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LATTICES OF PLUTONIUM-ENRICHED RODS IN LIGHT WATER
PART II - THEORETICAL ANALYSIS OF PLUTONIUM-FUELED SYSTEMS

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ABSTRACT

A theoretical analysis of $\text{UO}_2\text{-PuO}_2$ fueled, light-water-moderated lattice experiments has been performed to aid in establishing technical bases and design criteria for the utilization of plutonium bearing fuel in thermal power reactors. Results for UO_2 and Al-Pu lattices are included in order to understand the effects due to uranium and plutonium separately. The problems involved in calculating critical experiments are discussed. Estimates of the effects of various approximations inherent in the theoretical methods and/or analysis procedures are included along with the consequence on the results of the correlation. Uncertainties in the measurements and the neutron cross-section data are related to uncertainties in the calculated values of k_{eff} . Areas which should be investigated in future analyses are also identified.

Suggested running head: Plutonium Lattice Calculations

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LATTICES OF PLUTONIUM-ENRICHED RODS IN LIGHT WATER

PART II - THEORETICAL ANALYSIS OF PLUTONIUM-FUELED SYSTEMS

R. C. Liikala, V. O. Uotinen, and U. P. Jenquin*

I. INTRODUCTION

The need for establishing technical bases and design criteria for plutonium recycle cores is clearly recognized in light of the anticipated large-scale recycle of plutonium in thermal power reactors. A thorough knowledge of the neutronic characteristics of plutonium systems is essential if one is to establish valid bases and criteria. One should not expect that design methods that have been normalized for uranium cores will be valid for plutonium-enriched cores.

The neutronic analysis of light-water reactors fueled with plutonium-enriched rods is expected a priori to be less accurate than an analysis of light-water reactors fueled with uranium-enriched rods. First of all there are more isotopes present in plutonium-enriched fuel than in uranium-enriched fuel. In addition the cross sections of the plutonium isotopes have significant resonance structure at thermal and near thermal energies. This resonance structure complicates the calculation of neutron spectra in plutonium fueled reactors. In mixed-oxide fuels the interaction of the resonances of uranium and plutonium isotopes in the resonance energy region further complicates the analysis. Finally, neutron self-shielding effects due to the particulate nature of the plutonium in mixed-oxide fuels add to the calculational problem.

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Uniform lattice experiments have always played a major rôle in the development of reactor physics design methods. The calculational methods are evaluated to determine how well they can predict the behavior of these simple lattices. Then the technology is developed further by building upon this base and extending the evaluation to include other more complex features of the design problem. The mathematical models are ultimately developed to the point where they can be used with confidence in designing power reactor systems. Thus, the uniform lattice experiments form the base for the evaluation and development of physics design methods.

The analysis presented in this paper is based mainly on the available experimental data for uniform lattices of plutonium rods. Since the mixed-oxide fuels are the fuels of commercial interest, we concentrate on lattices of mixed-oxide rods. However, in order to make valid judgements concerning the adequacy of the theoretical methods and analytical procedures for mixed-oxide fuels, it is necessary to understand the effects due to uranium and plutonium separately. Therefore, our theoretical analysis includes experiments where the core is fueled with plutonium-only fuels (aluminum-plutonium alloy), uranium-only fuels (uranium dioxide), and mixed-oxide fuels (uranium dioxide-plutonium dioxide).

In this paper we give results of a theoretical analysis of plutonium-fueled light-water-moderated critical experiments and describe the problems involved in calculating k_{eff} for these small assemblies. The paper is based on extensive experimental and theoretical studies which have been carried out as part of a program⁽¹⁾ conducted at Battelle-Northwest to aid in establishing technical bases for the utilization of plutonium bearing fuel in thermal power reactors. The technical approach used in

this study is explained in Section II. The experiments analyzed and the results of a theory-experiment correlation are given in Section III. The effects of certain approximations which are either inherent in the theoretical methods and/or made in the analysis are estimated in Section IV along with their consequences on the results of the correlation. The final section of the paper summarizes the findings of our studies, presents the conclusions, and delineates some areas of concern for future analyses.

II. TECHNICAL APPROACH

The technical approach that has been used in this study needs explanation to orient the reader with respect to the results that will be presented in Section III and IV.

The results of uniform lattice critical experiments have historically been used as the basis for evaluating the accuracy of the neutron cross sections and/or theoretical methods employed in the calculation of the spectrum of neutrons slowing down and thermalizing in a unit cell.

In the choice of calculational methods for calculating the multi-group spectrum in unit cells, there are a number of possibilities. A standard approach which is used fairly widely in the industry today, is to use multigroup transport theory methods to calculate the spectrum-averaged cross sections for unit cells. These codes require a cross section library. In the choice of a set of multigroup neutron cross sections, one generally chooses one of the sets which were derived from a basic file of evaluated cross-section data. Finally, a calculational method must also be selected for computing the neutron balance for the critical assembly. In the calculation of the leakage from small critical assemblies, the choice of methods ranges from zero dimensional buckling prescriptions to multigroup multidimensional transport theory or Monte Carlo methods.

The cross sections used in this study were derived from the Battelle Northwest Master Library.⁽²⁾ The unit cell calculations were performed

using the multigroup transport theory codes HRG3⁽³⁾ and BRT-I.⁽⁴⁾

The neutron balance calculation for the critical assembly was performed using the one-dimensional diffusion theory code, HFN.⁽⁵⁾ Detailed information about these cross sections and methods are given in Appendix A. In Section III, we present the results that are obtained when these methods are used to calculate k effective for a large number of critical experiments.

Within this framework (an evaluated set of cross sections, transport theory cell methods, and diffusion theory leakage calculation) there is a broad range in the choices made on particular aspects of the calculations. Exact theoretical methods and analysis procedures generally are not used in reactor design because they demand an excessive amount of computer storage capacity and running time. In practice, various assumptions and approximations are made to simplify the calculation of cell averaged parameters. The particular assumptions and approximations that are made may lead to error. It is usually hoped that on the average, the errors due to various approximations act in opposite directions resulting in cancellation of errors. However, biases do exist in calculational methods. Therefore, attention must be given to evaluating the effects of major approximations that are contained in the methods, to determine whether or not they introduce a bias into calculated results.

The particular assumptions and approximations that are contained in the methods used in Section III are examined in Section IV. The material presented in Section IV does not represent a detailed evaluation of the effects of all of the assumptions and approximations for all of the lattices

that have been considered, but rather a limited study of the effects of the major assumptions and approximations on some particular lattices. We do not report the total bias for the lattices, but rather give examples of calculations for particular lattices which serve to point out which assumptions and approximations are most important to be evaluated in detail.

In addition to bias being introduced by the use of approximations, and assumptions, uncertainties exist in calculated results as a result of uncertainties in physical parameters, both experimental and analytical. These uncertainties exist in the basic data, such as microscopic neutron cross sections, and in mathematical definitions of multigroup constants, such as the transport cross section, and in experimental physical parameters, such as axial buckling values, dimensions, and contents of lattice components. In Section IV, we also discuss the uncertainties introduced into calculated values of k effective as a result of uncertainties in the physical parameters used in the analysis.

To summarize the philosophy, or the technical approach, of this study, we have chosen a calculational model and have calculated the values of k effective for a number of critical experiments. The assumptions and approximations contained in our calculational model appear on the surface to be reasonable and are in fact, similar to assumptions and approximations that are typically made in the industry. No claim is made that the particular choice of assumptions and approximations represent the best possible choice. Fortunately, as illustrated by the results presented in Section III, our particular choice of assumptions and approximations results in reasonably good agreement between measured and calculated values

of k_{eff} for a large range of UO_2 and $\text{UO}_2\text{-PuO}_2$ lattices. However, by examining the biases that one should expect to be present in the calculated values as a result of various assumptions and approximations that are contained in the methods, the conclusion is reached that this reasonably good agreement is the result of cancelling errors. Moreover if one were to use more exact assumptions and approximations the good agreement between calculated and measured values of k_{eff} would be destroyed. The calculation of the reactivity of these small plutonium lattices is a very basic problem, and our conclusion is that it is not yet on as sound a theoretical footing as is desirable.

III. CORRELATIONS

The results of measurements of the critical size for uniform arrays of fuel rods in a light water moderated lattice form the base upon which the calculational methods are tested. The combination of methods described in Section II consisting of the HRG3 and BRT-I cell codes and the one dimensional diffusion theory code, HFN, is evaluated by comparing calculated and measured values of k_{eff} in this section.

A. Experiments Correlated

The selection of experiments for this analysis was limited to those critical assemblies which are considered uniform, clean systems. The critical assemblies included both lattices and homogeneous reactor systems.

1. Lattices

As mentioned above, the experiments reported in the companion paper ⁽⁶⁾ provide the base of data for the theory-experiment correlation. These included three enrichments of plutonium in aluminum-plutonium alloy fuels and five enrichments of plutonium in plutonium dioxide-uranium dioxide fuels. To this base are added the series of lattices containing UO_2 -6.6 wt% PuO_2 fuel rods, in which k_{eff} was measured by Westinghouse. ⁽⁷⁾ These experiments allow us to extend the range of plutonium enrichments covered in our study. The pertinent experimental results

obtained from these experiments are given in Table I. In the calculations, it was assumed that all of the plutonium fuels in these experiments were solid solution (i.e., no Pu particles) fuel.

A number of slightly enriched UO_2 lattice critical experiments were also included in the analysis.⁽⁸⁻¹²⁾ Having data on assemblies which contain only plutonium in the fuel (the Al-Pu fueled systems) and on assemblies which contain only uranium in the fuel (the UO_2 fueled systems) allows us to gain insight into the combined effects of uranium and plutonium in the mixed oxide fueled assemblies. The UO_2 lattices were selected to cover a range of enrichments, lattice spacings and clad types. A summary of the key experimental results is given in Table II.

2. Homogeneous Criticals

Some aqueous solution critical experiments were included in the evaluation of the calculational methods. They consist of four experiments conducted at Oak Ridge using uranyl (^{235}U) nitrate solution⁽¹³⁾ and two experiments conducted at Battelle-Northwest using plutonium nitrate solution.⁽¹⁴⁾ The Oak Ridge experiments were large bare systems. The results have been used extensively throughout the years as benchmark experiments for ^{235}U systems.⁽¹⁵⁾ The fact that they are homogeneous, bare, spherical, and physically large systems makes them attractive for calculational benchmarks

because of their simplicity. The plutonium nitrate systems consist of one bare and one fully reflected sphere. An extensive analysis of plutonium nitrate solution criticals has been made previously.⁽¹⁶⁾ The intent in our analysis was to bridge the gap resulting from the use of different theoretical methods and cross sections in the previous analysis of these plutonium nitrate critical experiments. The experimental results for these homogeneous criticals are given in Table III.

B. Results

The adequacy of our calculational model in predicting k_{eff} for the various experiments is shown in Tables IV through VII where we show the calculated k_{eff} for each individual experiment and also the mean value of k_{eff} for each series of experiments.

1. Lattices

Looking first at the plutonium only systems, it is seen that the calculated results for the Al-Pu criticals shown in Table VII are high. The calculated values of k_{eff} for the Al-1.8 wt% Pu and Al-5 wt% Pu fueled lattices range from 0.04 to 1.13% high with no apparent discernible trend with lattice spacing. Adding boron to the moderator for the 1.05 inch lattice containing Al-5 wt% Pu fuel does not significantly perturb the result of the correlation. The purpose of conducting the measurements using boron in this lattice was to evaluate the

effect of neutron leakage from the lattice since adding boron requires more rods to maintain critical which in turn lowers the radial leakage. The rationale rests on the assumption that the only parameters which change significantly with boron addition are the thermal utilization, f , and the neutron leakage, both being reduced. Therefore, if the calculational trends do not change systematically with boron addition, then it can be inferred that both of these quantities (f and DB^2) are being calculated correctly, or incorrectly with the errors just compensating. Since the results for the lattices do not produce a corresponding systematic effect,

it could be concluded that the leakage calculation is adequate, assuming f is likewise calculated correctly. The results for the Al-2 wt% Pu series are approximately 2% higher than the other results. Because the discrepancy for this particular series of experiments is so much greater than for any of the other experiments, it was suspected that something could be systematically wrong with the experiments. The fuel rods have been nondestructively and destructively re-examined⁽¹⁷⁾ A chemical and an isotopic analysis were made to determine plutonium concentration and composition, and a spectrochemical analysis was performed in search of impurities. This re-examination of the fuel did not produce any new information that could explain why the discrepancy would be so much larger for this series of experiments than for the other experiments. The correlation results remain, as they always have over the years,⁽¹⁸⁾ unexplainable in terms of the difference from the results obtained for the 1.8 wt% and 5.0 wt% Pu fueled experiments. An explanation of the cause of the discrepancy remains an open question.

The calculated results of k_{eff} for the uranium dioxide criticals, shown in Table V, range from about 0.5% low to about 0.4% high. A trend such that the calculated k_{eff} value decreases with increasing lattice pitch is noticeable for the six 2.734 wt% ²³⁵U fueled lattices. The span of this trend is 0.66% $\Delta k/k$.

The correlations for the mixed oxide systems, shown in Tables VI and VII show some systematic trends. For the UO₂-1.5 wt% PuO₂ fueled lattices, a general trend with lattice spacing is discernible for the spacings from 0.55 in. to 0.90 in.; however, k_{eff} increases slightly for the 0.93 in. lattice. The results for the UO₂-2 wt% PuO₂ fueled criticals are sort of a random set of numbers. There is no trend with lattice spacing

and it doesn't appear that the effect of changes in Pu composition exhibit any noticeable trend either. Similar results are obtained for the UO_2 -4 wt% PuO_2 , and UO_2 -6.6 wt% PuO_2 fueled systems as shown in Tables VI and VII respectively.

Lattice criticals containing slightly enriched fuel rods are typically high leakage systems. Since leakage is one of the more obvious candidates as a source of error in the theoretical analysis, it is instructive to examine the results in terms of leakage to determine if systematic effects are evident. The calculated values of k_{eff} for all of the lattices are plotted as a function of the buckling in Figure 1 for the UO_2 fueled lattices, in Figure 2 for the Al-Pu fueled lattice, and in Figure 3 for the mixed oxide fueled lattices.

Examining the results plotted in Figures 1-3 no noticeable trends are evident for the UO_2 , Al-Pu and UO_2 - PuO_2 fueled assemblies. Thus, lacking trends, it would appear that our analysis of leakage from these assemblies is adequate, or if an error exists it is being compensated for by errors somewhere else in the analysis.

One of the reasons for conducting critical experiments using many different lattice spacings with the same fuel rods is to provide data which covers a range of moderator-to-fuel volume ratios. Having data in which the only variable that changes is the ratio of moderator to fuel allows evaluating theoretical models for systematic errors. It is generally conceded that a calculation made for overmoderated lattices is the least susceptible to calculational error because the effects of the many approximations made in the theoretical analysis are much smaller for these types of assemblies. Therefore, it is

instructive to examine the results of the calculation to see if a trend exists when k_{eff} is plotted as a function of moderator-to-fuel ratio. A plot of calculated k_{eff} versus hydrogen-to-uranium-235 atom ratio is shown in Figure 4 for the UO_2 fueled experiments. Plots of k_{eff} versus hydrogen-to-plutonium atom ratio are shown in Figures 5 and 6 for the plutonium fueled critical experiments.

The only trends noticeable are for the UO_2 fueled lattices. Neglecting the point at $\text{H}/^{235}\text{U}$ of 330 which appears out of line, a trend is observable in the curve (Figure 4) for the UO_2 fueled lattices. The larger the $\text{H}/^{235}\text{U}$ ratio the lower the calculated k_{eff} . Using the argument presented above concerning which lattices should be the easiest to calculate, we would arrive at the judgment that our theoretical methods are causing about a -0.5% error in k_{eff} since this is the discrepancy for open lattices having $\text{H}/^{235}\text{U}$ ratios of > 500 .

The results of this analysis do not show very many systematic variations in calculated values of k_{eff} . The only trends which are discernable are: (1) the calculated values of k_{eff} are consistently larger than the measured values for the Al-Pu fueled lattices, and (2) the calculated values of k_{eff} for the UO_2 fueled lattices are dependent on the moderator-to-fuel ratio.

2. Homogeneous Criticals

VIII The calculated values of k_{eff} for the aqueous solution critical experiments are shown in Table VIII. The calculated values of k_{eff} are systems lower by ~0.5% than the measured values for the uranyl nitrate solutions. The calculated values of k_{eff} for the 27.24 in. diameter sphere and the 48.04 in. diameter sphere are about identical; therefore, reactor size does not appear to be an influence on the calculation. When these results are compared to those obtained for the UO_2 lattice criticals we note that the mean values are ~0.5% different. However, if these points were plotted on the curve of k_{eff} as a function of hydrogen-to- ^{235}U uranium atom ratio, (Figure 4,) then the

Results are consistent with those for the UO_2 lattices. That is, a -0.5% discrepancy exists in calculated values of k_{eff} at $\text{H}/^{235}\text{U}$ ratios >500. These solution criticals have $\text{H}/^{235}\text{U}$ ratios ranging from 972 to 1835 as shown in Table III. Thus, a bias is evident in the theoretical methods which is related to hydrogen-to-fuel ratio.

The calculated values of k_{eff} for the plutonium nitrate systems are both high by 1.3% $\Delta k/k$. Since the bare and fully reflected spheres have nearly the same calculated multiplication it doesn't appear that the reflector adds to the calculational problem. Richey's analysis⁽¹⁶⁾ gave calculated results using diffusion theory which were within $\pm 0.4\%$ of experiment using the GAMTEC-II⁽¹⁹⁾ and HFN computer codes. Since we used the same diffusion theory code in this analysis, the reactivity difference between Richey's results and ours is due to the difference in spectrum average cross sections (GAMTEC-II versus HRG3/BRT-1) and amounts to about 1.3% $\Delta k/k$. The major difference between the spectrum average cross sections is the result of using different basic cross sections for ^{239}Pu below 1.0 eV. Richey used data which were normalized to a 2200 m/s value for ^{239}n of 2.093⁽²⁰⁾ whereas the ^{239}Pu cross sections used in our analysis were normalized to the 1965 IAEA evaluated ^{239}n value of 2.114.⁽²¹⁾ This difference in values for ^{239}n at 2200 m/s is about the order of the difference in the k_{eff} values. Other slight differences in the calculated values of k_{eff} are due to differences in calculational methods and cross sections, but these effects tend to cancel. Thus, our findings are consistent with Richey's when the calculational differences due to ^{239}n at 2200 m/s are taken into account.

Superimposing the calculated values of k_{eff} for these two plutonium nitrate criticals on the curve where k_{eff} is plotted as a function of H/Pu atom ratio (Figure 5) for the Al-Pu fueled systems, we note that they are consistent with those for the Al-Pu fueled lattices (i.e., there is

a discrepancy with the measured values, but there is no evident trend with H/Pu ratio).

C. Summary of the Correlation

The mean value of k_{eff} and the standard deviation of a typical value are shown in Table IX for each series of experiments. With the exception of the Al-2.0 wt% Pu fueled experiments and the plutonium nitrate experiments the calculations are all less than 1% in error. Two trends were observable in the results of this analysis. Systems fueled with plutonium-only have calculated values of k_{eff} which are consistently larger than experiment and systems fueled with uranium-only have calculated values of k_{eff} which are dependent on the H/ ^{235}U atom ratio.

The major components of k_{eff} for the plutonium-only systems are the neutron leakage (DB^2) and the thermal reaction rate ($\bar{\eta}f$) because the values of the resonance escape probability (p) and the fast fission factor (ϵ) are near unity. The discrepancies in the results are probably due to errors in the calculation of one or both of the major components (i.e., DB^2 or $\bar{\eta}f$).

The discrepancy for the Al-2 wt% Pu fueled systems is larger than the discrepancy for the Al-1.8 wt% Pu and Al-5 wt% Pu fueled systems. There is no logical explanation for this fact because the fissile content of the Al-2 wt% Pu fuel is similar to that of the Al-1.8 wt% Pu fuel while the ^{240}Pu content is similar to that of the Al-5 wt% Pu fuel and actually the Al-5 wt% fuel has more total ^{240}Pu .

The uranyl nitrate solution experiments are also well-thermalized and physically large that the major component of k_{eff} is the thermal reaction rate ($\bar{\eta}f$). The calculated value of k_{eff} is about 0.5% low which suggests that an error of this magnitude exists in the thermalization calculation.

All of the components of k_{eff} are important for the UO_2 fueled lattices. The mean value for the UO_2 lattices is 1.000 ± 0.003 which is better than expected based on the results of the aqueous solutions. The comparison of measured and calculated values of k_{eff} for these lattices shows a discrepancy which is dependent on moderator-to-fuel ratio. The calculated values of k_{eff} approach the aqueous solution values as the $\text{H}/^{235}\text{U}$ atom ratio increases. The calculated values of k_{eff} are not buckling-dependent.

Of the four factors of k_{∞} (η , f , p , and ϵ), we would expect to be able to calculate $\bar{\eta}$ and f more accurately than p and ϵ in uranium systems. The value of η for ^{235}U is nearly constant in the thermal energy region so that errors in the spectrum calculation do not significantly affect the cell average value of η . Most of the isotopes present in these lattices have cross sections which exhibit a $1/v$ dependence; therefore, the only error in the calculation of f is that propagated by errors in the calculation of the spatial flux within a lattice cell. Thus, we feel that the observed trend in k_{eff} with $\text{H}/^{235}\text{U}$ atom ratio is the result of an error in the calculation of the resonance escape probability, p ,

(principally the ^{238}U resonance absorption rate) and/or an error in the calculation of the fast fission factor, ϵ (principally spatial flux considerations).

It might be expected that the calculated values of k_{eff} for the mixed oxide lattices would lie "in-between" the results obtained for the uranium only (UO_2) and plutonium only (Al-Pu) fueled assemblies because the discrepancies would tend to cancel. However, this is not so, for the discrepancies for uranium and plutonium fueled systems do not combine linearly in the mixed oxide fueled systems. When we go back and start delineating the approximations which we have made in the analysis, the sheer number of these strengthens the suspicion that significant cancellation of errors is present in the analysis. To gain additional insight regarding the accuracy of our analysis, we examine potential sources of bias and error, and make estimates of their magnitude, in the next section.

IV. AREAS OF CALCULATIONAL UNCERTAINTY

As stated above, any calculational model which is used in reactor design contains certain simplifying assumptions and approximations. Many of the approximations in the theoretical methods are made simply to make the mathematics tractable. Also, many assumptions are made to make the calculational task less time-consuming and/or costly. It is recognized that the use of numerous approximations can be a source of error in the calculations. It is usually hoped that on the average, the errors due to various approximations act in opposite directions resulting in cancellation of errors. However, biases generally do exist in calculational methods. Therefore, attention must be given to evaluating the effects of major approximations that are contained in the methods, to determine whether or not they introduce a bias into calculated results.

In addition to a possible bias being introduced by the use of approximations and assumptions, uncertainties exist in calculated results as a result of uncertainties in physical parameters, both experimental and analytical. These uncertainties exist in the basic data, such as the microscopic neutron cross sections, in mathematical definition of multi-group constants, such as the transport cross section, and in experimental physical parameters, such as axial buckling values, dimensions, and contents of lattice components.

In part A of this section we present results of some studies which are aimed at determining the magnitude of the bias in calculated values of k_{eff} due to various approximations and assumptions.

In part B we discuss the uncertainties introduced into the calculated values of k_{eff} as a result of uncertainties in the physical parameters used in the analysis.

A. BIAS FROM ASSUMPTIONS IN CALCULATIONS

The calculational procedure involves both a description of the physical theory and a modeling of the geometric detail of the problem. In both of these areas certain simplifying assumptions are made. The calculational assumptions that have been investigated fall into four categories: the slowing-down calculation; the thermalization calculation; the leakage calculation; and modeling of the geometric details. The assumptions included in these four categories are listed below.

1. Slowing-down Calculation
 - Spatial fast effect neglected
 - Resonance overlap neglected
2. Thermalization Calculation
 - Reflecting cell boundary condition assumed
 - Energy detail
 - Upper energy limit of thermalization calculation
 - Approximation of anisotropy
3. Leakage Calculation
 - Axial leakage representation
 - Spatial detail
 - Energy detail
 - Diffusion theory assumed accurate
4. Assumptions Regarding the Geometric Detail of Assemblies
 - Fuel assumed homogeneous
 - Lattice hardware ignored

1. Slowing-down Calculation

We mention here two expected sources of error arising from approximations that are made in the theory of the slowing down calculation. These are neglecting the spatial fast effect and neglecting the effects of resonance overlap.

Spatial Fast Effect

The slowing down code used in our analysis (HRG3) assumes the lattice to be a homogeneous mixture of fuel, cladding and moderator. The fast flux is assumed to be spatially flat throughout the unit cell. In reality the fast neutron flux is peaked in the fuel rod and depressed in the moderator (i.e., the opposite of the thermal neutron flux distribution). Thus, a correction should be made to the calculated fast neutron cross sections to account for the lattice heterogeneity. The effects on criticality due to approximating the lattice cell in a homogeneous fashion have been investigated by Dwivedi⁽²²⁾ for the UO_2 lattices studied here. His results show that lattice multiplications increase by 0.2-0.5% when a correction for heterogeneity is made to the calculated fast fission factor. These results are consistent with the results of other investigations of the spatial effects of fast fission events in ^{238}U .^(23,24)

The mixed oxide fuels and the UO_2 fuels in our study are similar from the standpoint of fast fission events because of similar ^{238}U contents in the fuels. The magnitude of the correction is a function of lattice spacing⁽²³⁾ with the largest effect expected at the most open lattices. Based on our study, we would estimate the bias in calculated values of k_{eff} to be of the order of -0.2 to -0.5% when spatial effects are neglected in calculating fast fission events.

Resonance Overlap

The HRG3 code does not take into account the effects of resonance overlap. The overlap of ^{238}U and ^{239}Pu resonances, for example, is expected (25,26,27) to cause a reduction in the effective resonance integrals. Hellens (27) has made an estimate of the effect on k_{eff} of the resonance overlap of ^{239}Pu and ^{238}U for the UO_2 -2 wt% PuO_2 (8% ^{240}Pu) fuel. Hellens' results indicate an error ranging from -0.1 to -0.4% in k_{eff} can be attributed to neglecting this effect. The largest effect is in the tightest lattice. On the basis of this limited information, we assume that a bias exists in calculated values of k_{eff} for the UO_2 - PuO_2 fueled lattices, which is of the order of 0.0 to -0.5% $\Delta k/k$.

2. Thermalization Calculation

Boundary Conditions

In our thermal model, reflecting boundary conditions were used in the one dimensional cylindrical cells. Other investigations (28,29) have shown that these boundary conditions could lead to serious errors in the spatial flux for tightly packed uranium-water lattices. Further shown was that disadvantage factors obtained from the one dimensional cell calculation agree favorably with two dimensional calculations when the outer boundary of the one dimensional cell has a pure heavy scattering material surrounding it (i.e., neutrons returned isotropically). (29) Subsequent investigations on the effects of cell boundary approximations have shown that a so-called white boundary (30) leads to significant improvements in the description of thermal neutron distributions in space and energy. A white boundary condition was incorporated in the BRT-I code after most of our calculations were completed. To assess whether the use of reflecting boundary conditions

causes errors in our calculated values of k_{eff} , some of the BRT-I problems were rerun using the white boundary conditions incorporated in the BRT-I code. The conclusion from these calculations is that we indeed expect that calculated values of k_{eff} contain a bias when reflecting cell boundary conditions are used in the thermalization calculation. The bias is expected to be of the order of -0.1 to -0.5% for the lattices studied. The effect is largest at the most open lattices. It also increases as the enrichment increases.

Energy Detail

We have used thirty groups to span the energy region from 0.0 to 0.683 eV. To check if this provided enough detail for the reaction rate calculation, the thermalization problems for the 0.55 in. lattice using UO_2 -1.5 wt% PuO_2 fuel and the 0.75 in. lattice using Al-2 wt% Pu fuel were run using 40 energy groups. Most of the extra detail provided by the 10 additional groups was concentrated in the mesh covering the ~ 0.3 eV ^{239}Pu resonance. Comparison of calculated cell average values of $\bar{\eta}$ from the 30 and 40 energy group problems showed differences of the magnitude of 0.1% $\Delta k/k$.

Thermal Group Upper Boundary

We have assumed that the thermalization region extends to only 0.683 eV and that neutron upscattering to energies above this in H_2O systems can be accounted for by an approximate correction to the hydrogen cross section in HRG3. Evidence of molecular binding in the neutron energy region above 0.683 eV is well founded.⁽³¹⁾ One of our early attempts was to include the region from 0.683 to ~ 2 eV in our thermalization calculations using the THERMOS type code. Though we were not limited as to the number of energy groups, the results of early studies we made⁽³²⁾ showed that extending the Nelkin kernel for H bound in water to energies above 0.683 eV resulted in oscillating behavior in the calculated water cross sections and in the flux in a medium

comprised of only H_2O . Attempts to "connect" a gas model to account for downscattering with a Nelkin model to account for upscattering were unsuccessful. Since these results were obtained prior to the availability of the ENDF/B library data for H_2O kernels, it was decided that the most prudent approach was to try to account for this effect by an approximation which could be accommodated in the slowing down calculation in the HRG3 code. Determinations of the magnitude of the effect of the approximation which was included with the HRG3 code were made for purposes of evaluation and the results are presented in Table X.

The change in k_{eff} is always negative when H_2O upscattering is introduced. The change is negligible for the UO_2 lattice calculations. For the lattices containing plutonium, the effect is significant, ranging up to $-0.7\% \Delta k/k$. The change in k_{eff} is due primarily to the increased absorption rate in the ^{240}Pu 1.056 eV resonance. The effect is largest for the tightest lattices. It also increases as the ^{240}Pu content in the plutonium increases. The base calculations reported in this paper utilized the approximation for H_2O upscattering in HRG3. No estimate of the accuracy of this approximation has been made, but the results of our study give an indication of the significance of H_2O upscattering in the various lattices.

Neill and Prezbindowski subsequently made a study⁽³³⁾ of the effects of different group structures and H_2O scattering kernels for the Al-5 wt% Pu fueled - 1.30 in. lattice. The results of their study showed that the calculated value of k_{eff} was insensitive ($\pm 0.1\% \Delta k/k$) to scattering models (Haywood-II, McMurray-Russell, and Nelkin) or to including more groups than 30 groups below 0.683 eV. However, their study did show that a change in k_{eff} somewhere in the neighborhood of $+0.3$ to $+0.7\% \Delta k/k$ occurs when the thermal

cutoff is increased from 0.683 to 3.059 eV. In Table X we show that the upscattering correction incorporated in the HRG3 code leads to a reduction in k_{eff} of $-0.117\% \Delta k_{\text{eff}}$ for this lattice. Thus, the results of Neill's and Prezbindowski's study show an opposite effect from our results. It is possible that in a thermalization calculation which spans this energy region there are multiple effects such that upscattering alone may cause a negative reactivity effect, but including the ^{240}Pu resonance in the thermalization calculation may affect the reaction rates in the energy region below the resonance which causes the reactivity to increase, thus overriding the negative effect of upscattering.

Anisotropy

We also approximate the effects of anisotropy in the thermalization calculation by altering the diagonal elements of the scattering kernel so that the sum of the matrix at each initial energy added to the absorption cross section yields the transport cross section at each energy. Previous studies⁽³⁴⁾ have shown that this approximation has a significant effect on k_{eff} for certain lattices. Lacking more definitive evidence, we estimate no bias in the results of our analysis due to this approximation. We assume the anisotropy effect has been accounted for adequately in our calculations.

3. Leakage Calculation

Axial Leakage Representation

We have represented axial leakage as the neutrons emerging from the top and bottom of a cylindrical homogeneous core which is fully reflected with H_2O . This representation does not account for the possibility of neutrons leaking

from the assembly via streaming in the fuel and moderator channels in the lattices. For the systems we have studied, the largest possibility for calculational errors of this type is for the Al-Pu fueled lattices because the fuel rods are mainly aluminum. We have not made an analysis of the existence or the magnitude of this effect. However, other investigators have studied this phenomena both experimentally and analytically (35,36). Based upon their findings, we state that this effect is real and unaccounted for in our analysis. We estimate the bias in analysis of the Al-Pu fueled systems may be as large as $+0.5\% \Delta k/k$ when streaming is neglected. The sign is positive because we would underestimate the fast neutron leakage from the core with our homogeneous model which would lead to overestimating k_{eff} . We likewise estimate a bias of the order of $+0.25\% \Delta k/k$ for the UO_2 and UO_2 - PuO_2 fueled lattices. We expect a smaller error in the oxide fuel because these fuel rods are less susceptible to streaming.

Concerning the representation of axial leakage in our calculational model, the further assumption is made that a one dimensional (radial) diffusion theory calculation, in which the axial leakage is represented by the measured axial buckling, is adequate. When we compared the results of such a calculation with the results of a two-dimensional (r,z) diffusion theory calculation using the EXTERMINATOR code (37) we found that the two-dimensional calculation resulted in values of k_{eff} $\sim 0.3\%$ lower than the results of the one-dimensional calculation. This calculation was for the 1.05 in. lattice of Al-5 wt% Pu rods, and represents an extreme case because of the shortness of these rods. For the other lattice experiments, the difference is expected to be smaller than 0.3%.

We do not have enough information to conclude whether the inconsistency

that exists between results of one- and two-dimensional diffusion theory² calculations is due to an incorrect value of axial buckling, or whether it is due to an incorrect assumption regarding the separability of the axial and radial components of the flux. All we can conclude is that there is this inconsistency, and that it further illustrates the problem of calculating the leakage from these typically high-leakage assemblies.

Spatial Detail

In our standard one-dimensional diffusion theory calculation, 50 mesh points were used in the core and 50 in the reflector. The adequacy of this mesh spacing was investigated by changing the mesh to 30 in both core and reflector, and then to 70 in both core and reflector. The results indicated a negligible ($\sim 0.1\%$) change in the calculated value of k_{eff} between the 30 and 50 mesh point cases and no change between the 50 and 70 mesh point cases. Thus we conclude that our choice of 50 mesh points in both core and reflector is adequate.

Another aspect of the question of the adequacy of our description of spatial detail is the number of regions used to describe the reactor in the diffusion theory calculation. All of our analyses have been made using a two-region radial model of the reactor, namely, a homogeneous core and a homogeneous reflector. In reality, the spectrum changes as the boundary between core and reflector is approached. A calculation was performed to determine what change, if any, would occur in the calculated value of k_{eff} when three regions are used to describe the reactor instead of just two. This three-region model consists of a uniform core, an inner reflector (one lattice unit thick) and an outer reflector. The cross sections for hydrogen and oxygen in the inner reflector region were taken directly from the

HRG3 and BRT-I cell calculations and thus are averaged over a spectrum characteristic of the core. The non-thermal constants were cell-average values and the thermal constants were averages over the moderator portion of the unit cell. The calculation was performed for the 0.85 inch triangular lattice of UO_2 -2 wt% PuO_2 (8% ^{240}Pu) rods. The calculated k_{eff} increased from 0.9954 for the two-region reactor to 1.0062 for the three-region reactor. We conclude from this that if we were to change from a 2-region model to a more detailed description we could expect changes in calculated values of k_{eff} at least as large as 1%. The three-region calculational method mentioned above gave much-improved agreement between measured and calculated radial power density distributions.⁽³⁸⁾ In the study reported in Reference 38, the value of k_{eff} obtained for a UO_2 - PuO_2 lattice (0.75 cm square), using the three-region reactor model was ~1% greater than that obtained using a two-region model. For a UO_2 lattice the three-region model yielded a k_{eff} ~0.5% greater than that given by the two-region model.

Energy Detail

Our analysis assumed that four groups of neutrons were sufficient in describing the neutron leakage from the assemblies. To test the validity of this assumption, we performed some calculations using 18 groups of neutrons in the HFN code. The groups were selected such that extra energy detail was provided in the region above 11.7 keV, the one fast group in the 4-group analysis. The problems selected for the evaluation were the highest leakage systems: the 1.05 in. Al-5 wt% Pu fueled lattice and the plutonium nitrate criticals.

The effect of increasing the number of groups from four to eighteen

is to increase the calculated value of k_{eff} . The magnitude of the effect is 0.5% for the Al-5 wt% Pu fueled lattice, and less than 0.1% for the plutonium nitrate criticals for both the bare and reflected systems. From these results we conclude that the maximum expected bias in our four group model using diffusion theory is $\sim 0.5\%$ in k_{eff} .

Diffusion Theory Assumed Adequate

The diffusion theory solution of neutron leakage from typically high leakage assemblies may itself be introducing errors in the analysis. Richey's analysis of the plutonium nitrate criticals showed that transport theory yielded multiplication values which were consistently larger than values derived using diffusion theory⁽¹⁶⁾. To determine if a similar correspondence exists for our analysis, some calculations were repeated on the same basis. The calculations were made for the highest leakage systems (the 1.05 in. lattice of Al-5 wt% Pu and the plutonium nitrate systems), using the aforementioned eighteen group structure and the DTF-IV computer code (P_1 , S_4).

The comparison indicates differences between values of k_{eff} calculated using diffusion and transport theory. The differences in k_{eff} range from approximately 0.4% for the Al-5 wt% cases to about 2% for the reflected nitrate system. Dwivedi⁽³⁹⁾ has made an analysis to determine the dependence of calculated k_{eff} on energy and angular detail for the two nitrate systems. He concludes that a ten energy-group and an S_8 order DTF-IV calculation is sufficiently accurate to calculate the leakage from these systems. The effect of going from S_4 to S_8 would be to decrease slightly (approximately $0.2\% \Delta k/k$) the calculated values of k_{eff} . Neill and Prezbindowski's analysis for the 1.30 in. lattice containing the Al-5 wt% Pu fuel show that k_{eff} increased by $\sim 3.6\%$ when transport theory was used relative to diffusion theory.⁽³³⁾ Using the results of these analyses we conclude that the use of

diffusion theory tends to overestimate the leakage for the critical experiments analyzed in this study. Thus, our leakage calculation is suspect even though no trends were evident when k_{eff} was plotted against buckling (Figures 1-3).

4. Assumptions Regarding Physical Details of Assemblies

Fuel Assumed Homogeneous

The assumption that the fuel is homogeneous in the UO_2 - PuO_2 fueled experiments is a known source of error⁽⁴⁰⁾ in our calculations. It has been demonstrated experimentally⁽⁶⁾ that the fuels used in these experiments contain PuO_2 particles whose average size is 25 microns, and that a reactivity defect occurs⁽⁴⁰⁾ as a result of having these particles. Having the PuO_2 in the form of finite size particles results in a reactivity change relative to homogeneous fuel mainly because of changes in ^{239}Pu fission, ^{239}Pu capture, and ^{240}Pu absorption. The changes in ^{239}Pu fission and capture are mainly in the energy range below 0.683 eV while the change in ^{240}Pu absorption is primarily in the range of the 1.056 eV ^{240}Pu resonance. As pointed out in Reference 40, self-shielding of ^{239}Pu with increasing PuO_2 particle size reduces the ^{239}Pu fission reaction rate in the fuel, thus producing a negative reactivity effect. The thermal-spectrum-average value of the ^{239}Pu capture-to-fission ratio, $\bar{\alpha}^{239}$, is also reduced, due to a larger proportionate increase in shielding of the 0.3 eV resonance. This produces a positive reactivity effect. A positive reactivity change is also contributed by the increased shielding of the 1.0 eV resonance of ^{240}Pu . The magnitude of this positive reactivity contribution depends on the concentration of ^{240}Pu in the particle. The net reactivity effect due to shielding within the PuO_2 particles can be negative or positive; depending on the spectrum, the isotopic composition of plutonium, and the size of the PuO_2 particle.

We have made an assessment of the magnitude of the bias incurred in our

calculations because of neglecting the particulate nature of the fuel. The codes GRANIT and EGGNIT, which are described in the Appendix were used to calculate unit cell group constants for selected lattices assuming PuO_2 grains with diameters of zero (i.e., homogeneous) and 25 microns. These four-group constants were then used in HFN to regenerate values of k_{eff} . The change[†] in calculated values of k_{eff} between zero and 25 micron fuel cases is shown in Figure 7 for each fuel type.

The reactivity effect, because of neutron self-shielding in the particles, is seen to be dependent on: H/Pu atom ratio or lattice pitch, plutonium content, plutonium composition, and rod size. The largest effect occurs for the UO_2 -1.5 wt% PuO_2 rods because these are smaller diameter rods than the others. The reactivity effect is in the range of 0.1-0.7% $\Delta k/k$ and is negative for all the cases studied, but it can clearly be seen that at tighter pitches the effect would be expected to be positive. Also, for mixed oxide fuels containing higher concentrations of ^{240}Pu , one would expect the entire curve to shift toward the positive direction. These results indicate that our calculated values of k_{eff} presented in the previous section for the mixed oxide lattices are all too high because we have assumed the fuel to be homogeneous. The smallest bias is in our tight lattice calculations and the largest is in our loose lattice calculations.

Lattice Hardware Ignored

In the calculations we have used the as-measured critical sizes for all lattices. No corrections were made to account for the presence of lattice grid plates and other hardware in the assemblies. The most significant of the neglected items are the lattice grid plates. In most of the lattices the grid plates were of Lucite ($\text{C}_5\text{H}_8\text{O}_2$)⁽⁴¹⁾. The presence of Lucite in the core

[†] The experimental evidence shows a linear change in reactivity with particle size; therefore, we use simply the difference in k_{eff} s.

produces an effect which is essentially a voiding effect. Thus, in tight lattices we would expect a slight negative reactivity effect and in loose lattices a slight positive reactivity effect due to the presence of the Lucite. The magnitude of the reactivity effect has been determined experimentally⁽⁴²⁾ for a few lattices and is of the order of 0.2% Δk or less. In a few of the lattices some grid plates of aluminum were included and in these cases one would expect a slight negative reactivity effect. For the Hanford experiments using Al-1.8 wt% Pu and Al-2.0 wt% Pu rods, the rods were enclosed in Lucite sleeves⁽⁴³⁾. Subsequent measurements^(44,45) indicated that the reactivity effect of the Lucite sleeves was of the order of 0.1-0.2% in k_{eff} .

B. UNCERTAINTIES IN PHYSICAL PARAMETERS

Most of the physical parameters used in the analysis are measured quantities, or are deduced from measured quantities. As such, they are not known exactly, but have associated with them uncertainties. These uncertainties propagate through the mathematics of the analysis and result in uncertainties in the calculated parameters. There are also uncertainties in mathematical definitions of multigroup constants, such as the transport cross section. In this section we discuss the uncertainties arising from:

1. Uncertainties in neutron cross sections of the isotopes;
2. Uncertainties in definition of diffusion coefficient;
3. Uncertainties in the axial buckling that is used to describe the axial leakage;
4. Uncertainties due to manufacturing tolerances (dimensions, contents, etc.) of fuel rods and lattice components.

1. Uncertainties in Neutron Cross Sections

In considering what effects uncertainties in basic neutron cross sections have on calculated values of k_{eff} , two approaches are taken. The first approach is to consider the actual experimental uncertainties associated with the best evaluated measured cross-section data, and to calculate the changes in k_{eff} that come about when the cross sections are varied within their limits of uncertainty. In this approach one attempts to determine how accurately one should legitimately expect to be able to calculate k_{eff} , knowing the quoted precisions of the basic cross sections. The second approach is to consider the latest cross-section set to be "exact", and then calculate changes in k that come about when the latest set of cross sections is substituted for some earlier set. This then is a measure of the "uncertainty" in the earlier set.

Effects of Experimental Uncertainties in Cross Sections

Uncertainties in the nuclear data propagate through the calculational procedures and lead to uncertainties in calculated values of k_{eff} . Calculations have been performed to determine the sensitivity of k_{eff} to changes in the cross sections of uranium and plutonium isotopes.^(46,47) The results of these earlier studies are summarized in Table XIV. Estimated uncertainties in the "best" evaluated cross sections have been reduced somewhat throughout the years, but the results shown in Table XIV are still representative. The uncertainties listed in Table XIV are for the lattice of each type of fuel which exhibits the largest sensitivity to the cross section uncertainty.

Since the largest uncertainties are in the non-thermal data, the uncertainty in calculated values of k_{eff} is greatest for the tight lattices which

have a greater proportion of non-thermal neutrons, and is reduced as the assemblies become more thermal, i.e., as the moderator-to-fuel volume ratio increases. Uncertainties for fission and absorption cross sections are expected to be correlated but no effort has been made to evaluate the correlation effects.

The thermal data for ^{239}Pu contains a large resonance at 0.3 eV in which the capture-to-fission ratio varies as a function of energy. Reference 17 contains results of calculations utilizing two sets of ^{239}Pu data with different shapes for the cross-section curve in this energy region. One shape was that given by Schmidt in Reference 48 and the other shape was that suggested by Leonard and given in Reference 49. The two different shapes can be taken as representative of the uncertainty in the exact shape of the cross-section curves. The values of k_{eff} calculated using the different shapes differ by $\sim 0.5\%$ for plutonium lattices.

In summary, our estimates of the uncertainties in calculated values of k_{eff} due to experimental uncertainties in the cross sections are the following: For the Al-Pu lattices the uncertainty in k_{eff} is about $\pm 1\%$. For the UO_2 lattices the uncertainty in k_{eff} ranges from about $\pm 1.5\%$ for tight lattices to about ± 0.5 for loose lattices. For the $\text{UO}_2\text{-PuO}_2$ lattices the uncertainty in k_{eff} ranges from about $\pm 2.0\%$ for tight lattices to about $\pm 1.0\%$ for loose lattices. These numbers are estimates of how accurately one should legitimately expect to be able to calculate the reactivities of light water lattices using "exact" methods and knowing the quoted precisions of the basic cross sections.

Effect of Changing Basic Cross Sections

Some of the calculations were repeated using cross sections derived from ENDF/B-II. If ENDF/B-II data were not available for a particular isotope, the BNWML data were used. Thus, differences in results can be ascribed to

differences between the cross sections for certain isotopes from ENDF/B-II and the BNWML. The source of the data for these calculations is summarized in Table XII.

The results of these calculations are shown in Table XIII along with the corresponding calculations based on the BNWML data. For both the UO_2 and $\text{UO}_2\text{-PuO}_2$ systems, the resulting values of k_{eff} , using ENDF/B-II data, are significantly less than those obtained using the BNWML data. The difference ranges from 0.7% for loose lattices to 3.8% for tight lattices. For the Al-Pu systems the differences in k_{eff} are not as large. The calculated values of k_{eff} using BNWML data are closer to experimental values than those obtained using ENDF/B-II data. However, because of biases in the calculational methods, which have been discussed above, one cannot use the results in Table XIII as a basis for deciding that the BNWML data are better than ENDF/B-II data.

The thermal values of neutron multiplication, $\bar{\eta}f_2$, agree in all cases within 0.3% for the two sets of data. Thus, for the UO_2 and $\text{UO}_2\text{-PuO}_2$ cases essentially all of the difference in the calculated value of k_{eff} must be due to the nonthermal parameters. The nonthermal parameters $\bar{\eta}f_1$ and p_1 are significantly less using ENDF/B-II cross sections. The changes in $\bar{\eta}f_1$ and p_1 are due primarily to larger epithermal spectrum-average ^{238}U cross sections (about 10% larger) using ENDF/B-II data.⁽⁵⁰⁾ As lattice spacing increases, the ^{238}U cross section has a diminishing effect on p_1 and, hence, on k_{eff} .

The calculated infinite dilute resonance capture integrals are 269.5 barns for BNWML data and 276.9 barns for ENDF/B-II data. The difference of 2.7% is magnified into a difference of about 10% in the effective resonance integral. The shielded portion of the effective resonance is about 15 barns for both sets of data. The non-shielded portion of the resonance integral (floor) is 3.90 barns for BNWML data and 6.21 barns for ENDF/B-II data. This difference of 2.31 barns gives a difference of about 10% in the effective resonance capture integral and, hence, 10% in the spectrum average cross section

The BNWML data does not contain any p-wave cross sections in the resolved and unresolved resonance regions (1 eV to 2.5 keV). The p-wave cross-section data on ENDF/B-II in this energy range consists of 0.41 barns on the smooth file and 0.89 barns on the resonance parameter file. Thus, about 1.30 barns of the difference (2.31 barns) between the HRG3 floors using BNWML and ENDF/B-II cross-section data are attributable to omission of p-wave cross-section data on the BNWML. The remainder of the difference is due to different evaluations of the data. If the identification of the p-wave resonances in ^{238}U is correct, the description of the ENDF/B-II cross section data is better than the BNWML cross-section data. If the difference between the two sets of cross-section data is considered to be an "uncertainty" in the nuclear data, then the resulting uncertainty in calculated values of k_{eff} ranges from 3.8% for tight lattices to 0.7% for loose lattices of UO_2 and $\text{UO}_2\text{-PuO}_2$ systems. The uncertainty in calculated values of k_{eff} for Al-Pu systems would be 0.3%.

2. Uncertainties in Definition of Diffusion Coefficient⁽⁵¹⁾

In our calculation of the non-thermal multigroup parameters using the HRG3 code, we employ the "consistent" definition of the macroscopic transport cross section. The definition is obtained by equating the second of the P_1 or B_1 equations to Ficks' Law. In terms of cross sections, the consistent definition for a group g is

$$\Sigma_{\text{tr},g} = \alpha_g \Sigma_{t,g} - \Sigma_{1,g}^{\text{in}} \quad (5)$$

where $\Sigma_{t,g}$ is the current weighted total cross section, $\Sigma_{1,g}^{\text{in}}$ is the current weighted P_1 component of the scattering cross section from all energies into an energy in group g , and α_g is a parameter in the second B_1 equation ($\alpha = 1$ for the P_1 approximation). Specifically, $\alpha_g = X^2 A_0 / 3(1-A_0)$ where $X = B/\Sigma_{t,g}$,

$\Lambda_0 = \tan^{-1} X/X$, and B is the square root of the buckling. The "standard" definition of the macroscopic transport cross section is

$$\Sigma_{tr,g} = \alpha_g \Sigma_{t,g} - \Sigma_{1,g}^{out} \quad (6)$$

where $\Sigma_{1,g}^{out}$ is the current weighted P_1 component of the scattering cross section of an energy in group g into all energies, and the other parameters are as above. In the limit of a single energy group solution, these two definitions yield identical values for the transport cross section. However, in a multigroup solution, the values may differ considerably.

Calculations were made using ENDF/B-II cross sections to determine how sensitive the multiplication constant is to this difference in values of the transport cross section (more specifically, the diffusion coefficient). Results are given in Table XIV for two representative systems of mixed oxide fuels. As shown, the reactivity effect is indeed significant. Also given are the three nonthermal broad group diffusion coefficients. The standard definition of the transport cross section gives a higher diffusion coefficient in group 1 and lower diffusion coefficients in groups 2 and 3.

The consistent transport cross section is the more rigorous of the two definitions, and we feel it is the better one for diffusion calculations. However, the standard transport cross section is a valid definition and is widely used. It is the only one calculated by some slowing-down codes. Since both definitions of the transport cross section are valid, the resulting difference in k_{eff} (0.5%) should be treated as a representative uncertainty in the leakage calculation. Other definitions of the transport cross section, such as using a flux-weighted rather than a current-weighted Σ_t , may result in calculated values of k_{eff} which do not fall between the values shown in Table XVII.

3. Uncertainties in Axial Buckling

The axial bucklings, B_z^2 , that were used in the one-dimensional radial diffusion theory calculations to account for neutron leakage in the axial direction were determined by the simple prescription:

$$B_z^2 = \left(\frac{\pi}{H + 2\lambda} \right)^2 \quad (7)$$

where H is the physical height of the fuel and λ is a measured reflector savings. The quoted uncertainties in the measured reflector savings are typically less than $\pm 1\%$.⁽⁶⁾ These uncertainties result in uncertainties of less than $\pm 0.2\%$ in the axial bucklings. Such small uncertainties in the axial buckling result in negligible uncertainties (less than $\pm 0.01\%$) in calculated values of k_{eff} .⁽⁵¹⁾

There is an additional consideration concerning the use of axial bucklings derived from the measured reflector savings reported in Reference 38. The values reported for reflector savings are biased because of assumptions⁽⁵²⁾ that were made in deducing the reflector savings from measured data. The assumptions were that the reflector savings are the same in both axial and radial directions, and that the radial reflector savings are the same for the critical core and the exponential (approximately 50% critical mass) core. The reflector savings are expected to be somewhat larger in the radial direction than in the axial for these rather small assemblies.⁽⁵³⁾ Also, the radial reflector savings are expected to be larger for the exponential core than for the critical core.⁽⁵⁴⁾ Thus, the value deduced for the axial reflector savings by the method described in Reference 6 is expected to be too large. The magnitude of the bias is expected to vary from lattice to lattice, but it is estimated that the

effect on the calculated values of k_{eff} would be only of the order of 0.1% in the worst case when only the axial leakage is represented by a DB_z^2 term.

4. Uncertainties Due to Manufacturing Tolerances

As in other manufacturing situations the manufactured materials are built to within specified tolerances. Usually these tolerances are selected so that one reaches a meaningful balance between cost of manufacturing and the effect of the tolerance on the predicted performance of the product. Some items that are subject to statistical variations within certain tolerance limits are the height of the fuel, density of fuel, composition of fuel, cladding thickness, and lattice spacing.

Variations within the specified tolerances may result in local perturbations in the fine detail within individual unit cells. However, when the variations are distributed randomly over the entire core, the various effects tend to cancel. Thus, we assume that no significant uncertainties are introduced into calculated values of k_{eff} as a result of variations of dimensions, etc., within the manufacturing tolerances.

V. CONCLUSIONS AND RECOMMENDATIONS

The results of the analysis illustrate the importance of performing a detailed evaluation of calculational methods. Given only the summary of results presented in Table XII, it could be concluded that the cross sections, theoretical methods, and analysis procedures are adequate to establish valid design bases and criteria for plutonium cores. However, k_{eff} is an integral parameter which is made up of many components. A study of the uncertainties in calculating these components indicates many potential sources of error. We have attempted to identify and estimate the magnitude of the major uncertainties and biases in our calculations. The scope of this paper has been confined to the problem of calculating k_{eff} for small plutonium lattices. There are many other important parameters, such as power distribution, reactivity coefficients, control rod worth, and burnup, that need to be investigated in connection with plutonium recycle. However, the reactivity calculation, is still a very basic problem and our conclusion is that it is not yet on as sound a theoretical footing as is desirable. We feel that further study is needed in several areas. Firstly, there is a need for improvement in the precision of measured cross sections. Secondly, there is a need for improvement in the methods used to calculate cell-average parameters. Finally, there is a need for improvement in the method of calculating the leakage from these small critical lattices.

A. CROSS SECTIONS

The expected uncertainty in k_{eff} due to experimental uncertainties in the cross sections is significant. For UO_2 lattices this uncertainty in

k_{eff} ranges from about $\pm 1.5\%$ for tight lattices to about $\pm 0.5\%$ for loose lattices. For Al-Pu lattices the uncertainty in k_{eff} is about $\pm 1\%$. For the $\text{UO}_2\text{-PuO}_2$ lattices the uncertainty in k_{eff} ranges from about $\pm 2\%$ for tight lattices to about $\pm 1\%$ for loose lattices. Thus, if the theoretical methods and analytical procedures used in a calculation were "exact," these uncertainties are estimates of how accurately one can legitimately expect to be able to calculate k_{eff} .

The cross sections making the largest contribution to the uncertainty in k_{eff} are the nonthermal data for ^{238}U and ^{239}Pu . Since ^{238}U is present in such high concentrations, it would be desirable to know the background (floor) cross section data, as well as the resonance parameters, more precisely than they are known at present.

B. CELL METHODS

Exact theoretical methods and analysis procedures generally are not used in reactor design because they would demand an excessive amount of computer storage capacity and running time. In practice, various assumptions and approximations are made to simplify the calculation of cell-average parameters, and this should be expected to result in a bias in the calculated results. When designing reactor cores, it is important to estimate the net bias that one would expect from the particular assumptions and approximations that he has made in his cell methods. However, the scope of this paper has not included an evaluation of the effect of every assumption and approximation on the calculated result for every lattice. Rather, the purpose of the studies presented in Section IV has been to illustrate the importance of various assumptions and approximations for a few selected lattices. Some of the important assumptions which result in a bias in our results are neglecting resonance overlap effects, fast fission effects, streaming, the grain size of PuO_2 particles, assuming a reflecting boundary condition

in BRT-I, and a thermal energy-group upper boundary of 0.683 eV instead of an energy above the 1.056 eV resonance of ^{240}Pu . It is not necessary for the reactor designer to include all of these items in his calculation. However, they all need to be evaluated so that the designer can apply a correction to his calculated results to account for the neglected items.

Because of the limited nature of the results in Section IV, we are not in a position to report the total expected bias for the lattices considered in this paper. However, if we were to piece together what information we have, we would estimate that for UO_2 lattices the net bias due to assumptions and approximations made in the cell methods is a few tenths of a percent in the negative direction. For the tightest mixed oxide lattices we would estimate the bias to be of the order of 2% in the negative direction. Thus, if we were to correct the results of Section III for the net bias (using BNWML data) we would expect to predict k_{eff} for UO_2 lattices quite satisfactorily (within a few tenths of one percent). However, for mixed-oxide lattices we would expect to overestimate k_{eff} , in the worst case by as much as 2%.

C. LEAKAGE CALCULATION

In our analysis we have used a one-dimensional four-group diffusion theory calculation to predict the leakage. We have found that using 4 energy groups instead of 18 groups in diffusion theory leads to a bias of about -0.5% in k_{eff} . We have found that using 18-group diffusion theory instead of 18-group transport theory leads to a further negative bias. Our analysis also indicates that a two-region reactor model yields values of k_{eff} somewhat lower than a more detailed, three-region reactor model. Thus, if an 18-group transport theory calculation using a three-region reactor model

can be considered to be closer to the "exact" solution than a 4-group diffusion theory calculation using a two-region reactor model; then there is evidence of a significant negative bias in our calculated values of k_{eff} as a result of approximations regarding the leakage. We would conclude from this that if the cross sections and cell methods were "exact," we would expect to calculate values of k_{eff} for these critical lattices that were consistently low by approximately 1-2%.

Historically, critical experiment correlations have been used to evaluate either cross sections or cell methods or both. The problem of calculating the leakage, although it has been pointed out as a problem area, has usually been ignored. That is, it has been assumed generally that the leakage can be predicted adequately by a simple one-dimensional (and in some cases even by a zero-dimensional) calculation. It is our opinion that a detailed analysis must be made of the leakage from these small assemblies if one is to have confidence in the use of these lattices as bench-marks for testing design methods. On the basis of our analysis it appears that diffusion theory is definitely questionable, and that a higher order calculation (perhaps even Monte Carlo) is necessary to assure a proper calculation of the leakage.

TABLE I

SUMMARY OF EXPERIMENTAL RESULTS
FOR UO_2 -6.6 wt% PuO_2 FUELED LATTICES⁽¹⁾

<u>Lattice Spacing (in.)</u>	<u>Moderator-to- Fuel Volume Ratio</u>	<u>Critical Number of Rods</u>	<u>Geometrical₁ Buckling, m^{-2}</u>
0.52	1.68	472	108.8 ± 1.3
0.56	2.15	337	122.1 ± 1.1
0.735	4.72	151	159.3 ± 2.2
0.792	5.66	133	159.3 ± 2.2
1.04	10.73	117	128.4 ± 1.4

TABLE II
SUMMARY OF UO_2 FUELED EXPERIMENTS

Laboratory	Reference	Fuel		Clad		Lattice Spacing (in.)	Moderator-to-Fuel Volume Ratio	Experimental Results	
		wt% ^{235}U	Pellet Dia. (in.)	Material	Thickness (in.)			Critical Number of Rods	Geometrical Buckling, m^{-2}
WAPD	8	2.734	0.300	304-SS	0.01608	0.405	1.048	3043	40.75
"	8	"	"	"	"	0.435	1.405	1351	53.23
"	8	"	"	"	"	0.470	1.853	1301	63.26
"	8	"	"	"	"	0.573	3.357	826	65.64
"	8	"	"	"	"	0.615	4.078	790	60.07
"	8	"	"	"	"	0.665	4.984	813	52.92
BNW	9	2.350	0.440	A1	0.0300	0.750	2.408	385	94.3
BAPL	10	1.328	0.383	A1	0.0280	0.613*	1.330	2308	32.59
"	10	"	0.383	A1	0.0280	0.711*	2.235	1706	34.22
B&W	11	2.490	0.4054	A1	0.0320	0.595	1.371	190	70.1

* triangular lattices; all others are square.

TABLE III

SUMMARY OF EXPERIMENTAL RESULTS FOR
AQUEOUS SOLUTION EXPERIMENTS (13,15)

Uranyl Nitrate Solution

<u>Experiment #</u>	<u>Sphere Diameter (in.)</u>	<u>H/²³⁵U Atom Ratio</u>	<u>Corrected Measured Value of k_{eff}</u> (15)
1	27.24	1378	1.00026
2	27.24	1177	0.99975
3	27.24	1033	0.99994
4	27.24	972	0.99924
10	48.04	1835	1.00031

Plutonium Nitrate Solution

<u>Sphere Diameter (in.)</u>	<u>H/Pu Atom Ratio</u>	<u>Reflector</u>	<u>Measured k_{eff}</u>
15.2	553	H ₂ O	1.0000
15.2	668	None	1.0000

TABLE IV

CALCULATED VALUES OF k_{eff} FOR AL-Pu CRITICALS^a(MEASURED $k_{\text{eff}} = 1.0000$)

Lattice Spacing (in.)	Al-1.8 wt% Pu		Al-2.0 wt% Pu	
	H/Pu Atom Ratio	k_{eff}	H/Pu Atom Ratio	k_{eff}
0.75	630	1.0086	578	1.0182
0.80	810	1.0099	743	1.0240
0.85	1000	1.0079	918	1.0213
0.90	1204	1.0072	1104	1.0198
0.95	1418	1.0045	1300	1.0189
Mean =	1.0076 $\pm$ 0.0020		Mean =	1.0204 $\pm$ 0.0026

Lattice Spacing (in.)	Al-5 wt% Pu		
	Boron in H ₂ O (wppm)	H/Pu Atom Ratio	k_{eff}
0.85	0	355	1.0067
1.05	0	665	1.0113
"	48	665	1.0004
"	101	665	1.0072
"	164	665	1.0042
"	229	665	1.0029
"	285	665	1.0050
1.30	0	1150	1.0069

Mean = 1.0056 $\pm$ 0.0032

- a. The uncertainties assigned to the mean values are standard deviations for a typical value rather than for the mean value.

TABLE V

CALCULATED VALUES OF k_{eff} FOR UO_2 LATTICES^a

Lattice Spacing (in.)	H/U Atom Ratio	H/ ²³⁵ U Atom Ratio	Enrichment (% ²³⁵ U)	Pellet Dia.(in.)	k_{eff}
0.405	3.06	112	2.734	0.300	1.0035
0.435	4.11	150	2.734	0.300	1.0017
0.470	5.42	198	2.734	0.300	1.0002
0.573	9.86	361	2.734	0.300	0.9989
0.615	11.93	436	2.734	0.300	0.9980
0.665	14.57	533	2.734	0.300	0.9969
0.750	7.85	334	2.35	0.440	1.0028
0.6134*	4.06	306	1.328	0.383	0.9962
0.711*	6.82	514	1.328	0.383	0.9952
0.595	3.96	159	2.490	0.4054	1.0013

Mean = 0.9995 ± 0.0029

*triangular pitch; all others square.

- a. The uncertainties assigned to the mean values are standard deviations for a typical value rather than for the mean.

TABLE VI

CALCULATED VALUES OF k_{eff} FOR $\text{UO}_2\text{-PuO}_2$ CRITICALS ^a(Measured $k_{\text{eff}} = 1.0000$)

Lattice Spacing (in.)	H/Pu Atom Ratio	$\text{UO}_2\text{-2 wt% PuO}_2$		
		k_{eff}		
		8% ^{240}Pu	16% ^{240}Pu	24% ^{240}Pu
0.80	238	0.9920	--	0.9942
0.93	391	0.9979	0.9982	0.9963
1.05	554	0.9913	0.9931	0.9981
1.143	693	0.9992	1.0000	1.0007
1.32	991	0.9999	0.9995	0.9985
1.386	1113	0.9979	0.9964	0.9971
Mean = 0.9964 $\pm$ 0.0043		0.9974 $\pm$ 0.0024	0.9975 $\pm$ 0.0022	

$\text{UO}_2\text{-4 wt% PuO}_2$			$\text{UO}_2\text{-1.5 wt% PuO}_2$		
Lattice Spacing (in.)	H/Pu Atom Ratio	k_{eff}	Lattice Spacing (in.)	H/Pu Atom Ratio	k_{eff}
0.85	153	0.9964	0.55	230	1.0035
0.93	203	0.9940	0.60	326	0.9988
1.05	289	1.0035	0.71	567	0.9988
1.143	414	1.0024	0.80	794	0.9968
1.386	578	1.0062	0.90	1077	0.9971
1.60	805	1.0047	0.93	1169	0.9989
1.70	922	1.0031	Mean = 0.9990 $\pm$ 0.0013		
Mean = 1.0015 $\pm$ 0.0045					

- a. The uncertainties assigned to the mean values are standard deviations for a typical value rather than for the mean value.

TABLE VII

Calculated Values Of K_{eff} For UO_2 -6.6 wt% PuO_2 Criticals^a

<u>Lattice Spacing*</u> <u>(in.)</u>	<u>H/Pu Atom Ratio</u>	<u>k_{eff}</u>
0.52	75	1.0094
0.56	97	1.0081
0.735	210	0.9996
0.792	253	<u>1.0041</u>

Mean = 1.0053 ± 0.0053

* These were all square pitch lattices.

- a. The uncertainties assigned to the mean values are standard deviations for a typical value rather than for the mean value.

TABLE VIII

VALUES OF k_{eff} FOR AQUEOUS SOLUTION CRITICALS^aHomogeneous Uranyl Nitrate Spheres

<u>Experiment No.</u>	<u>Sphere Diameter</u>	<u>Measured k_{eff}</u>	<u>Calculated k_{eff}</u>
1	27.24 in.	1.00026	0.9955
2	27.24 in.	0.99975	0.9959
3	27.24 in.	0.99994	0.9936
4	27.24 in.	0.99924	0.9954
10	48.04 in.	1.00031	0.9944

Mean = $0.995 \pm .001$ Homogeneous Plutonium Nitrate Spheres
(Measured Values = 1.0000)

<u>Case No.</u>	<u>Sphere Diam. (in.)</u>	<u>H/Pu Atom Ratio</u>	<u>Calculated k_{eff}</u>
1 (Reflected)	15.2	553	1.0135
2 (bare)	15.2	668	1.0127

Mean = $1.013 \pm .001$

- a. The uncertainties assigned to the mean values are standard deviations for a typical value rather than for the mean value.

TABLE IX

MEAN VALUES AND STANDARD DEVIATION
FOR LATTICE MULTIPLICATION STUDIES

<u>Loading</u>	<u>Number of Data Points</u>	<u>Mean Value</u>
Lattice		
Al-1.8 Pu	5	1.008 ± 0.002
Al-2.0 Pu	5	1.020 ± 0.003
Al-5.0 Pu	8	1.006 ± 0.003
UO ₂ -1.5 PuO ₂	6	0.999 ± 0.001
UO ₂ -2.0 PuO ₂ (8% ²⁴⁰ Pu)	6	0.996 ± 0.004
UO ₂ -2.0 PuO ₂ (16% ²⁴⁰ Pu)	5	0.997 ± 0.002
UO ₂ -2.0 PuO ₂ (24% ²⁴⁰ Pu)	6	0.998 ± 0.002
UO ₂ -4.0 PuO ₂	7	1.002 ± 0.004
UO ₂ -6.6 PuO ₂	4	1.005 ± 0.005
UO ₂	10	1.000 ± 0.003
Homogeneous		
Large Uranyl Nitrate Spheres	5	0.995 ± 0.001
Small Plutonium Nitrate Spheres	2	1.013 ± 0.001

REACTIVITY EFFECT OF USING WATER UPSCATTERING IN HRG3

TABLE X

CALCULATED VALUES OF k_{eff} FOR VARIOUS CRITICAL EXPERIMENTS

Lattice Spacing in.	$\frac{N^H}{N^{fiss}}$	$\frac{\Delta k_{eff} \times 10^3}{H_2O \text{ Upscattering}}$
---------------------------	------------------------	--

UO₂ (2.734% ²³⁵U) 0.3 in. rods (Yankee)

0.405	113	-0.41
0.435	151	-0.38
0.470	200	-0.33
0.573	363	-0.31
0.615	439	-0.24
0.665	537	-0.09

Al-5 wt% Pu (5% ²⁴⁰Pu) 0.5 in. rods

0.85	384	-2.68
1.05	722	-1.74
1.30	1242	-1.17

UO₂-4 wt% PuO₂ (18% ²⁴⁰Pu) 0.5 in. rods

0.85	156	-5.98
------	-----	-------

UO₂-2 wt% ²⁴⁰Pu (8% ²⁴⁰Pu) 0.5 in rods

0.800	185	-4.35
1.143	541	-2.31
1.386	868	-1.50

UO₂-2 wt% ²⁴⁰Pu (24% ²⁴⁰Pu) 0.5 in. rods

0.800	213	-6.72
1.143	620	-3.57
1.386	996	-2.50

TABLE XI

UNCERTAINTIES IN NEUTRON MULTIPLICATION OF LATTICE EXPERIMENTS
DUE TO UNCERTAINTIES IN ISOTOPIC CROSS SECTIONS

Isotope and Type of Integral	Estimated Uncertainty in I_{∞} , %	Uncertainty in k_{eff} , %		
		<u>UO₂</u>	<u>Al-Pu</u>	<u>UO₂-PuO₂</u>
²³⁵ U fission	6.0	0.8	-	0.3
²³⁵ U absorption	10.0	0.9	-	0.3
²³⁸ U absorption	5.0	0.9	-	1.0
²³⁹ Pu fission	10.0	-	0.6	1.2
²³⁹ Pu absorption	12.0	-	0.6	0.8
²⁴⁰ Pu absorption	8.0	-	0.3	0.4
Isotope and Type of Cross Section	Estimated Uncertainty in 2200 m/sec Values, %			
²³⁵ U fission	0.4	0.4	-	<0.1
²³⁵ U absorption	0.4	0.2	-	<0.1
²³⁸ U absorption	2.0	0.2	-	0.1
²³⁹ Pu fission	0.5	-	0.5	0.5
²³⁹ Pu absorption	0.5	-	0.4	0.4
²⁴⁰ Pu absorption	7.0	-	0.2	0.2

TABLE XII

SOURCE OF CROSS-SECTION DATA
FOR CROSS-SECTION SENSITIVITY CALCULATIONS

<u>Isotope</u>	<u>HRG3</u>	<u>BRT-I</u>
Oxygen	BNWML	BNWML
Water		ENDF/B-II
Zirconium		BNWML
Aluminum		ENDF/B-II 2200 m/s Value
Iron	ENDF/B-II	
Nickel		
Chromium		
^{235}U		ENDF/B-II
^{238}U		
^{238}Pu		BNWML
^{239}Pu		ENDF/B-II
^{240}Pu		
^{241}Pu		
^{242}Pu		
^{241}Am		BNWML

TABLE XIII

EFFECT OF CHANGING CROSS SECTIONS

ON CALCULATED VALUES OF k_{eff}

Fuel Type	Lattice Spacing, in.	Calculated Value of k_{eff}	
		BNWML	ENDF/B-II
2.734 wt.% UO_2	0.405	1.0035	0.9658
	0.470	1.0002	0.9770
	0.573	0.9989	0.9850
	0.665	0.9969	0.9861
A1-1.8 wt.% Pu	0.75	1.0086	1.0113
	0.85	1.0079	1.0112
	0.95	1.0045	1.0083
A1-2 wt.% Pu	0.75	1.0182	1.0214
	0.85	1.0213	1.0249
	0.95	1.0189	1.0226
A1-5 wt.% Pu	0.85	1.0067	1.0065
	1.05	1.0113	1.0119
	1.30	1.0069	1.0074
UO_2 -1.5 wt.% PuO_2	0.55	1.0035	0.9654
	0.71	0.9988	0.9823
	0.93	0.9989	0.9914
UO_2 -2 wt.% PuO_2 (8% ^{240}Pu)	0.80	0.9920	0.9634
	1.05	0.9913	0.9778
	1.386	0.9979	0.9898
UO_2 -2 wt.% PuO_2 (16% ^{240}Pu)	1.05	0.9931	0.9799
	1.386	0.9964	0.9884
UO_2 -2 wt.% PuO_2 (24% ^{240}Pu)	0.80	0.9942	0.9676
	1.05	0.9981	0.9855
	1.386	0.9971	0.9893
UO_2 -4 wt.% PuO_2	1.05	1.0035	0.9920
	1.386	1.0062	0.9991

TABLE XIV Effect of Diffusion Coefficient Definition on the Leakage Calculation

1.05 in. UO_2 -2 wt% PuO_2

<u>Parameter</u>	<u>Consistent</u>	<u>Standard</u>
D_1	1.4660	1.5601
D_2	0.5895	0.5579
$\textcircled{D_2} \quad D_3$	0.5837	0.5206
k_{eff}	0.9778	0.9726

1.05 in. UO_2 -4 wt% PuO_2

D_1	1.4617	1.5556
D_2	0.5913	0.5582
D_3	0.5700	0.4963
k_{eff}	0.9920	0.9869

FIGURE 1 Variation of Calculated Multiplication With Buckling For UO_2 Lattices

FIGURE 2 Variation Of Calculated Multiplication With Buckling For Al-Pu Lattices

FIGURE 3 Variation Of Calculated Multiplication With Buckling For UO_2 - PuO_2 Lattices

FIGURE 4 Variation Of Calculated Multiplication With H/²³⁵U Atom Ratio For UO₂ Lattices

FIGURE 5 Variation Of Calculated Multiplication Ratio For Al-Pu Lattices

FIGURE 6 Variation Of Calculated Multiplication With H/Pu Atom Ratio
For UO_2 - PuO_2 Lattices

FIGURE 7 Reactivity Effect Of Finite PuO_2 Particles Relative To Homogeneous Fuel

APPENDIX ADESCRIPTION OF THE CROSS SECTIONS, THEORETICAL METHODS, AND ANALYSIS PROCEDURES

The theoretical methods that we have used for this analysis are based upon a combination of transport and diffusion theory methods. Transport theory methods are used for performing unit cell spectrum calculations. Diffusion theory is used for performing reactor neutron balance calculations to obtain multiplication values. In some instances, transport theory is also used for the latter type calculation to evaluate the differences between diffusion theory and transport theory solutions. The source of the basic cross sections is the Battelle-Northwest Master Library, BNWML.⁽²⁾ These cross sections are, with some exceptions, nearly identical to those contained in version I of ENDF/B.⁽⁵⁵⁾ The following is a summary of the more important cross section values and a brief description of each of the codes used.

A. Cross Sections

The BNWML (its genesis is the R. B. U. Basic Library)^(56,57) is a compilation of isotopic partial cross sections represented as point values covering the energy range from zero to 10 MeV. A computer code^(58,59) was developed to read and interpret this basic file and provide cross-section values at specific energy points or group averages using the appropriate flux weighting. The cell codes described below derive their multigroup libraries from the BNWML by this means. The most important cross sections in these calculations are summarized in Tables A-I and A-II.

1. Resonance Cross Sections

Age measurements have been used extensively to assist in determining the adequacy of the cross sections for the common moderating materials. Using the cross sections of the BNWML for hydrogen and oxygen we calculated the age from a fission source to indium resonance of neutrons in H_2O . The calculated value is compared to what we consider the best measured value in Table A-I. As shown, the agreement is excellent between the calculated value and the experimental value.

Measured values of the infinite dilution resonance integral have also played a useful role in evaluating cross sections. In part 2 of Table A-I we show how the values calculated from the BNWML compare with some of the measured values. For some of the isotopes wide variations exist in measured values; hence it is difficult to quote a best value. With the exception of ^{238}U and ^{242}Pu all of the calculated values are within the standard deviation shown for at least one of the measured values. The departure in values for ^{242}Pu is not significant for the critical assembly calculations presented in this paper. However, for ^{238}U the difference between the measured and calculated infinitely dilute resonance integrals is significant in terms of the impact on the critical assembly correlations. The calculated value of 269 barns using the cross sections from the BNWML is very nearly the value of 270.7 barns quoted for the ENDF/B - I cross sections. (60)

2. Thermal Cross Sections

The thermal cross sections for the fissile nuclides from the BNWML were normalized at 2200 m/s to the parameters recommended in the 1965 IAEA evaluation.⁽²¹⁾ The 2200 m/s absorption cross sections for the other materials of importance in our calculations were our best estimate values. These values are all shown in Table A-II.

The variation of the fissile nuclide cross sections with energy in the thermal region is also of importance.⁽⁶¹⁾ The shapes of these BNWML cross sections give the g values at 20.44°C shown in Section 2 of Table A-II for ^{235}U , ^{239}Pu and ^{241}Pu .

B. Cell Methods

The neutron distributions in space and energy within a unit lattice cell are computed using the multigroup transport theory codes HRG3,⁽³⁾ Battelle-Revised THERMOS (BRT-I),⁽⁴⁾ EGGNIT,⁽⁶²⁾ and GRANIT.⁽⁶³⁾ The spectrum-averaged multigroup cross sections are then collapsed to broad group values for subsequent use in the reactor calculations. The bulk of the calculations were made using HRG3 and BRT-I. The EGGNIT and GRANIT codes were used only for evaluating the effect of neutron self shielding due to particulate mixed oxide fuels.

1. The Thermalization Calculation

The computer code BRT-I is based on the original THERMOS⁽⁶⁴⁾ code, but contains certain revisions made at the Pacific Northwest Laboratory over the years.

The BRT-I code solves the integral transport equation in one dimension using a multigroup cross section library which was derived from the BNWML. The code was used in this analysis to compute the thermal neutron distribution in space and energy in a cylindrical geometry unit cell composed of three regions: fuel, clad, and associated moderator.

Twenty space points describe this unit cell with seven being allocated to the fuel, three to the clad, and ten to the moderator. The thermalization region is assumed to be from 0.0 to 0.683 eV. Thirty energy groups were used to describe the isotopic cross sections for this energy region. Reflecting boundary conditions were used in the calculations reported here.

In BRT-I the calculation of the thermal diffusion coefficient is based on the neutron current. An approximate method for correcting the scattering kernel to account for anisotropic scattering is available for all materials used in the cell calculation. This method involves altering the diagonal elements of the scattering kernel so that the sum of the matrix at each initial energy added to the absorption cross section yields the transport cross section at each energy. The scattering kernel that was used for H_2O is based upon the Nelkin model⁽⁶⁵⁾ and was calculated using the GAKER code.⁽⁶⁴⁾ The Brown-St. John⁽⁶⁶⁾ model is used for calculating scatter transfer from all other materials. The computed space-and energy-dependent flux and current solutions are used to average the multigroup cross sections to derive one thermal group flux/current weighted and volume weighted constants for the homogenized cell.

2. The Slowing-Down Calculation

The computer code HRG3 is used for calculating the fast and epithermal neutron spectrum in a homogenized system by solving the time independent Boltzmann equation with isotropic sources using either the P_1 or B_1 approximation. The energy range from 0.414 eV to 10 MeV is covered in 68 groups, each group one-fourth of a lethargy unit wide. With this calculated spectrum, the code forms broad group averages of parameters for use in spatial multigroup calculations. HRG3 is the latest of a series of versions which have evolved at Battelle-Northwest from GAM-1,⁽⁶⁷⁾ and still retains the basic characteristics of its predecessor.

For the calculations reported here the B_1 approximation was used with the measured geometrical buckling B_g^2 as the leakage factor. The fission spectrum for ^{239}Pu was used in all plutonium fueled lattices. For those lattices containing only uranium fuel, the ^{235}U fission spectrum was used. The effect of heterogeneity in the resonance region, that is, the shadowing caused by neighboring rods in the lattice, is accounted for using the method described by Carlvik.⁽⁶⁸⁾

The resonance integral is calculated by a modification⁽⁶⁹⁾ of the method of Adler, Hinman and Nordheim.⁽⁷⁰⁾ This includes an intermediate resonance approximation for both the resonance absorber and an admixed moderator,⁽⁷¹⁾ and the cross sections for resonances can be allocated to more than one fine group. An approximate correction to account for upscattering by hydrogen in water⁽⁷²⁾ is included in the calculation.

The intermediate resonance approximation, resonance allocation, and correction for upscattering in water are improvements to the slowing-down calculation that have been made since earlier reported correlations.^(73,74)

In HRG3⁽³⁾ there are two ways in which the transport cross section is calculated. These are referred to as the "standard" and "consistent" definitions. The latter definition was used in our analysis.

3. Calculation Of The Reactivity Effect Of PuO₂ Particles

The reactivity effect of the finite PuO₂ particles in the mixed oxide fuels was evaluated using the codes GRANIT and EGGNIT. These codes permit one to calculate the self-shielding within finite absorber grains embedded in a matrix of diluent material.

The GRANIT code is an extended version of THERMOS. It computes the position-dependent thermal neutron spectrum in a heterogeneous unit cell in which finite absorber grains (PuO₂ in our case) are imbedded in the fuel rod. The granular region is handled by extending the normal region-to-region collision probabilities, using an extension of the approximate method of Lane, Nordheim and Sampson,⁽⁷⁵⁾ to explicitly include particle and diluent interactions.

The EGGNIT code is a major revision of the GAMTEC-II code.⁽¹⁹⁾ Only the slowing down segment of the EGGNIT code was used in this study since the GRANIT code was used for the thermalization calculation. An iteration technique is incorporated in the slowing-down segment of EGGNIT which extends Nordheim's numerical integration method⁽⁷⁶⁾ to multiregion situations. A collision probability routine allows one to treat the problem of finite absorber grains embedded in a matrix of diluent material. The GRANIT and EGGNIT codes were run using the same cell conditions used in the BRT-I and

HRG3 calculations as explained in parts 1 and 2 of this subsection.

C. Reactor Methods

In most cases the solution of the reactor neutron balance equation was obtained using the HFN⁽⁵⁾ one-dimensional diffusion theory code. To evaluate the effects of neglecting anisotropy, a few solutions were obtained using the one-dimensional transport theory code DTF-IV.⁽⁷⁷⁾

The reactor model assumed for all of the critical assembly calculations is a simple two-region reactor consisting of a homogeneous core and a water reflector. A one-dimensional description of this model in the radial direction is used in calculating the neutron leakage and associated value of k_{eff} for the assembly. The radial neutron distribution in each broad group is determined exactly whereas the axial neutron distribution is approximated by using a monoenergetic transverse buckling, B_z^2 , in both the core and reflector regions. The transverse buckling is determined in each case from the physical height of the fuel, H , and measured reflector savings, λ , by the relationship:

$$B_z^2 = \pi^2 / (H + 2\lambda)^2 \quad (1)$$

1. Diffusion Theory Calculations

The HFN code solves the homogeneous or non-homogeneous, multigroup diffusion theory equation in one space dimension for its lowest eigenvalue and the corresponding direct and/or adjoint vectors, in both multiplying and non-multiplying systems. The code allows a maximum of 18 energy groups and 50 homogeneous regions. Provision to account for neutron leakage in directions transverse to the single coordinate being considered are included in the code.

The HFN code was run to obtain the direct flux solution and corresponding eigenvalue for a multigroup system. The mesh utilized was 50 points in the core and 50 points in the reflector. Thus, the mesh spacing in the core and reflector regions were dependent on the radius of the core. The convergence criteria used for the flux and eigenvalue solutions in HFN were 10^{-4} and 10^{-7} respectively.

2. Transport Theory Calculations

The DTF-IV code computes the neutron flux distribution as a discrete ordinates solution of the Boltzmann transport equation. The multigroup form of the transport equation with anisotropic scattering is solved in one-dimensional plane, cylindrical, or spherical geometry. The quadrature order and the order of anisotropic scattering are input variables which are left up to the user to select. The code allows a large number of energy groups and space points. Neutron leakage in directions perpendicular to the flux solution are accounted for by a DB^2 leakage term.

The transport theory calculations made with DTF-IV are analogous to the diffusion theory calculations made with HFN. The DTF-IV code was run in cylindrical geometry with various numbers of energy groups and quadrature orders. First order anisotropic scattering cross sections were used in all cases. A total of 100 mesh points were used with 50 mesh points used in the core and 50 mesh points in the reflector. A convergence criteria of 10^{-4} was used for both the eigenvalue and flux solutions.

D. Mockup Of The Critical Assembly

As mentioned above, the two region cylindrical reactor consisting of a homogeneous core and an H_2O reflector is equivalent to the fully inundated heterogeneous assembly. The analysis proceeds with the calculation of lattice constants for the homogeneous core and the reflector. The derivation of broad group parameters for the core was described above. Reflector cross sections were averaged over a neutron spectrum calculated for fission neutrons slowing down and thermalizing in an infinite medium of water. The non-thermal cross sections for water are obtained from the HRG3 code calculations assuming the P_1 approximation, no leakage, and a ^{239}Pu fission spectrum for plutonium fueled cores and a ^{235}U fission spectrum for uranium fueled cores.

Parameters for the reflector and homogenized core are obtained for four broad energy groups for use in the reactor calculation to obtain values of the multiplication factor k_{eff} . The energy boundaries for these

four broad groups are given in Table A-III. The score is assumed to be a right circular cylinder whose radius R_c is determined from the measured critical number of rods N_c , by conserving volume. The relationship is:

$$\pi R_c^2 = N_c A \quad (2)$$

where A is the area of a unit cell.

Thus for a square pitch lattice the critical radius is:

$$R_c = \ell \sqrt{N_c / \pi} \quad (3)$$

and for a hexagonal pitch lattice it is:

$$R_c = \ell \sqrt{N_c \sqrt{3} / 2 \pi} \quad (4)$$

where ℓ is the lattice pitch.

TABLE A-I

Summary Of Resonance Cross Sections

Quantity	Measured Value And Reference		Calculated From BNWML
	Value	Reference	
1. Age to Indium Resonance in H ₂ O (cm ²)	26.5 ± 0.3	78	26.5
2. Resonance Integrals, I _∞ (10 ⁷ to 0.5 eV) (barns)			
a. U-235 I _{∞c}	150 ± 6	79	140
I _{∞f}	292±11, 276±11	79, 80	280
α	0.514±0.016	79	0.500
b. U-238 I _{∞c}	286 ± 8	80	269
c. Pu-239 I _{∞c}	--		177
I _{∞f}	326±22, 301±10	80, 81	312
α	--		0.567
d. Pu-240 I _{∞a}	8370 ± 380	82	8467
e. Pu-241 I _{∞c}	--		164
I _{∞f}	581±33, 524±16	80, 83	517
α	--		0.317
f. Pu-242 I _{∞a}	1280 ± 60	84	1112

TABLE A-II

Summary Of Thermal Cross Sections

<u>Isotope</u>	<u>2200 m/s Value From BNWML, b</u>
1.	
a. Hydrogen	0.332
b. Boron	759.0
c. Nitrogen	1.88
d. Aluminum	0.235
e. Nickel	4.6
f. Zirconium	0.188
g. Stainless Steel	2.87
h. U-235 σ_a	679.9
σ_f	579.5
η	2.071
i. U-238 σ_c	2.72
j. Pu-239 σ_a	1008.1
σ_f	742.4
η	2.114
k. Pu-240 σ_c	281.1
l. Pu-241 σ_a	1391
σ_f	1009
η	2.154
m. Pu-242 σ_c	20.01

2.	<u>g Values For 20.44°C</u>
a. U-235 g_a	0.97696
g_f	0.97595
b. Pu-239 g_a	1.0787
g_f	1.0550
c. Pu-241 g_a	1.0463
g_f	1.0456

TABLE A-III

Boundaries of Neutron Energy Groups.

<u>Group</u>	<u>Energies</u>
1	10 MeV - 11.7 keV
2	11.7 keV - 2.38 eV
3	2.38 eV - 0.683 eV
4	0.683 eV - 0.0

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