^{12,13} The area absorption method utilizes the thermal and epithermal transmission probabilities to reduce the source strength for epithermal- and thermal-neutron groups. In this manner, the rod absorption can be considered without treating the rods as discrete regions.

* These measurements are part of the Nuclear Superheat Experimental Program being performed by Combustion Engineering, Inc., Windsor, Connecticut.

J. Adjoint Calculations

For perturbation and reactivity coefficient calculations, it is necessary to calculate the adjoint fluxes. Because no epithermal fission capture is assumed in the formulation, it is possible to transform the real flux equations into the adjoint equations by simply inserting artificial cross sections which are a linear combination of the real flux input data. In this manner, one computer code can perform both real and adjoint calculations.

If the following substitutions are made in Equation 1 which formally contain a first-group absorption term, Σ_{a1} , although it is zero for all real flux calculations, the adjoint equations shown below are produced.

$$\phi_1 = \Psi_3, D_1 = D_3, \epsilon \nu \Sigma_{f3} = \epsilon \nu \Sigma_{f3}, \Sigma_{a1} = \Sigma_{a3} - \Sigma_{sl2}$$

$$\phi_2 = \Psi_2, D_2 = D_2, \Sigma_{sl1} = \Sigma_{sl2}, \Sigma_{a2} = \Sigma_{a2} + \Sigma_{sl2} - \Sigma_{sl1}$$

$$\phi_3 = \Psi_1, D_3 = D_1, \Sigma_{sl2} = \Sigma_{sl1}, \Sigma_{a3} = \Sigma_{sl1}$$

$$\begin{aligned} -D_1 \nabla^2 \Psi_1 + \Sigma_{sl1} \Psi_1 &= \Sigma_{sl1} \Psi_2 \\ -D_2 \nabla^2 \Psi_2 + (\Sigma_{a2} + \Sigma_{sl2}) \Psi_2 &= \Sigma_{sl2} \Psi_3 \\ -D_3 \nabla^2 \Psi_3 + \Sigma_{a3} \Psi_3 &= \epsilon \nu \Sigma_{f3} \Psi_1 \end{aligned} \quad (20)$$

III. ANALYSIS OF CRITICAL EXPERIMENTS

The sole justification of the method is the ability to predict reactivity and to predict power distributions. Both of these quantities are readily measureable, and furnish a direct comparison with theory. At the same time, it is desirable that the individual subroutines that calculate reactor parameters agree with the measured values in order for the method to be valid for temperature and isotopic changes. However, a comparison between theory and experiment in regard to lattice parameters is much more difficult to interpret, since the lattice parameters may not be calculated under the conditions for which they are measured. Further, the measurements themselves may require much analysis to reduce them to simple parameters. In making the present comparison between theory and experiment, only a surface inspection has been made of the experimental quantities in order to ascertain how they are related to the corresponding analytical quantities. For example, the disadvantage factor is defined as the ratio of the thermal flux in the moderator to that in the fuel. However, the definition of the experimental thermal flux is not quite the same as that used in the theoretical analysis. Also, these definitions may vary from experiment to experiment. The theory values listed in the analysis of the critical experiments are calculated analytic values; when comparison is made with experiment, the most closely related experimental quantities are quoted.

Three critical experiments have been analyzed. These experiments represent the presently available experimental information for cores

consisting of low-enrichment oxide fuel, moderated with light water. These experiments are: the Westinghouse TRX Critical Experiments,^{7,14} the Westinghouse Yankee Critical Experiments,¹⁵ and the Babcock and Wilcox N.S. Savannah Critical Experiments.¹⁶ All these experiments used rod-type fuel elements, and covered a wide range of water-to-fuel ratios. The TRX experiment included a 1.3 per cent U^{235} enrichment, and utilized aluminum clad rods. The Yankee experiment included a 2.7 per cent U^{235} enrichment, and utilized stainless steel clad rods. The N.S. Savannah experiment included a 4 per cent U^{235} enrichment, and utilized both stainless steel clad rods and an aluminum and stainless steel box structure.

The analysis consists of calculating the individual parameters by the previously described methods, these calculations effectively homogenizing each of the fuel regions in the core. These parameters are then inserted in Equation 1. For complex geometries, the equations are solved numerically by the IBM-704 PDQ Two-Dimensional Code.¹⁷

It should be recognized that the computational codes and their applications introduce other uncertainties into the analysis. Two different codes seemingly solving the same equations with precisely the same input data may give slightly different answers because of the differences in mathematical methods used to solve the equations. Also, the same code analyzing the same problem can give slightly different answers, depending on the choice of mesh spacing used to describe the problem and depending on the convergence criterion. For all experiments that have been analyzed in this report, fairly coarse mesh spacings have been used in order to minimize the cost

of each problem. The standard that has been adopted is to use one mesh space in any direction for each fuel rod and to use two mesh spaces for a pure-water channel. The convergence criterion that is used for the PDQ code to terminate the iteration cycle is: $\epsilon = 0.05$. In determining the detailed power distribution, rod by rod, the resulting power distribution is averaged over each mesh space.

A. TRX Critical Experiments^{7,14}

Measurements of lattice parameters and critical configurations have been made for both slightly-enriched-uranium-metal-and-uranium-oxide-fueled lattices. Three measurements were made using high-density (10.53 g/cm^3) UO_2 rods enriched with 1.311-wt.% U^{235} . Each rod was made up of 0.383-in.-diameter pellets. These pellets were inserted into aluminum tubes of 0.028-in. wall thickness to form rods 48 inches in length. There is a 0.005-in. radial gap between the fuel and the aluminum. Three different lattice spacings were measured with a water-to-uranium-metal ratio of 2.9, 3.6, and 4.9. The comparisons between the measurements and calculations are, as follows:

<u>W/U</u>	<u>p</u>	<u>ϵ</u>	<u>$\frac{\phi_M}{\phi_F}$</u>	<u>M^2</u>	<u>δ_{radial}</u>	<u>δ_{axial}</u>
2.9 Theory	0.7865	1.0500	1.1086	45.07	7.72	15.44
Experiment	0.775 ± 0.004	1.046 ± 0.002	1.10 ± 0.01	45.8	7.86 ± 0.12	15.27 ± 0.41
3.6 Theory	0.8216	1.0422	1.1172	43.25	7.54	15.08
Experiment	0.815 ± 0.004	1.042 ± 0.002	1.13 ± 0.01	44.3	7.41 ± 0.13	14.69 ± 0.43
4.9 Theory	0.8609	1.0333	1.1301	41.32	7.33	14.66
Experiment	0.850 ± 0.004	1.034 ± 0.002	1.13 ± 0.01	40.6	7.10 ± 0.10	14.52 ± 0.17

Based on the measured critical bucklings, the calculated reactivity using Equation 18 is

<u>W/U</u>	<u>Reactivity</u>	
	<u>Theory</u>	<u>Experiment</u>
2.9	0.9961	1.000
3.6	0.9982	1.000
4.9	0.9999	1.000

B. Yankee Critical Experiments ^{*,15}

Measurement of lattice parameters, critical configurations, and power distributions were made for uranium oxide lattices with a U^{235} enrichment of 2.70 wt.% and a density of 10.2 g/cm³. Each fuel rod was made up of 0.300-in.-diameter pellets, clad with stainless steel tubing of 0.0161-in. wall thickness. There was a 0.0031-in. radial gap between the pellets and the tubing. The length of the fuel rod was 48.0 inches. Three different configurations were measured. The water-to-uranium ratios for these measurements were 2.2, 2.9, and 3.9. The lattice parameter measurements have not been reported as yet. The following table lists the calculated parameters:

<u>W/U</u>	<u>p</u>	<u>€</u>	$\frac{\phi_M}{\phi_F}$	<u>M²</u>
2.2	0.7204	1.0576	1.1182	41.93
2.9	0.7748	1.0473	1.1311	40.05
3.9	0.8186	1.0387	1.1447	38.67

* The author is indebted to P.W. Davison for having data made available that is more detailed than data presented in related reports.

The disadvantage factor of 1.127 ± 0.01 has been reported for the 3.9-water-to-uranium-ratio experiment.

The radial and the axial reflector savings have been measured, utilizing activation techniques. The following is a comparison of the theory with the experimental results for the activity induced in individual fuel rods:

<u>Water-to-Uranium Ratio</u>	<u>Radial Savings</u>	<u>Axial Savings</u>
2.2 (Theory)	7.39	14.78
(Experiment, Fuel Rods)	8.19 ± 0.18	13.84 ± 0.66
2.9 (Theory)	7.24	14.48
(Experiment, Fuel Rods)	7.04 ± 0.37	13.58 ± 0.83
3.9 (Theory)	7.07	14.14
(Experiment, Fuel Rods)	7.32 ± 0.10	13.72 ± 0.84

The critical configurations and the power distributions have been calculated for the three lattices with control rod followers in the core. For this calculation, the PDQ two-dimensional code was used. The following reactivities were calculated:

<u>Water-to-Uranium Ratio</u>	<u>Theory</u>	<u>Experiment</u>
2.2	0.9835	1.0007
2.9	0.9904	1.0006
3.9	0.9925	1.0002

The calculated power distributions along a 45-degree traverse for these calculations are shown in Figure 3, Figure 4, and Figure 5.

An additional experiment has been performed with the 2.2-water-to-uranium-ratio lattice to investigate water channel peaking.¹⁸ For this experiment, the central row of elements was removed from the core, and power traverses were made perpendicular to the water channel. Figure 6 describes the core configuration, and shows the comparison of the experimental measurement with the theoretical results. The channel peaking factor — defined as the ratio of the power in the rod adjacent to the channel with the channel present, to the power in the rod without the channel present — is calculated to be 1.50, as compared to a measured value of 1.47.

Another set of measurements of the lattice parameters using 4.4-wt.% enriched fuel — in a lattice otherwise similar to the 3.9-water-to-uranium-ratio lattice — has been reported.¹⁹ For this lattice, the comparison between theory and measurement is as follows:

	<u>p</u>	<u>ε</u>	$\frac{\phi_M}{\phi_F}$
Theory	0.8160	1.0392	1.2001
Experiment	0.805 ± 0.015	1.039 ± 0.003	1.25 ± 0.02

C. N.S. Savannah Critical Experiments^{*,16}

Measurements of critical configurations and power distributions have been performed with 4.02-wt.% U²³⁵-enriched fuel. The swaged stainless steel clad fuel rods had an OD of 0.500 in., including a stainless steel jacket of 0.0283 in. wall thickness. The active

* The author is indebted to R. M. Ball and A. M. MacKinney for having data made available that is more detailed than data presented in related reports.

length of fuel rod was 66.5 inches. The density of the UO_2 was 9.45 g/cm^3 . Two lattice spacings have been investigated, one having a water-to-uranium ratio of 2.7, the other a water-to-uranium ratio of 3.6.

The disadvantage factors for moderator and cladding have been measured for these lattices. In addition to the hand calculation method, Equation 8, a P-3 calculation using the CEPTR code²⁰ with cross sections hardened by Equation 2 has been carried out for the 3.6-water-to-uranium-ratio lattice.

<u>Water-to-Uranium Ratio</u>	$\frac{\phi_M}{\phi_F}$	$\frac{\phi_{Cl}}{\phi_F}$
2.7 Theory	1.2170	1.1085
Experiment	1.29 ± 0.06	1.19 ± 0.06
3.6 Theory	1.2578	1.1299
Theory (P-3)	1.2656	1.1125
Experiment	1.40 ± 0.03	1.09 ± 0.03

For the 2.7-water-to-uranium-ratio lattice, two different critical measurements were performed. One core, designated Core II, contained 0.83-in. water channels and 0.156-in. stainless steel walls. The other core, designated Core III, had 0.83-in. water channels and 0.130-in. aluminum walls. There are 192 fuel rod positions within a box, 14×14 lattice, with the four corner rods missing. The comparison of the calculated reactivity with experiment is

	<u>Reactivity</u>	
	<u>Theory</u>	<u>Experiment</u>
Core II	1.0010	1.0006
Core III	0.9985	1.0017

The calculated rod-by-rod power distribution in Core II is given in Figure 7. The water channel peaking factor -- equal to the ratio: power in the corner rod with the channels, to power in the rod without channels -- is 1.81. There is no published measured power distribution for this core. However, for the same lattice in a larger core, a channel peaking factor of 1.77 can be inferred from the measurements.²¹

For the 3.6-water-to-uranium-ratio lattice, three different critical measurements were performed. One core, designated Core IV, contained 0.83-in. water channels and 0.130-in. aluminum walls. The second core, designated Core V, contained no fuel assembly walls or water channels. The third core, designated Core VI, contained 0.83-in. water channels and 0.156-in. stainless steel walls. There were 165 fuel rod positions within a box, 13 x 13 lattice, with the four corner rods missing.

The comparison of the calculated reactivity with experiment is

	Reactivity	
	<u>Theory</u>	<u>Experiment</u>
Core IV	0.9981	1.0011
Core V	0.9950	1.0012
Core VI	0.9979	1.0013

The calculated rod-by-rod power distribution in Core VI are given in Figure 8. The water channel peaking factor is 1.59. There is no published measured power distribution for this core; however, for the same lattice in a larger core, a channel peaking factor of 1.57 can be inferred from the measurements.²¹

IV. DISCUSSION OF RESULTS

Although experimental critical configurations can be determined to a very high degree of accuracy, there always exists an uncertainty as to the detailed composition of the core. The mechanical tolerances on fuel pellets, fuel cladding, and structural material as well as uncertainties in the purity of materials introduce uncertainties of the order of $0.5\% \Delta k$ in any composition. Therefore, one should not expect an analytical method to duplicate criticality measurements to better than about $0.5\% \Delta k$. The "package" method described here gives a good correlation for the existing experimental information; all cases check to within $2\% \Delta k$, most cases to within $1\% \Delta k$.

What is usually desired in core analysis is the prediction both of the lower limit of reactivity in the hot operating condition with no control elements present and of the upper limit of the reactivity in the cold clean condition with all control elements present. These two conditions determine the reactivity lifetime and the shutdown safety margin. The comparison of the calculational method with cold clean experiments without control rods does not directly evaluate the accuracy of the method for either of these conditions. However, the initial cold clean condition with control rods present does not appear to furnish too much difficulty. It is practical to determine directly the epithermal transmission probability for the rod directly from critical experiments (see Section II, I — Control Rod Calculations). In this manner, the cold control rod calculations should be of the same order of accuracy as the cold, no-control-rod calculation. On

the other hand, the accuracy of the reactivity calculation for the initial hot operating condition cannot be extrapolated from the cold calculations. Nevertheless, since both the cold experiments and the analysis have been carried out over a wide range of enrichment, water-to-uranium-fuel ratio, and geometry, it is expected that the same degree of accuracy will be maintained. Furthermore, it should be noted that in almost all comparisons with experiment the analysis underestimates the reactivity, the system being more reactive than calculated. Therefore, this systematic deviation acts as a small safety factor in predicting the minimum reactivity in the hot condition.

The agreement of the power distributions with experiment indicates that this method is capable of calculating the rod-by-rod power distributions, although more detailed comparisons with experiments are required to estimate the accuracy. It should be noted that the initial assumption neglecting epithermal fissions has a tendency to overestimate the local peaking factors, since the epithermal diffusion length is much longer than that which occurs at thermal energies.

For burnup calculations, it is necessary to provide cross sections for the plutonium isotopes — Pu-239, Pu-240, and Pu-241. Each of these isotopes has its own peculiarities, and each requires special attention. It would appear that the thermal and epithermal effects of plutonium can be handled by calculating equivalent thermal cross sections for the isotopes, using the entire method as previously described. This approach is presently being employed. However, experimental confirmation is required, especially for high burnups, where plutonium content is a major fraction of the fuel concentration.

Finally, some remark should be made in regard to how changes are to be made in the entire calculational procedure. Obviously, it will prove necessary to devise -- for grossly different reactor configurations, such as those which involve annular fuel elements -- new subroutines to calculate lattice parameters. Also, future experimental information at elevated temperatures and with high plutonium concentrations may indicate that it is desirable to make changes in the over-all analytical "package." However, changes cannot be made arbitrarily to satisfy a new condition. Any change or addition must be made in such manner as to maintain the internal consistency of the method and to agree with previous experiments.

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**SUPPLEMENTARY STUDY
RELATED TO BONUS AND NUCLEAR SUPERHEAT
PROGRAMS**

ILLUSTRATIONS

Figure 1. Self-Shielding Factor for a Cylinder As a Function of the Product of Macroscopic Cross Section and Radius³

Figure 2. $\Delta \left(\frac{R_o}{\lambda} \right)$ for a Cylinder⁴

Figure 3. Radial Power Distribution for 2.2/1 W/U Yankee Experiment

(1,833 fuel rods and four control rod followers in core)

Figure 4. Radial Power Distribution for 2.9/1 W/U Yankee Experiment

Figure 5. Radial Power Distribution for 3.9/1 W/U Yankee Experiment

0.405-in. Water Channel Bisecting Core of 2.2/1 W/U Yankee Experiment

(2,874 fuel rods and four control rod followers in core)

Figure 6. Comparison of Calculated and Experimental Radial Power Density

Average Core Power Normalized
to Unity

(1,416 fuel rods, 0.83-in. water channels, and
0.156-in. stainless steel box walls in core)

**Figure 7. Two-Dimensional Rod by Rod Radial Power
Distribution for 2.7/1 W/U N.S. Savannah Experiment**

Average Core Power Normalized
to Unity

(948 fuel rods, 0.83-in. water
channels, 0.156-in. stainless
steel box walls in core)

Figure 8. Two-Dimensional Rod by Rod Radial Power
Distribution for 3.6/1 W/U N.S. Savannah Experiment