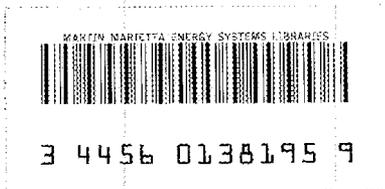


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## **A Discussion About Modeling the Effects of Neutron Flux Exposure for Nuclear Reactor Core Analysis**

D. R. Vondy

OPERATED BY  
MARTIN MARIETTA ENERGY SYSTEMS, INC.  
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*Stephanie Raby*  
Stephanie Raby  
Engineering Physics and  
Mathematics Division

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ORNL/TM-9860

Engineering Physics and Mathematics Division

**A DISCUSSION ABOUT MODELING THE EFFECTS OF NEUTRON FLUX EXPOSURE  
FOR NUCLEAR REACTOR CORE ANALYSIS**

D. R. Vondy

Date of issue: April 1986

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## TABLE OF CONTENTS

Abstract .....	v
Introduction .....	1
Simple Geometric Modeling .....	3
The Lifetime Core History .....	3
The Equilibrium State or Quasi-Equilibrium Repeating Cycle .....	3
The Detailed Core History Model .....	4
Viewpoint .....	4
The Equations .....	5
Radioactive Decay .....	5
Neutron Interaction Effects .....	7
Reaction Rate Simulation .....	8
The Nuclide Chain Equations .....	9
Considering Different Contributions .....	11
Nuclide Travel .....	12
Solution Methods .....	14
The Explicit Chain Solution .....	14
The Average Generation Rate Method .....	15
The Matrix Exponential Scheme .....	16
Example Problem .....	20
Modeling Considerations .....	24
Strategy for Modeling the Time Variable .....	24
Once Through Marchout Model .....	25
Recalculation Techniques .....	27
Geometric Modeling .....	28
The Neutron Energy Spectrum .....	30
Modeling Neutron Transport .....	31
Other Aspects, Auxiliary Calculations, and Generating Information .....	32
Cross-Section Variation .....	34
Cross-Section Dependence on Temperature .....	37
Strategy for Maintaining the Power Level .....	38
Local Power Density Importance .....	40
Fissile Material Accounting .....	41
Economic Importance .....	41
The Multiplication Factor .....	42
Modeling the Critical State .....	42
Fuel Management Capability .....	45
Accuracy, Importance and Uncertainty .....	45
Example of Implemented Capability .....	50
Task Assignments to Code Modules .....	52
Nuclide Chains for Reactor Core Analysis and Nuclide Importance .....	54
Results of Calculations .....	60
A Uranium Fuel Benchmark Exposure Problem With Feedback .....	60
A Fast Reactor Benchmark Core History Problem .....	60
Pressurized Water-Reactor Depletion Benchmark .....	65
Continuous Fueling Calculation .....	69
Shutdown Reactivity .....	73
Reactor History .....	74



## A DISCUSSION ABOUT MODELING THE EFFECTS OF NEUTRON FLUX EXPOSURE FOR NUCLEAR REACTOR CORE ANALYSIS

D. R. Vondy

### ABSTRACT

Methods used to calculate the effects of exposure to a neutron flux are described. The modeling of a nuclear-reactor core history presents an analysis challenge. The nuclide chain equations must be solved, and some of the methods in use for this are described. Techniques for treating reactor-core histories are discussed and evaluated.

#### NOTICE

This work was performed approximately two years ago and therefore does not reflect current efforts in the gas-cooled reactor program. It is published now on limited distribution to ensure that the considerable amount of research contained herein is fully documented for future reference.



## INTRODUCTION

The nuclide chain equations of the time dependence of the nuclide concentrations at a location in space are expressed in a compact mathematical form as the matrix equation

$$\dot{N} = -AN,$$

where  $N$  is the nuclide concentration, a vector,  $\dot{N}$  its time derivative, and  $A$  the appropriate loss, coupling matrix operator. This equation has the solution for a  $\Delta$  time interval of

$$N(\Delta) = N(0) e^{-\Delta A}$$

if the coefficients in  $A$  are fixed. This might seem to cover the calculation of the effects of exposure. The rather involved subject of modeling exposure is examined in some detail in what follows. The analysis of short-time effects, dynamics-kinetics-nuclear-stability-noise, is not addressed.

There are controllable variables in reactor-core analysis. These can be core-design details, a control-rod positioning schedule, fueling and refueling details (loading, distribution, recycle), burnable poison, soluble poison, etc. Most any calculation would limit the variables, tailoring the modeling to represent those features of most importance considering the desired results. The accounting of nuclide concentrations, specifically representing their variation in time, must be done discretely since a precise representation of the gradual changes that follow exposure to a neutron flux that varies in space is not possible. The analyst relies on experience in the selection of a calculational procedure and in describing the situation of interest as a model that can be treated mathematically.

A complication in the analysis of a situation involving radioactive material is that not only does the amount of the original material keep changing, but the daughter products propagate and accumulate. Neutrons in a reactor react with the various nuclei further complicating analysis. Occurrences outside of the fueled regions admit a somewhat simpler analyses there than is needed in the fuel. Thus the build-up of the products of neutron capture in the components of a pressure vessel or in other structural material located closer to the core may be readily followed with account for losses of the products through neutron interaction and decay. Of special concern when treating the nuclear fuel is following the neutron economy (reactivity state), and a complication is the build-up of the many nuclei that are produced by fission.

This is a discussion about calculating the effects of exposure to a neutron flux. There are several techniques in use and many aspects to consider in usual analysis. Treating the effects of exposure may be a primary part of the calculation, or this may be auxiliary, moving the core contents to a desired state. The objective of a calculation may be to predict fuel temperatures, power density peaking, controllability, fueling requirements, etc., and usually more than one of these is of interest. Such analysis directly supports the design or operation of a nuclear plant or projections for a system or the industry. Results are used to allow choices to be made from among the alternatives. Often comparative evaluation is used to assess the effects associated with each choice.

Various requirements are imposed on an analysis and on the methods of analysis that are applied. Different methods are used to assess different aspects, and different types of nuclear-core designs or specific situations invite the use of appropriate analysis techniques. Usually it is necessary and desirable to use available analysis capability familiar to the analyst.

Only a few of the actinides play much role in the neutron economy of a reactor core, so treating more than a few invites but a data handling burden unless additional ones are needed for a special purpose. Certain nuclides impact the handling of fuel waste and must be treated to support analysis in this area. Thus aspects of real importance interesting to the investigation are emphasized while others are downplayed. Whereas an estimate of detailed effects can be made treating over 1000 different nuclides at several thousand locations for one set of core conditions, carrying out such an analysis representing three dimensions would involve so much data and calculation as to be impractical and uneconomical, even if the capability to do so were available. Often computation costs are so high that rather coarse modeling is necessary; 100 locations are treated instead of 1000 or more, 30 nuclides are treated instead of 2000, and a coarse staging through time must suffice to describe the history.

Most calculations must be done on the computer due to the complexity of the problems. Certainly simple calculations are often in order, however, to promote the understanding of a situation and of primary aspects, and the results with a simple model may often be used as check points. Even in the use of the computer, the preference must be for a simple modeling of primary aspects applying familiar methods, not really to avoid complexities as such, but rather to avoid inconsistencies and errors, promoting reliability.

A rather unfortunate aspect regarding the subject under discussion is inadequate application of what is known to enhance analysis effort. The implemented capability may be hard to use due to unfamiliarity with its use or with the data requirements, or unwieldy to apply, or have poor availability, or be of questionable reliability. The computer codes and code systems contain limited capability and have limited applicability and flexibility for application. Rather obscure restrictions often come into play, especially when codes are used like black boxes with little understanding of the solution procedures by the user.

Often but a modest investment is made in implementing capability for exposure calculations. Naturally this limits what can be accomplished, especially regarding the flexibility for analysis and the reporting of useful auxiliary information.

Results of exposure calculations tend to be used either in a relative sense or an absolute one. With comparative evaluation, the differences in results may often be used directly. When results are to be used in an absolute way, often adjustments must be made to allow a reasonable interpretation. The multiplication factor calculated for control rod insertion is usually not as important as the difference in multiplication calculated for rods in and rods out. The modeling approximations cause distortion that needs to be corrected for an absolute interpretation of the results. For this correction to be made, an estimate is needed of the amount of the distortion. Is the peak power density underestimated or overestimated? How much reactivity should the model of the core exhibit at refueling time with the

rods out? Is it calculated to be positive or negative? An integral part of reactor core analysis is associating reliability and uncertainty with calculated results. Special calculations are normally required to allow the quantification of reliability.

A simple burn-up (depletion) code provides a capability to estimate the effects of exposure to a neutron flux for a period of time on a set of materials. The difference between a burn-up code and a calculational procedure for core analysis includes capability of the latter for

1. Modeling the situation and accounting for details that affect the history,
2. Maintaining the core state over the period in a way that simulates operation,
3. Producing auxiliary information essential for performance analysis, and
4. Close coupling with other analysis capability, separate or integrated, for engineering calculations, including thermal hydraulics.

Somewhat different techniques are applicable to different types of problems. Five quite different problems are discussed here

1. Simple exposure of material,<sup>1</sup>
2. The lifetime core history,<sup>2</sup>
3. The equilibrium state or quasi-equilibrium repeating cycle,<sup>3,4</sup>
4. The detailed core history modeling (design support)<sup>5,6,7,8</sup>
5. The detailed core history modeling to support operation.<sup>9,10</sup>

### **SIMPLE GEOMETRIC MODELING**

The effect of exposure to a representative neutron-flux spectrum and level is of interest to support other analysis. Simple geometric modeling may be used: a point for resonance-shielding calculations and a cell for fast-effect enhancement and thermal-flux suppression and spectrum hardening. This allows an elaborate treatment of the neutron energy and the consideration of many nuclides at an acceptable cost. Collapsed cross sections and correlating data for a few group representation are essential for core analysis. Auxiliary information can readily be generated to indicate the importance of specific aspects and support the modeling of other activities such as fuel processing and storage and elaborate economic assessment.

### **THE LIFETIME CORE HISTORY**

It is not practical or economical to carry out a lifetime history with a detailed core model. Thus economic analysis, fueling options, and study of aspects of importance are done with a simple model. There is a limit to how simple the model can be made. Reasonable neutron accounting is necessary, the critical core state effected and fuel accounting done by a nuclide mass balance. The exposure history of individual batches of fuel associated with partial core refueling may be followed. The conversion of mass to energy by the process of fission must be modeled accurately. Economic aspects may be stressed with elaborate treatment of the batch mass balance data.

### **THE EQUILIBRIUM STATE OR QUASI-EQUILIBRIUM REPEATING CYCLE**

The objective of this calculation is to resolve a condition of the core or a repeating cycle without addressing how it is approved. It is assumed that there is such a condition and that the procedure of

calculation produces a unique solution. In simple situations the uniqueness of a solution may be proven leaving only the question of whether or not a reported result is an accurate solution. More than one solution may exist in a complicated situation, so a result must be proven to be acceptable. A calculation may start by a reasonable representation of a freshly fueled core (or other point), and a simple iterative process used to affect a solution. In the case of an equilibrium state for continuous fueling, the history of the calculation does not resemble the early operating history. With fixed fuel, the early history may be followed. With quarter-core refueling, perhaps twelve cycles must be treated to approach the quasi-equilibrium state without recycle. (With recycle, some constraint is needed that fixes the solution rather than allowing the continuing buildup of non-separable product actinides such as  $^{236}\text{U}$ .)

Whatever the situation being modeled, some means is needed to accelerate the solution process. Simple extrapolation of successive iterate information is attractive. That is, given successive estimates of the detailed core contents at the start of cycle, these may be driven toward the solution. It would be essential for the situation to be truly repeating and full communication be established so as to avoid leaving something out. Successive quarter-core fuelings may be viewed as adding fuel to batches of zones 1, 2, 3, 4, 1, 2 ... . Full communication establishes on the fourth cycle, so data for cycles 4, 5, and 6 might be extrapolated, although the state of the error content may not allow its effective removal. If some desired end-of-cycle condition is to be satisfied, additional calculations would be necessary to move from an unacceptable but converged solution or to effect near an acceptable result each cycle by recalculation. Detailed fuel-element positioning often causes the quasi-equilibrium state to involve more than one cycle that may or may not be easy to model.

#### **THE DETAILED CORE HISTORY MODEL**

Very detailed calculations are done to support core design effort.

Operation is supported by following the core history. Two quite different requirements are satisfied: (1) regulations on operation and safety, and (2) operation support. The former has formal requirements to be satisfied with established set procedures not easily changed. The latter generates useful information and is available for projections such as would be needed to evaluate fueling options. Of special utility in any reactor operation is the modeling capability that is used to keep an up-to-date version of the core contents available for use. In either of these cases, it is usual to incorporate operating data into the calculation making the model current and adequate, even though this model may be rather coarse and perhaps the methods rather primitive.

Tailored calculational capability is required to allow the ready incorporation of information from the operation.

#### **VIEWPOINT**

The author has not been in the mainstream of water-reactor design, development, and operation support. Instead my background has been in reactor-core analysis and methods development and implementation for computer calculations in various areas of reactor analysis for other than water reactors. Therefore, this discussion is from a somewhat different than usual viewpoint. Of some consideration has been that a different and unfamiliar core concept always presents an analysis challenge, and the tendency is toward the use of a more basic and detailed approach than might be considered in a mature situation where experience allows emphasis and concentration on the more important aspects.

## THE EQUATIONS

### RADIOACTIVE DECAY

Radioactive decay is a process that exhibits a statistical variation. We apply methods that ignore the statistical variation, unless it is important. When a large number of events is involved, it is appropriate to represent only the aggregate. The differential equation that applies to the decay process of a packet of material fixed in space with no source is

$$\frac{dN_n}{dt} = -\lambda_n N_n , \quad (1)$$

where  $N_n$  is the concentration of a nuclide referenced  $n$ , and  $\lambda_n$  is its total decay constant,  $\text{sec}^{-1}$  for time  $t$  in seconds. A volume integral of the nuclide concentration would give the quantity of it. Equation (1) indicates that the amount of a nuclide at a location decreases at a rate proportional to its concentration. The solution to Eq. (1) is

$$N_n(t) = N_n(O) e^{-\lambda_n t} , \quad (2)$$

where the concentration with  $O$  argument,  $N(O)$ , refers to an initial condition, and  $N(t)$  refers to that at an elapsed time after the reference initial condition. The amount of a radioactive nuclide falls off exponentially, the exponent being proportional to the elapsed time. Here we should not ignore the popular characterizing quantity the half-life. When  $N_n(t) = 0.5 N_n(O)$ ,

$$1/2 = e^{-\lambda T_{1/2}} ; \quad (3)$$

$$T_{1/2} = \frac{1}{\lambda} \ln 2 .$$

We may consider two decay processes, perhaps  $\beta$  and  $\alpha$  to different daughter products,

$$\frac{dN_n}{dt} = -\lambda_{1,n} N_n - \lambda_{2,i} N_n . \quad (4)$$

Thus the individual processes contribute independently, and for any number so contributing, there is a sum,

$$\lambda_n = \sum_m \lambda_{m,n} . \quad (5)$$

A situation may exist where a nuclide is generated at a constant rate, or it may be so approximated over a short interval of time, leading to

$$\frac{dN_n}{dt} = -\lambda_n N_n + P_n , \quad (6)$$

where  $P_n$  is a generation (source) rate,

$$N_n(t) = N_n(O) e^{-\lambda_n t} + \frac{P_n}{\lambda_n} (1 - e^{-\lambda_n t}) . \quad (7)$$

If  $t \rightarrow \infty$ ,  $N_n$  goes to the steady state value of  $P_n/\lambda_n$ , i.e., the nuclide concentration changes from its initial values until the decay rate equals the source rate. How long it takes for the contribution from the initial concentration to lose importance relative to that generated depends on the decay constant, the initial concentration, and the generation rate.

The second term in Eq. (7) presents a computation difficulty. The result of evaluating  $e^{-x}$  and subtracting it from unity will be in error carrying a fixed number of digits, and this error becomes more significantly the smaller  $x$ . A more accurate form is needed for general application. Consider the expansion

$$e^{-x} = 1 - x + \frac{x^2}{2} - \frac{x^3}{6} + \frac{x^4}{24} - \dots \quad (8)$$

Note that for very small  $x$ , only the first two terms of the expansion of Eq. (8) are needed to evaluate  $e^{-x}$ . However, simply accumulating these terms leads to a significant error in the estimate of  $e^{-x}$  for large  $x$ . Consider  $x = 0.5$ . Accumulation of successive terms yields 1, 0.5, 0.625, 0.604167, ..., each result moving closer to the true answer of 0.606531 .... For  $x = 10$ , however, successive values are 1, -9, 41, -125.7, 291, -543.2, ..., compared with the solution of 0.0000453999 ..., and seven digits of significance are lost in the solution process.

An alternate expansion for  $e^{-x}$  is more practical,

$$e^{-x} = 1 - x \left[ 1 - \frac{x}{2} \left[ 1 - \frac{x}{3} \left[ 1 - \frac{x}{4} (\dots) \right] \right] \right] \quad (9)$$

and the calculation begins at the inside, so to speak, avoiding the significance difficulty of Eq. (7). The number of terms required for a desired significance is predictable, but a check of the significance of each added term is not possible as it is the case with the use of Eq. (8).

Alternatively, a continued fraction form is in common use, as used for the calculational procedure for the computer library routine for the exponential function; for example

$$e^{-x} = \frac{1}{1 - \frac{x}{1 + \frac{x}{2 - \frac{x}{3 + \frac{x}{2 - \dots}}}}} \quad (10)$$

Since  $1 - e^{-x} \rightarrow 0$  as  $x \rightarrow 0$ , the result obtained by evaluating  $e^{-x}$  and subtracting this from 1 has a relative error that increases as  $x$  becomes smaller. For small  $x$ , it is essential to use a more accurate form, and an expansion yields

$$\begin{aligned} \frac{1 - e^{-x}}{x} &= 1 - \frac{x}{2} + \frac{x^2}{6} - \dots, \\ &= \left[ 1 - \frac{x}{2} \left[ 1 - \frac{x}{3} \left[ 1 - \frac{x}{4} \left[ \dots \right] \right] \right] \right] \quad (11) \end{aligned}$$

so one of a variety of possible formulations may be used. Since

$$e^{-x} = \frac{e^{-\frac{x}{2}}}{e^{\frac{x}{2}}},$$

and for very small  $x$ ,

$$\frac{1 - e^{-x}}{x} \approx \frac{1}{1 + \frac{x}{2}}. \quad (12)$$

A simple parent-daughter relationship is often of interest, as for the reactor-shutdown state with  $^{135}\text{Xe}$  build up from  $^{135}\text{I}$  decay, and subsequent decline.

$$\begin{aligned} \frac{dN_1}{dt} &= -\lambda_1 N_1, \\ \frac{dN_2}{dt} &= +\lambda_{1,2} N_1 - \lambda_2 N_2, \end{aligned} \quad (13)$$

where  $\lambda_{1,2}$  may simply be  $\lambda_1$ . This set of chain equations may be solved to yield ( $\lambda_1 \neq \lambda_2$ )

$$\begin{aligned} N_1(t) &= N_1(O) e^{-\lambda_1 t}; \\ N_2(t) &= N_2(O) e^{-\lambda_2 t} + N_1(O) \lambda_{1,2} \left[ \frac{e^{-\lambda_1 t} - e^{-\lambda_2 t}}{\lambda_2 - \lambda_1} \right]. \end{aligned} \quad (14)$$

In the case of reactor shutdown, there is interest in the amount of peak absorption by  $^{135}\text{Xe}$ , maximum  $N_2$ , because compensating reactivity would have to be available to make the core critical to allow restart at this time. This peak occurs at  $dN_2/dt = 0$ , when the time satisfies

$$t_{N_2, \max} = \left[ \frac{1}{\lambda_2 - \lambda_1} \right] \ln \left\{ \frac{\lambda_2}{\lambda_1} \left[ 1 + \left( \frac{\lambda_1 - \lambda_2}{\lambda_{1,2}} \right) \frac{N_2(O)}{N_1(O)} \right] \right\}. \quad (15)$$

This time the second nuclide in the chain peaks is thus dependent on the ratio of the nuclide densities at the time of shutdown. This ratio, of course, varies with time but takes on an asymptotic value after much operation that is associated with the specific data involving the yield from fuel fission and the flux level.

Given the time of maximum  $^{135}\text{Xe}$  concentration, the concentration may be estimated applying Eq. (14). The neutron absorption rate in  $^{135}\text{Xe}$  is approximately proportional to its concentration. However, more elaborate calculations are often done to generate specific results for the reactivity override capability.

The time when  $N_2(t)$  returns to its initial value  $N_2(O)$  may be determined by solving Eq. (13) by trial and error, or iteratively if it is recast, the core multiplication thereafter increasing above what it was at shutdown due to decay of the poisoning  $^{135}\text{Xe}$ .

## NEUTRON INTERACTION EFFECTS

Several neutron-nuclide reactions are of interest. In any specific situation there may be special reaction types that must be treated. For the usual reactor core calculation,  $\sigma_c$ ,  $\sigma_f$  and  $\sigma(n, 2n)$  describe

the most important processes. For general purposes, an absorption cross section is defined as the sum of all the different cross sections involving reactions that add one neutron to the nucleus thereby altering the isotope. Although various daughters and states may be involved, we consider simply

$$\sigma_a = \sigma_c + \sigma_f + \sigma(n, 2n) , \quad (16)$$

where  $\sigma_c$  is the sum of all capture cross sections. Special reactions may be adequately accounted for in this framework for usual reactor core analysis.

Most neutronic codes do not carry the  $(n, 2n)$  reaction data separately. Rather than burden the code with quite unnecessary data handling, usually an artificial absorption cross section is carried to account for the net effect of one excess neutron each reaction,

$$\sigma_b = \sigma_a - 2\sigma(n, 2n) , \quad (17)$$

and the group-to-group scattering data equivalent to the  $(n, 2n)$  product are added to the group-to-group cross sections for the elastic-inelastic total scattering. Thereby an adequate representation of the primary macroscopic effect is achieved with somewhat jimmied data. Note that to properly account for the total loss rate of a nuclide,

$$\sigma_a = \sigma_b + 2\sigma(n, 2n) \quad (18)$$

would be calculated requiring data for the  $(n, 2n)$  loss cross section, even though this data is not needed by the neutronics code. The accounting of the concentration of such a nuclide as  $^{238}\text{U}$  requires consideration of the  $(n, 2n)$  cross section and thus the use of  $\sigma_a$ , not  $\sigma_b$ , because the  $(n, 2n)$  reaction changes  $^{238}\text{U}$  to  $^{237}\text{U}$ .

More than one capture reaction in a nuclide may be represented. For example, the concentration of  $^{149}\text{Sm}$  may be of interest, especially at a high power density, because this nuclide has a large cross section. Also it is stable and builds up after shutdown from its two precursors,  $^{148}\text{Pm}$  and the isomeric state  $^{148m}\text{Pm}$  at different decay rates depending on the individual precursor source strengths. Accounting for the primary aspects requires treating the individual capture rates of  $^{147}\text{Pm}$  to  $^{148}\text{Pm}$  and of  $^{147}\text{Pm}$  to  $^{148m}\text{Pm}$ . Typically a total capture cross section is specified for  $^{147}\text{Pm}$  as is needed for a neutronics solution, and data for the fraction of total capture are used in the exposure calculation. (A diagram showing key fission products and chain coupling is shown later.)

It is interesting to note that had exposure methods development preceded that for neutronics, the burden of unraveling the information might well have been placed on the neutronics codes. Perhaps of most concern to note here is that what can be modeled with available computational capability is often limited. Coded procedures must usually be applied as they exist, with the exception of the case where enhancement is allowed. Enhancement is especially difficult when new data requirements are imposed. The fact that the use of qualified and familiar procedures may produce better information than altered procedures inadequately qualified tends to limit the changing of methods that are implemented and qualified for the application.

## REACTION RATE SIMULATION

It should be noted that the local total-reaction rate in a nuclide from an integral over energy (one group data) is (1)  $N_n \sigma_{a,n} \phi V$ . Quite generally this must be conserved as well as the specific reaction rate (2)  $\sigma_{a,n} \phi$  to conserve the effect of neutron absorption. Therefore  $N_n V$  and  $\sigma_{a,n} \phi$  must be conserved. If exposure were not involved it could be practical to effect (1) while ignoring (2). An example of this would be weighting of cross sections for an isotopic mixture to use the naturally

occurring density of the mixture. Thus natural boron may be used when exposure is not treated, but  $^{10}\text{B}$  must be depleted. Fine scale heterogeneity can be eliminated and the actual nuclide density may be smeared for discretized volume elements

$$\bar{N}_n = \frac{\sum_j N_{n,j} V_j}{\sum_j V_j} \quad (19)$$

The neutron flux may vary considerably in space and energy. Adequate weighting for a simple situation is given by

$$\bar{\sigma}_{a,n} = \frac{\sum_j N_{n,j} V_j \int dE [\sigma_{a,n}(E) \phi(r,E)]}{\sum_j N_{n,j} V_j \int dE \phi(r,E)} \quad (20)$$

where the flux-per-unit energy form is used for simplicity, and the discretized volume elements are considered for consistency with the nuclide concentration weighting above. Note that special consideration must be given to the desired results when applying Eq. (20) to a situation where the nuclide concentration is zero or it is zero in some locations of interest.

#### THE NUCLIDE CHAIN EQUATIONS

For such a nuclide as  $^{238}\text{U}$  having no source, the appropriate equation is

$$\frac{dN_n}{dt} = -(h_n + \lambda_n)N_n, \quad (21)$$

$h_n$  being the specific total loss reaction rate,

$$h_n = \int_E \sigma_{a,n}(E) \phi(E) dE, \quad (22)$$

at some location, where the neutron-flux-per-unit energy is shown as  $\phi(E)$ . Since discretization in both energy and space is usual, essential indeed for most calculations, within a discretized range at some reference time

$$h_n(r) = \sum_g \sigma_{a,n}(g,r) \phi(g,r) \quad (23)$$

where the sum-over-energy groups is indicated for the local specific absorption rate,  $\phi(g,r)$  being an energy group and discretized special volume average of the neutron flux. To be explicit, for location  $r$ ,

$$\frac{dN_n(r,t)}{dt} = -a_n(r) N_n(r,t), \quad (24)$$

where

$$a_n(r) = h_n(r) + \lambda_n. \quad (25)$$

Most nuclides are generated by the neutrons capture in or decay of a precursor, or through fission, and the appropriate source terms must be included,

$$\frac{dN_n(r,t)}{dt} = a_n(r)N_n(r,t) + \sum_j q_{j,n}(r) , \quad (26)$$

where more than one precursor source  $q_{j,n}$  is allowed. Nuclides often have more than one source, for example,  $^{135}\text{Xe}$  is produced by decay of  $^{135}\text{I}$  as well as by fission of any nuclide. Each source term here is limited to a nuclide precursor that decays, transmutes through a (neutron, nuclide) reaction, or fissions. Only the simple source and loss terms shown are considered. Special situations such as the fixed neutron source or circulating fuel can not be treated with these equations.

The set of Eq. (26) for all of the nuclides to be treated is often referred to as the nuclide chain equations, since groups of nuclides are linked together one after the other by the coupling equation. Thus successive neutron captives move up the  $^{239}\text{Pu}$ ,  $^{240}\text{Pu}$ ,  $^{241}\text{Pu}$ ,  $^{242}\text{Pu}$  chain, important in most reactor-core calculations.

For generalization, the generation of fission products must be represented,

$$q_{j,n}(r) = \int_E y_{j,n}(E) N_j(r) \sigma_{f,j}(E,r) \phi(r,E) dE , \quad (27)$$

but this is usually simplified to

$$q_{j,n}(r) = y_{j,n} N_j(r) \sum_g \sigma_{f,j}(g,r) \phi(g,r) , \quad (28)$$

and these equations would be summed over the fissioning nuclides for use directly in Eq. (26). Since there is some variation in the energy of the fission-product yield values, the sum-over-energy groups could be divided into bands. More common, however, is the use of effective yield data weighted over an appropriate neutron energy spectrum.

The coefficients in Eqs. (26) and (28) do not remain constant although they usually vary slowly in time. Usual solution methods ignore the time variation over a short enough time interval between points in time, and discrete changes are introduced as appropriate.

The reference to a spatial location will not be carried further in this discussion. The equations would apply to each of the individual locations considered, and several locations must be considered to account for the differences, as-loaded or as the consequence of exposure. With quarter-core refueling, the coarsest possible model is four locations, one for each of the different ages of the fuel. This would have to be increased to 240 or more locations for three-dimensional modeling. Symmetry conditions are imposed whenever possible to reduce the size of the problem, especially the size of the neutronics problem that must be solved.

Equation (26) applies to each of the nuclides to be treated at each location. The set of these equations was expressed in matrix notation as Eq. (1). Given  $I$  nuclides, operator  $A$  is of size  $I^2$  and contains many zero entries. If 2000 nuclides are treated at a location, the size of  $A$  is 4,000,000. Techniques are used to reduce the size of  $I$  and often some limitations are imposed. Of course as the computers are made larger, such limitations become relaxed.

Several schemes are in use for modeling the effects of the fission products. A single nondepleting pseudo nuclide representation has been popular, possibly because of its simplicity. Its use is somewhat

more reasonable in fast-reactor analysis than for the thermal core. For the latter, likely  $^{135}\text{Xe}$  must be treated explicitly, often at equilibrium.

The two-pseudo-nuclide model has also found use. The common lumping is of those fission products that tend to saturate slowly into one lump and the other nonsaturating into another. By slow saturation is meant that the cross sections are large enough that significant loss occurs so the rate of neutron absorption deviates significantly from a straight line growth with time, and indeed it would become constant given enough time. The time when equilibrium of the slowly saturating lump would occur is much longer than the usual core exposure time, compared with but a few days for  $^{135}\text{Xe}$  to reach equilibrium. Including a secondary effect tends to improve the modeling accuracy; the capture in the slowly saturating lump coupled into the nonsaturating lump as a precursor. The two-nuclide model is used with explicit representation of several of the fission product nuclides, as is indicated later.

Another two-lump-nuclide model may be more accurate. Consider that neutron capture in an odd-number nucleus makes an even-number nucleus. The nuclides having an odd atomic number tend to have similar nuclear properties while so do those having an even atomic number. Thus the natural model to apply is  $N_1 \rightleftharpoons N_2$ ;

$$\begin{aligned}\frac{dN_1}{dt} &= -a_1 N_1 + a_{2 \rightarrow 1} N_2 + Y_1, \\ \frac{dN_2}{dt} &= -a_2 N_2 + a_{1 \rightarrow 2} N_1 + Y_2,\end{aligned}\tag{29}$$

where usually  $a_1 = a_{1 \rightarrow 2}$  and  $a_2 = a_{2 \rightarrow 1}$ . Unfortunately these equations require a special solution formulation preventing their modeling with a generalized explicit solution. Alternative solution methods, such as the matrix exponential, can be used. It is interesting that summing the above equations,

$$\frac{dN_1}{dt} + \frac{dN_2}{dt} = Y_1 + Y_2,$$

although this is of little utility for solving the equations, it provides a check,

$$N_1(T) + N_2(T) = (Y_1 + Y_2) T.$$

#### CONSIDERING DIFFERENT CONTRIBUTIONS

Advantage may be taken of the fact that with a linear differential equation, different contributions add independently to the solution. Consider

$$\frac{dN_1}{dt} = -a_1 N_1 + S_1 + S_2,\tag{30}$$

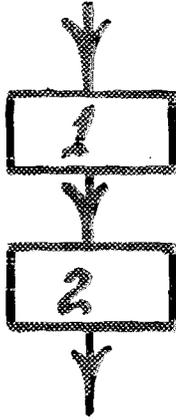
and its solution

$$N_1(T) = N_1(O)e^{-a_1 T} + \frac{S_1}{a_1}(1 - e^{-a_1 T}) + \frac{S_2}{a_1}(1 - e^{-a_1 T}).\tag{31}$$

thus the total result given here may be arrived at by separate calculations that cumulate the parts. This is especially important in applying the explicit chain-solution scheme in that it extends the application from treating only a single chain to coverage of a variety of situations involving chain couplings.

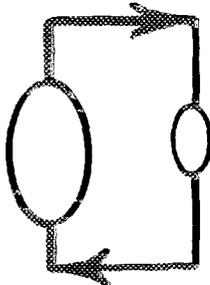
## NUCLIDE TRAVEL

Usual calculations consider the materials to be fixed in space. When the fuel circulates or coolant flow is involved, the equations must take a form appropriate to the situation. A few situations are considered here to be informative.



Consider first the simple situation of continuous fuel movement through a reactor core with the core held at a true equilibrium condition being supplied continuously with a fixed feed composition. A representative traverse through the core is divided into intervals, and here two intervals are chosen for illustration. Material enters 1 at the feed composition and leaves 1 with a new composition. The feed to 2 is the discharge from 1, and the discharge composition from 2 leaves the core. If the material in 1 were fixed, an exposure calculation would apply average conditions to determine the composition after an exposure period  $\Delta$ . Given a residence time  $\Delta$ , the exposure of the feed material for this period to average conditions converts it to the composition leaving 1.

Thus usual exposure capability can be altered to treat the fuel movement case by taking account of the material entering and the material leaving the discrete volumes along each flow path. An additional complication comes from the need for returning to the neutronics code the average composition in each zone. Given a sufficiently fine discretization, the average between the feed and discharge compositions may be used. Only a few or many flow paths may be followed to effect representative modeling. Such aspects as multiple passes, delayed recycle, and more than one stream along each path (countercurrent fueling for example) are readily modeled. Implementation amounts to coding the alternative accounting without significant changes to the exposure equations. Cores having azimuthal symmetry are modeled simply in two dimensions, an annular design requiring only the addition of a inner plug and reflector. Up to 60 passes of pebbles along the flow paths have been treated to represent a continuously fueled pebble-bed core.



The equations to model the flow through an external loop are not a simple interpretation of the usual equations applied to fixed material, although certain simple approximations may be useful. Consider the core with an outside loop. Using subscripts  $c$  for core,  $l$  for loop and  $t$  for total, the amount of any material is given by

$$N_{n,t}V_t = N_{n,c}V_c + N_{n,l}V_l \quad (32)$$

where  $N$  is the average concentration and  $V$  the volume with any necessary adjustment included for appropriate volume fractions. Note that the total amount of material in the system relative to that in the core is given by

$$\frac{N_{n,t}V_t}{N_{n,c}V_c} = 1 + \frac{N_{n,l}V_l}{N_{n,c}V_c} \quad (33)$$

These equations do not account for exposure effects. Such accounting is, however, important. Even in a fixed system there is fuel on hand that should be accounted for in this way for fuel management and economic analysis.

Consider a reactor core and an external loop with feed and discharge of material. There are several ways to model these, and what may be adequate in one situation may not be in another.

A first approximation would ignore the loop and simply model the core. Ignoring spatial effects, a point model is applied that takes the form of a mass accounting,

$$\frac{d(N_{n,c}V_c)}{dt} = F_n - D_n + G_n - C_n \quad (34)$$

where  $F$  is the feed rate,  $D$  the discharge rate,  $G$  the generation or loss rate,  $C$  the consumption rate, and  $V$  the volume. Performing an integration for a fixed volume,

$$N_{n,c}(t) = N_{n,c}(0) + \int_0^t dt \{F_n - D_n + G_n - C_n\} . \quad (35)$$

thus the concentration of a nuclide increases at the sum of the rates of its net input into the system (feed - discharge) and its net production (generation - consumption). The modeling is completed by replacing the symbolic rate terms with appropriate equations expressing the effects of exposure in the core and decay in the core and in the loop, involving the chain relationships.

A very useful approximation, at least for coarse analysis, is to consider the system of the core and the loop as a whole. A point model for this system, Eq. (32) above, reduces to the usual chain equations with two changes,

1. Feed and discharge rates are added, where rate terms are relative to the system volume, and
2. The neutron flux level is decreased by multiplying it by the ratio to the residence time in the core to the total system transit time.

If it is appropriate to assume rapid mixing, then a single concentration of each nuclide is appropriate. Considering the core and loop separately and a fixed flow rate coupling the two of  $r$ , the set of coupled equations is

$$\begin{aligned} V_c \frac{d N_{n,c}}{dt} &= r(N_{n,l} - N_{n,c}) + G_{n,c} - C_{n,c} , \\ V_l \frac{d N_{n,l}}{dt} &= r(N_{n,c} - N_{n,l}) + G_{n,l} - C_{n,l} + F_l - D_n \end{aligned} \quad (36)$$

Thus the rate of movement of material, feed and discharge rates, and the volumes are involved. The appropriate equations must be solved for an accurate representation.

An alternate representation is to consider a once-through pass without mixing. If this is done for the loop, the composition along the path can be related to the entering composition, and the location and time after entering are simply related allowing the form

$$\frac{d}{dt} N_{n,l}(t') = G_{n,l}(t') - C_{n,l}(t') . \quad (37)$$

Of most interest likely is the composition returning to the core (since for most purposes only a coarse estimate of loop concentrations is adequate), the return concentration to the core without feed or discharge is

$$N_{n,l}(t + t_l) = N_{n,l}(t)e^{-\lambda t} + \int_t^{t+t_l} [G_{n,l}(t') - C_{n,l}(t')] dt' , \quad (38)$$

simply a solution of the chain equations for the loop-transit time considering only decay without exposure. With fixed feed and discharge rates,

$$N_{n,l}(t + t_l) = N_{n,l} \left[ 1 - \frac{V_d}{V_l} \right] e^{-\lambda t} + N_{n,f} \left[ \frac{r_f}{r_l} \right] + \int_t^{t+t_l} [G_{n,l}(t') - C_{n,l}(V')] dt' , \quad (39)$$

where subscripts on the rates are *d* for discharge, *f* for feed, and *l* for loop, and for consistency here  $r_f = r_d$ .

## SOLUTION METHODS

The objective is to simulate a specific situation as accurately as is economically feasible. Fissile material is consumed in a core, and the decrease in the fissile inventory must usually be compensated with an elevation of the neutron flux to hold the power level up. This change in the flux level could be included in the equations, at least as a linear approximation, but such complexity is likely unwarranted, and the correction is usually not known in advance. Thus, simple solution schemes are of interest, and consideration is given to doing complicated things with simple capability. The chain-equation solutions shown here assume fixed coefficients implying constant specific neutron-reaction rates.

### THE EXPLICIT CHAIN SOLUTION

The general explicit solution is used extensively for the chain equations with simple chain coupling. For reactor-core calculations it is appropriate to consider a nearly constant power level. Then the fission-product generation would be constant, except as the fissioning nuclide concentrations shift and as fission rates vary locally. The actinide chains may be solved first, and then the fission-product yield rate can be determined from a simple average of the start and end fissile nuclide concentrations,

$$\bar{N}_l \approx \frac{1}{2} [N_l(O) + N_l(T)] . \quad (40)$$

The explicit solution of Eq. (26) for an exposure period *T* is

$$N_n(T) = N_n(0)e^{-a_n T} + Y_n \left[ \frac{1 - e^{-a_n T}}{a_n} \right] + \sum_j \sum_{i=1}^{n-1} [N_i(O)Q_{j,n,i} + Y_{j,i}U_{j,n,i}] , \quad (41)$$

where

$$Q_{j,n,i} = \sum_{m=i}^{n-1} \left[ \frac{e^{-a_m T} - e^{-a_n T}}{(a_n - a_m)} \right] b_{j,m \rightarrow m+1} \prod_{\substack{k=i \\ k \neq m}}^{n-1} \frac{b_{j,k \rightarrow k+1}}{(a_k - a_m)} , \quad (42)$$

and

$$U_{j,n,i} = \left[ \frac{1 - e^{-a_n T}}{a_n} \right] \frac{n-1}{m-i} \frac{b_{j,m \rightarrow m+1}}{a_m} - \sum_{m=i}^{n-1} \left[ \frac{e^{-a_n T} - e^{-a_i T}}{a_m(a_n - a_m)} \right] b_{j,m \rightarrow m+1} \frac{n-1}{\substack{k=i \\ k \neq m}} \frac{b_{j,k \rightarrow k+1}}{(a_k - a_m)}. \quad (43)$$

Adequate results should be obtained with single precision on a long word (64 bit) computer for most uses, but double precision is essential on a short word machine (<48 bit). Significance tests can be made and extraneous contributions discarded. When two specific loss rates are found to be identical, they can automatically be separated by a slight adjustment to avoid the gross error that results from the use of an incorrect equation.

To achieve the necessary precision, terms should be changed from the form

$$\frac{e^{-zt} - e^{-yt}}{y-z} \text{ to } e^{-zt} \left[ \frac{1 - e^{-(y-z)t}}{(y-z)t} \right]$$

and the approximation of Eq. (11) used. This is important as  $(y-z)t$  approaches 0.

Flexible application of the explicit chain-solution method requires that some sophistication be included in the calculational procedure. Chain intercoupling is permitted by allowing the contributions from different sources to be added. For the other solution methods, parent-daughter relationships with processes are given, while for the explicit chain-solution method, the chain members and coupling processes must be described.

#### THE AVERAGE GENERATION RATE METHOD

Simplifying Eq. (26) to the form

$$\frac{dN_n(t)}{dt} = -a_n N_n(t) + P_n, \quad (44)$$

where  $P_n$  is an effective or average generation rate, the exposure period  $T$  is divided into a fine scale of  $L$  intervals of time  $\Delta$  each,  $\Delta = T/L$ . A typical value for  $L$  would be 100 but a value much larger may be necessary in some applications to get a desired accuracy. An elementary finite-difference solution of Eq. (44) is

$$\frac{dN_n(t)}{dt} = \left[ \frac{N_n(\Delta) - N_n(0)}{\Delta} \right] \approx -a_n \left[ \frac{N_n(\Delta) + N_n(0)}{2} \right] + P_n,$$

$$N_n(\Delta) = N_n(0) \left[ \frac{1 - \frac{a_n \Delta}{2}}{1 + \frac{a_n \Delta}{2}} + \frac{\Delta P_n}{1 + \frac{a_n \Delta}{2}} \right],$$

or

$$N_n(\Delta) = N_n(O) \left[ \frac{2 - a_n \Delta}{2 + a_n \Delta} \right] + \left[ \frac{2\Delta}{2 + a_n \Delta} \right] P_n . \quad (45)$$

When appropriate,  $a_n \Delta$  large, a higher order formulation can be used which comes directly from integration of Eq. (44),

$$N_n(\Delta) = N_n(O) e^{-a_n \Delta} + \left[ \frac{1 - e^{-a_n \Delta}}{a_n} \right] P_n . \quad (46)$$

Use of the higher order form is especially desirable to avoid serious inaccuracy for nuclides which have a large specific loss rate  $a_n$  and approach an equilibrium condition rapidly,

$$\frac{dN_n}{dt} = 0; \quad N_n = \frac{P_n}{a_n} .$$

To improve the estimate of the average generation rate,  $N_n(\Delta)$  for the precursors may be used to calculate  $P_n$  if  $e^{-a_n \Delta} < 0.1$  for exposure calculations or if  $< 0.01$  for shutdown calculations. A selected weighting for calculating  $P_n$  from the precursors is

$$N_n(O, \bar{\Delta}) = \alpha N_n(O) + (1 - \alpha) N_n(\Delta) , \quad (47)$$

where the parameter  $\alpha$  may be specified, but typically 0.5 is used simply averaging the concentrations.

The equation coefficients are assumed to not change with time and therefore are calculated only once. Passing through the specifications, the end of step concentrations will be the same as start of step concentrations for those nuclides not yet treated, so the results depend on the order of processing. The actinide nuclides might be treated first, preferably down the coupling chains, and then the fission products last.

#### THE MATRIX EXPONENTIAL SCHEME

Consider a simple situation where there are no coupling terms, no generation rates,

$$\frac{dN_n}{dt} = -a_n N_n .$$

After an exposure period  $\Delta$ , the nuclide concentrations are given by

$$N_n(\Delta) = N_n(O) e^{-a_n \Delta} .$$

Expansion of the exponential terms gives

$$N_n(\Delta) = N_n(O) \left[ 1 - a_n \Delta + \frac{1}{2} (a_n \Delta)^2 - \frac{1}{6} (a_n \Delta)^3 + \dots \right] ,$$

or

$$N_n(\Delta) = N_n(O) \left\{ 1 - a_n \Delta \left[ 1 - \frac{1}{2}(a_n \Delta) \left[ 1 - \frac{1}{3}(a_n \Delta)[1 - \dots] \right] \right] \right\}. \quad (48)$$

Consider the meaning of  $e^{-\Delta A}$ , where  $A$  is a matrix;

$$\begin{aligned} e^{-\Delta A} &= I - \Delta A + \frac{\Delta^2}{2} A^2 - \frac{\Delta^3}{6} A^3 + \dots \\ &= I - \Delta A \left[ I - \frac{\Delta}{2} A \left[ I - \frac{\Delta}{3} A [I - \dots] \right] \right]. \end{aligned} \quad (49)$$

With no coupling,  $A$  contains only diagonal entries, so Eq. (48) is the desired solution. The operation  $AA$  simply squares the diagonal terms.

For the general problem, the off-diagonal terms in  $A$  are coupling terms, and Eq. (26) is to be solved. With fixed entries in  $A$ , all positive terms  $a_{nn}$  on the diagonal, and the  $-a_{m,n}$  terms,  $m \neq n$ , off the diagonal (all negative), this equation has the solution<sup>11</sup>

$$\begin{aligned} N(\Delta) &= e^{-\Delta A} N(O) \\ &= \left\{ I - \Delta A + \frac{\Delta^2}{2} A^2 - \frac{\Delta^3}{6} A^3 + \dots \right\} N(O) \\ &= \left\{ I - \Delta A \left[ I - \frac{\Delta}{2} A \left[ I - \frac{\Delta}{3} A [I - \dots] \right] \right] \right\} N(O), \end{aligned} \quad (50)$$

for an exposure period  $\Delta$ , where  $I$  is the unit matrix. A single term  $(I - \Delta A)$  can not be used because there is inadequate propagation through the coupling terms. Indeed matrix  $A$  contains only near-chain coupling.  $A^2$  increases this by one nuclide, so if the coupling band is  $n+1$  nuclides,  $n$  couplings,  $A^n$  is needed to effect propagation through the whole chain, evidently a minimum requirement.

An advantage of the matrix exponential solution method is that it properly accounts for the full coupling between nuclides; alpha-decay feedback along a chain and multiple routes can not be fully accounted for with explicit solutions for individual chains. It should be noted that the nuclide-to-nuclide coupling (transmutation) terms include the fissile nuclide, fission product nuclide coupling, so the generation of fission products is modeled directly.

A procedure of calculation is desired that tends to minimize the amount of storage required, the amount of data transferred during calculation, and the amount of arithmetic involved. Consider the solution cast in the form

$$N(\Delta) = \sum_{j=0}^{\infty} (-1)^j \left[ \frac{1}{j!} \right] (\Delta A)^j N(O). \quad (51)$$

Let  $E = \Delta A$ ,  $H_j$  be a working column vector, and  $M_j$  be the estimate of the solution column vector, where  $j$  is a running index of the sweeps through the equations. Setting

$$\begin{aligned}
M_0 &= H_0 = N(O) , \\
H_j &= - \left[ \frac{1}{j} \right] E H_{j-1} , \\
M_j &= M_{j-1} + H_j .
\end{aligned} \tag{52}$$

An acceptable solution is identified,  $N(\Delta) = M_j$ , and the calculation terminated at  $j = J$  when the ratio of any term in  $H_j$  to the associated solution estimate (term in  $M_j$ ) is  $< 10^{-6}$ . A minimum value of  $J$  may be set by various ways, such as  $J = \max(\Delta a_n)$  plus the square root of the number of actinide nuclides plus the square root of the number of fission-product nuclides. The matrix  $E = \Delta A$  need not be set up as a square matrix. Instead, two major components may be stored separately:

1. the diagonal entries  $\Delta a_n$
2. the set of coupling terms  $\Delta b(m \rightarrow n)$  plus the fission product yield terms, the latter typically being

$$\Delta b(\ell \rightarrow k) = \Delta \sum_{g=1}^G y(\ell, k, g) \sum_{u \in g} \sigma_{f, \ell, u} \phi_u .$$

Underflow may be prevented by setting any entry in  $H_j$  equal to zero (after it has been used) if it is within  $10^{25}$  of the smallest number that can be stored.

The convergence rate of the calculation can be accelerated a small amount for usual problems by a simple transformation. Consider

$$\begin{aligned}
N &= e^{-\alpha \Delta} Z , \\
A e^{-\alpha \Delta} Z &= - \frac{d}{dt} [e^{-\alpha \Delta} Z] , \\
B Z &= - \dot{Z} , \\
\text{where } B &= (A - \alpha) ; \\
N(\Delta) &= e^{-\alpha \Delta} [e^{-\Delta B} N(O)] .
\end{aligned} \tag{53}$$

The procedure described above is used with  $E = \Delta(A - \alpha)$ , and the solution is  $N(\Delta) = e^{-\alpha \Delta} M_j$ . The main diagonal term  $\alpha$  is a selected constant, a reasonable choice being

$$\alpha = \frac{1}{2} \max a_n . \tag{54}$$

The use of  $e^{-\alpha \Delta}$  evaluated precisely at the end causes a slight distortion of the results. (An expansion of  $e^{\Delta \alpha}$  to the number of terms used in the calculation and use of its reciprocal instead of  $e^{-\Delta \alpha}$  was found to be less accurate, apparently inconsistent.)

Another procedure is of interest because of a slight gain in the significance of the results for large coefficients at a slight increase in computation cost. Consider the expansion

$$e^{-x} = 1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} + \frac{x^4}{4!} - \dots$$

## Grouping adjacent terms

$$e^{-x} = 1 + \frac{x}{2!}(x-2) + \frac{x^3}{4!}(x-4) + \dots$$

By such grouping the result is obtained by summing numbers which have greater differences in magnitude. Integer subtraction can, of course, be done precisely. For small  $x$ , the approximation monotonically decreases from unity and for large  $x$  it increases monotonically to a peak and then monotonically decreases. The procedure is as follows with the transformation introduced above. Let

$$\begin{aligned} B &= \Delta(A - \alpha) , \\ M_0 &= N(O) , \\ \text{for } i = 1, \quad E_1 &= \frac{1}{2} ZN(O) ; \\ \text{for } i > 1, \quad Y_i &= ZE_{i-1} , \text{ and} \\ E_i &= \left[ \frac{1}{2i} \right] \left[ \frac{1}{2i-1} \right] BY_i ; \end{aligned}$$

Then

$$\begin{aligned} F_i &= B - (2i)I , \\ H_i &= F_i E_i , \text{ and} \end{aligned}$$

$$M_i = M_{i-1} + H_i . \quad (55)$$

The solution  $N(N) = M e^{-\alpha \Delta}$  would be obtained upon truncation at required convergence,  $I \approx J/2 + 1$ . About 15% more calculation is incurred by this procedure over the simpler one above, although testing has shown no significant increase in the required computer time in usual short chain application. Early termination of the expansion must be avoided because the combination of successive terms may make a small if not zero contribution, so a minimum number of terms is required to avoid false convergence indication,  $I > \alpha \Delta / 2$ .

If an entry in  $A$  exceeds some value, the results from these procedures would not have adequate significance due to subtraction of numbers of nearly the same magnitude. The problem is illustrated by the expansion

$$e^{-x} = 1 - x + \frac{x^2}{2!} - \dots$$

This expansion peaks when

$$\frac{x^n}{n!} \approx \frac{x^{n-1}}{(n-1)!} ,$$

$$x \approx n ,$$

and since the signs of the successive terms alternate, the largest value involved is  $x^n/n!$ , while the answer we seek is  $e^{-x}$ . For six-digit significance in  $e^{-x}$ , it is required that the number of machine significant digits used to store the largest value be six more than the desired remainder considering the difference  $x^n/n! - e^{-x}$ . If  $x$  is 12, the difference is  $18,614 - 0.0000061$ , a loss of 10 digits requiring  $9 + 6 = 16$  machine significant digits. If the effect of coupling coefficients is considered and the largest term is

nearly equal to the largest diagonal (loss) term, then  $x$  above is twice the largest diagonal loss coefficient, the sum of the absolute values of the entries in columns of matrix  $A$ , or if  $x = 12$ ,  $\max(a_n) = 6$ . (The  $e^{x\Delta}$  transformation distorts the operator norm evaluation.)

In simple situations it is reasonable to assume that a nuclide having a large value of  $a_n$  will take on the end-of-exposure steady state solution. An alternate procedure is practical for modeling this. Given nuclide  $n$  having large  $a_n$  for all  $m$  having coupling ( $m \rightarrow n$ ) and all  $l$  having coupling ( $n \rightarrow l$ ), replace all ( $n \rightarrow l$ ) with coupling coefficients

$$a_{m,l} = a_{m,n} \left[ \frac{a_{n,l}}{a_{n,n}} \right], \quad (56)$$

drop nuclide  $n$  from the calculation, and finally set

$$\begin{aligned} \left. \frac{dN_n}{dt} \right|_{t=\Delta} &= 0 = -a_n N_n(\Delta) + P_n(\Delta), \\ N_n(\Delta) &= \max \left[ \frac{1}{a_n} P_n(\Delta), e^{-a_n \Delta} N_n(0) \right], \end{aligned} \quad (57)$$

where  $P_n$  is the generation rate of nuclide  $n$  from all sources. It may be possible to eliminate one or even several nuclides in this manner. There is loss of conservation of mass introduced by Eq. (56).

Advantage may be taken of another solution form. If the full solution matrix is retained without multiplying in the nuclide concentrations, as was done above, the solution may be recast in the matrix notation form<sup>12</sup>

$$N(A) = N(0) \left[ e^{-\frac{\Delta}{n} A} \right]^n. \quad (58)$$

That is, the result is obtained for the exposure step  $\Delta/n$ ,  $n$  being large enough to ensure accuracy for the significant digits carried, and this result raised to the  $n$  power. Computation may be held down by taking advantage of  $x \cdot x \cdot x \cdot x = (x^2)^2$ , etc.

### EXAMPLE PROBLEM

As an example, a simple situation is treated here involving three nuclides,

$$\begin{aligned} \frac{dN_1(t)}{dt} &= -a_1 N_1(t) \\ \frac{dN_2(t)}{dt} &= -a_2 N_2(t) + a_1 N_1(t) \\ \frac{dN_3(t)}{dt} &= a_2 N_2(t). \end{aligned} \quad (59)$$

There is no loss of material because loss shows up as source to the next nuclide and the last nuclide has no loss. One measure of the accuracy of a calculation is the loss of material from the closed system. Initial conditions selected are

$$\begin{aligned}
 N_1(0) &= 0.7 \\
 N_2(0) &= 0.3 \\
 N_3(0) &= 0.0 \\
 \text{Sum} &= 1.0
 \end{aligned}$$

The explicit results for an exposure step  $T$  are

$$\begin{aligned}
 N_1(T) &= N_1(O)e^{-a_1 T}, \\
 N_2(T) &= N_2(O)e^{-a_2 T} + N_1(O) \left[ \frac{a_1 e^{-a_2 T}}{a_1 - a_2} \right] \left[ 1 - e^{-(a_1 - a_2)T} \right], \\
 N_3(T) &= N_2(O) \left[ 1 - e^{-a_2 T} \right] + N_1(O) \left[ 1 - \frac{a_2 e^{-a_1 T} - a_1 e^{-a_2 T}}{(a_2 - a_1)} \right]. \tag{60}
 \end{aligned}$$

For comparing solutions with various methods, selected values are  $T=1.0$ ,  $a_1=0.4$ , and  $a_2=0.3$ . These data give higher specific reaction rates than those typical of usual application. An explicit solution of the equations yields the following results precise to the digits shown,

$$\begin{aligned}
 N_1(T) &= 0.46922403 \\
 N_2(T) &= 0.41964036 \\
 N_3(T) &= 0.11113561 \\
 \text{Sum} &= 1.0
 \end{aligned}$$

For the average generation rate method, consider first the lower order finite difference approximation,  $e^{-x} \approx 1 - x$ ,

$$\begin{aligned}
 N_1(t + \Delta) &= N_1(t)(1 - a_1 \Delta) \\
 N_2(t + \Delta) &= N_2(t)(1 - a_2 \Delta) + a_1 \frac{\Delta}{2} [N_1(t) + N_1(t + \Delta)] \\
 N_3(t + \Delta) &= N_3(t) + \frac{a_2 \Delta}{2} [N_2(t) + N_2(t + \Delta)] \tag{45}
 \end{aligned}$$

The dependence of the results on the number of steps taken over the exposure period is shown here,

Steps	1	2	4	8
$N_1(T)$	0.42	0.448	0.45927	0.464394
$N_2(T)$	0.434	0.42465	0.421173	0.420604
$N_3(T)$	0.1101	0.11150	0.111455	0.111349
TOTAL	0.9641	0.98415	0.991908	0.996347

Thus doubling the number of steps essentially halves the error in this example. This is a relatively slow rate of error reduction. Of critical importance for producing accurate results is that all  $a_i\Delta \ll 1$ .

Next consider the use of average generation rates with a precise integration of the differential equations,

$$\begin{aligned}
 N_1(t+\Delta) &= N_1(t)e^{-a_1\Delta} , \\
 N_2(t+\Delta) &= N_2(t)e^{-a_2\Delta} + \frac{a_1}{2a_2} [1 - e^{-a_2\Delta}][N_1(t) + N_1(t+\Delta)] , \\
 N_3(t+\Delta) &= N_3(t) + \frac{a_2\Delta}{2} [N_2(t) + N_2(t+\Delta)] .
 \end{aligned} \tag{61}$$

The dependence of the results on the number of steps taken over the exposure period is shown here,

Steps	1	2	4	8
$N_1(T)$	0.4692	0.46922	0.469224	0.469224
$N_2(T)$	0.4243	0.42079	0.419928	0.419712
$N_3(T)$	0.1086	0.11053	0.110984	0.111098
TOTAL	1.0021	1.00054	1.000135	1.000034

The result for the first nuclide is, of course, precise (not shown entirely displaying few digits).

Thus the error is much smaller than it was with the lower-order formulation, and a relatively fast rate of error reduction is associated with the calculated nuclide concentrations. Doubling the number of steps reduces the error by a factor of four.

For the matrix exponential approach, we consider the matrix

$$A = \begin{bmatrix} 0.4 & 0 & 0 \\ -0.4 & 0.3 & 0 \\ 0 & -0.3 & 0 \end{bmatrix},$$

$$I - \Delta A = \begin{bmatrix} 0.6 & 0 & 0 \\ 0.4 & 0.7 & 0 \\ 0 & 0.3 & 1.0 \end{bmatrix}; \quad (62)$$

and the results as dependent on the number of terms taken in the expansion are

Terms	0	1	2	4	8
$N_1(T)$	0.7	0.42	0.476	0.468533	0.469280
$N_2(T)$	0.3	0.49	0.4055	0.421417	0.419476
$N_3(T)$	0	0.09	0.1185	0.11005	0.111244
TOTAL	1.0	1.0	1.0	1.0	1.0

Here the total is conserved. Measuring the error level as the square root of the sum of the squares of the differences of the final nuclide concentrations from fact, the error goes down as 0.08843, 0.01732, 0.002194, and 0.000204 for the increasing number of terms used in the expansion; doubling the number of terms decreases the error level by about a factor of ten after full coupling is effected.

The simple transformed matrix exponential method is now applied. Let  $\alpha = \frac{1}{2} \max(a_n) = 0.2$ ,

$$B = \begin{bmatrix} 0.2 & 0 & 0 \\ -0.4 & 0.1 & 0 \\ 0 & -0.3 & -0.2 \end{bmatrix} \quad (63)$$

The dependence of the results on the number of terms of the expansion is shown here,

Terms	0	1	2	3	4
$N_1(T)$	0.7	0.458489	0.469951	0.469187	0.469226
$N_2(T)$	0.3	0.450302	0.417143	0.419777	0.419635
$N_3(T)$	0	0.073686	0.111757	0.110979	0.111138
TOTAL	1.0	0.982477	0.998851	0.999943	0.999999

The expansion is more rapidly convergent, although conservation of the total was lost. For  $\alpha = 0.3$ , the results obtained are

Intervals	0	1	2	3	4
$N_1(T)$	0.7	0.4667	0.469931	0.469222	0.469224
$N_2(T)$	0.3	0.4297	0.41930	0.419649	0.419640
$N_3(T)$	0	0.0667	0.10779	0.110863	0.111120
TOTAL	1.0	0.9631	0.99640	0.999734	0.999984

Here 0.2 is judged superior to 0.3 for  $\alpha$ . Increasing the value of  $\alpha$  tends to reduce a weighted error level of the results with termination at a set number of terms up to some point where the error grows, the optimum depending on both the coupling coefficients and the magnitudes of the nuclide concentrations.

## MODELING CONSIDERATIONS

### STRATEGY FOR MODELING THE TIME VARIABLE

Here the representation of exposure to a neutron flux over a period of time is considered. Typically the level and energy spectrum of the flux vary in space and over time. Thus in a reactor-core calculation those changes that occur that affect the space, energy neutron-flux distribution are to be accounted for. The accuracy of the modeling that is needed depends on the type of calculation, the desired reliability of the results, and the importance of each aspect taken collectively. The effects of changes or differences are generally of more importance and interest than absolute results in many applications. For example, a bias factor may be required to adjust the calculated multiplication factors to an absolute result. It is common practice to adjust a calculated multiplication in this way to estimate requirements for the critical conditions and performance at that state.

A calculation is to be done for the period between refuelings. Generally the required fuel loading and distribution, burnable poison, and control positioning or soluble poison are not known for a desired exposure period. Alternately, the period of time before refueling is not known. Complications may include operation toward the end of the period at a reduced power level to maximize the amount of energy extracted from the fuel. Quite generally the fuel and cladding temperatures must be held within design limits, and since the economic considerations drive up the power rating, heat extraction must be effected by the coolant with a favorable power density distribution. The power density in fresh fuel assemblies after partial refueling, and especially near reflectors, may be kept down by the use of burnable poison. Likely much is known about how much fuel and burnable poison are needed and about a reasonable special variation in these. Optimizing the power-density distribution presents a challenge and generally requires experience and experimentation since direct assessment employing

importance techniques considering time must yet come into common use. The objective function for such analysis tends to be rather involved causing simple solution procedures to lack utility. Implemented capability is adequate only for producing an incomplete solution at best or an estimate of results requiring further calculation of the trial-and-error type. When thermal hydraulic considerations are involved, constraining temperatures are only crudely approximated by constraining the power-density distribution, although a reasonable approximation of the correspondence between temperatures and power density may, of course, be useful. Primary calculations with elaborate core modeling are supported by the results obtained with simple models.

A direct calculation of the required concentration of burnable poison is attractive for a pressurized-water core (when applicable). When control rods are to be positioned during the history, it may be most practical to use a preset schedule of positioning the control rods with adjustment and recalculation when necessary. Enhancing such a procedure to effect automated optimization remains a challenge. Still even modest improvements to a preselected rod positioning schedule should be worth some investment in methods development and implementation.

Typically the time when refueling must take place is not known and must be established. Since exposure of materials is needed precisely to this time, a procedure is needed that effects just that. Some scheme of projection from known information is needed, or the ability to back up to some previous point and redo the exposure to the desired time.

Concern in the discussion here is primarily about modeling-time effects. The experienced analyst is wary about using a time interval between neutronics solutions that is too long. There may or may not be difficulties depending mostly on the core size and makeup. A large core containing a low specific loading of the actinides may be weakly coupled. The neutron-flux distribution can be sensitive to differences. It is possible, for example, for the thermal flux to be high on one side and low on the other, and for this condition to reverse after some period of operation. The cases of very high-fuel burnup and high poisoning that burns out should be suspect. Evidently the modeling is somewhat more complicated when radical flux changes are involved. Instead in some calculations it has been found that radical flux shifting was a consequence of coarse calculational modeling and not a phenomenon to be expected in real operation.

The space, energy neutron-flux distribution would be expected to be somewhat different after refueling than when the cycle ends for the next refueling. (Without a significant change over the cycle, the modeling would be simple.) Considering the application of basic capability separate neutronics and exposure calculations, considerable variation is possible, but the most attractive possibilities are limited to:

1. Once through, marchout, successive neutronics, exposure calculations, or
2. recalculation techniques.

The first involves breaking the exposure period (cycle) into  $n$  intervals and performing a neutronics calculation at each node point ( $n+1$  calculations) with exposure done in between. The recalculation technique can be applied by initially carrying out the exposure calculation to the end of the period (perhaps the full cycle) using the neutron-flux distribution obtained initially, calculating the flux at the end, then repeating the exposure calculation with a weighting of the endpoint flux values, and finally repeating the final neutronics calculation. These schemes are addressed in some detail below.

#### **ONCE THROUGH MARCHOUT MODEL**

The once-through marchout calculation is a look-ahead procedure. A neutronics solution is obtained for the core contents at some reference time, and the neutron flux distribution that is calculated is

assumed to apply over a following period of time. The desired power level should and can be effected over this interval as is discussed later. Computation costs force the use of long exposure intervals between neutronics problem solutions while the approximation is more accurate the shorter the exposure period. Thus accuracy is sacrificed as necessary to allow adequate results to be obtained at a reasonable cost. (Other compromises are also involved including the detail of the geometric model, the neutron energy discretization, and the fueling and control representation.) The requirement is to account for the feedback effects of exposure that alter the space, energy neutron-flux distribution. This may be a severe requirement in some situations but not in others. If temperature peaking tends to moderate from a worst condition after refueling, then a coarse modeling thereafter may be quite adequate. Pushing the design and operation such that design limits are approached is to be expected, and modeling accuracy then increases in importance.

The choice of the exposure period between neutronics problems is dependent on several aspects. Control-rod positioning, change in coolant density, and high-fuel burnup can cause special flux shifts. Changes in nuclear data due to shift in the fissile nuclides may have to be accounted for. So the reaction rates over the core must be adequately resolved to satisfy the accuracy requirements of the task at hand. How easy this is to say and yet how hard it is to quantify beforehand unless there is specific experience that is applicable. If the end of the cycle is to be established when refueling is required, then shorter intervals may be necessary for projecting or to allow accurate interpolation. Techniques are used to hold down the flux shifts that would otherwise occur, such as preferential fuel loading and repositioning and the use of burnable poison. The analyst tends to overkill when the error levels and the nature of the error are unknown and when accurate methods of error compensation or extraction are not known.

A two-dimensional heterogeneous fast-reactor core exposure problem was solved without control-rod representation. The results for a traverse across the fuel assemblies shown in Table 1 were obtained for an exposure period of 511 days with fixed microscopic cross sections. The error in the solution obtained with the marchout scheme is proportional to the reciprocal of the number of periods. (Additional information is presented later for this problem and the results obtained with recalculation are discussed in the next section). The results show that there is a significant fractional error in the calculated reactivity swing associated with coarse representation in time. This is due in part to the small magnitude of the reactivity swing. The rate of error reduction obtained with the use of more exposure steps is significant, doubling the number of steps halves the error. (Other modeling approximations can contribute more error, as is shown later for this problem).

**Table 1. Reactivity Swing Calculated for a Fast Reactor Cycle**

Calculational Method	Numbers of Intervals	Neutronics Problems Solved	Processor time (min)	Reactivity Swing	Relative Fractional Error	Error $\times$ Time
Marchout	1	2	0.31	-0.0043916	0.46	0.14
Marchout	2	3	0.48	-0.0036944	0.23	0.11
Marchout	6	7	0.92	-0.0032468	0.08	0.07
(Extrapolated)				-0.00301	-----	
Recalculation	1	3	0.42	-0.0030999	0.03	0.013

## RECALCULATION TECHNIQUES

By recalculation is meant that information generated from a calculation is used in repeating the calculation, hopefully improving the results. A special advantage of recalculation is that the model is not limited to a look-ahead approximation. The most appropriate cross-section data, temperatures, etc. may be used to achieve accurate modeling. Of course a long exposure period might have to be treated in steps to achieve a high accuracy and to produce adequate information about the performance. The objective of recalculation is to effect an improvement in the solution by improving the estimate of the specific reaction rates on the average over the interval. A disadvantage of this technique is that a convergent process is not assured; successive iterate results may oscillate. It may not be simple to judge whether or not an exposure calculation for a long interval is accurate. Another disadvantage may be the lack of adequate data for predetermining the time when refueling should occur, although an iterative procedure may be used to establish this.

A number of techniques can be used. Fundamentally different procedures are applicable to the cycle-by-cycle calculation and to the one-cycle quasi-equilibrium state. Survey calculations admit the use of a flux solution at a single point in time, or at most two, with a single-exposure period. Detailed analysis may require treating two or more exposure steps between fuelings.

Consider a simple model for survey calculations. The core is to be partially refueled annually with operation at a load factor below design, and it will be assumed that a truly repeating cycle will be established requiring identical fuel element removal, repositioning and insertion at each refueling. The state at the time of refueling before fuel removal is taken as the reference for which a critical condition is required with the control rods nominally removed. A trial-and-error (iterative) solution procedure may be used to effect an acceptable solution for the exposure period between successive fuelings. The required fuel enrichment must be determined each cycle and an effective cycle-average neutron flux estimated. Typical applications show that the period between successive fuelings needs to be broken into at least a few exposure periods when there is high fuel burnup so that the flux-level increase required to effect the desired power level, fuel consumption compensation, is modeled accurately. Starting with an initial flux estimate, likely for the startup case with a fresh-fuel loading, the calculation would proceed through the successive cycles with a specified convergence level satisfied at each by recalculation. The amount of calculation is minimized by using only the initial and the end-of-cycle flux distributions. Improving this with a midcycle flux solution requires two additional neutronics problems be solved each cycle iteration. Note that with recalculation done for two intervals, five neutronics problems must be solved, an increase of only 67% over three neutronics problems for one interval with recalculation once. Not only are techniques needed to accelerate the rate of convergence but also the data for the past history should be made available and recovered to hold down computation costs. The latter is especially important for those problems for which the result moves into a repeating, quasi-equilibrium condition.

The geometric model is tailored to the situation. Although one-dimensional models find some use, a two-dimensional model of a traverse through the fuel assemblies is usually essential to model reaction rates and reflector effects and to generate power density data, and the third dimension is often synthesized in some way. Modeling this third dimension is especially important to allow representative heat-removal calculations to be done to determine temperature distributions and to establish fueling, burnable poison and control-positioning requirements and effects. Only as much geometric detail need be represented as necessary to produce results of adequate quality for the purpose at hand.

The point-reactor model is useful and interesting. Exposure of the materials is to a neutron flux having an energy spectrum appropriate to the mixture, an effective core flux. Separate exposure calculations for the individual batches achieves individual accounting. If one-fourth of the core is to be refueled each time, then it contains four different types of material, one at each of the four basically

different ages of exposure. With annual refueling, these ages are at the time of shutdown for refueling 1, 2, 3, and 4 years, and after refueling they are of 0, 1, 2 and 3 years. The point model ignores spatial variation in the flux including the tendency for the flux level to be high in fresh fuel (unless burnable poison is used) and low where high burnup lowers the fuel concentration. An effective core neutron loss rate must be supplied for realistic neutron accounting. Different batch sizes are seldom allowed in such a model. On the other hand, informative low-cost calculations are possible with fissile accounting. The net fuel consumption can be made to be correct for the energy generated within the limit of the accuracy of fissile generation.

The investment of effort on methods development in support of any major project generates useful analysis capability. Attention to the specific project needs should tailor the capability toward solving those problems of most interest efficiently and economically.

One of the difficulties in applying special calculational techniques to reactor history calculations is the possibility that the model was inadequate. As modeling complexity increases, the likelihood of a discrepancy may increase and reliability may be hard to establish or test. Sensitivity and importance data are useful, as well as is redoing a calculation with some parameter changed.

The fast-reactor core-exposure problem discussed in the previous section was solved applying the recalculation technique. Initial and final flux values for a single exposure step (over the 511 days) were averaged, the exposure calculation was redone, and a final neutronics problem was solved. The original calculation of two neutronics problems and one exposure treatment was thereby increased to three neutronics problems and two exposure treatments at an increase of 35% in the computer processor time. The error in the calculated reactivity swing was essentially eliminated as is shown in Table 1. The error is much less than was achieved with two marchout intervals and is well below that achieved with six intervals. Thus the recalculation technique is shown to be a preferred technique in this case, and the added computational cost is certainly justified if the error content of the result obtained with the coarse model is of any consequence.

Computation requirements for the different techniques may be compared. Generally the computer time required for the exposure calculation is considerably less than for the neutronics problem. Letting  $E$  be the time for the minimum exposure calculation, one step, and  $F$  be that for the neutronics, a simple forward step-out calculation for  $m$  intervals takes  $F+m(F+E)$ . While subdividing each interval into  $n$  steps for power level renormalization increases this to  $F+m(F+nE)$ . To allow for repeat calculations, let  $j$  be the number of times each step is done,  $j = 2$  for one repeat, the time is increased to  $F+jm(F+nE)$ . Note that for  $F \gg E$ ,  $n$  can be large with little penalty. However, it would be usual for  $n$  to be 3 without repeat and perhaps only 1 with repeat, while  $j$  may need not be more than 2 or perhaps 3.

## GEOMETRIC MODELING

A core model is selected that will be adequate for the situation. Two dimensions will be treated rather than three to hold down analysis costs, if the effects associated with the third coordinate can be estimated or done without. An appropriate model depends on the task at hand, the core design, the quality of the results and detail that are needed, and the available analysis capability. Useful results can be obtained with a point-core model and rather sophisticated modeling capability that could not be produced with a one-dimensional model.

A particularly useful three-dimensional model in some applications is a two-dimensional slice through adjacent fuel assemblies representing the different ages with partial core refueling plus a full axial traverse to allow the assessment of heat extraction, fuel enrichment variation, burnable poison use, and control positioning. A full section through all of the fuel assemblies across the core is not taken, rather a reduced section, considerably simplifying the model by reducing its size and reducing the number of different compositions that must be taken into account.

Fine scale heterogeneity, as of fuel pins, is eliminated by homogenization. Care must be taken to effect an adequate representation. Given a choice, materials that are quite different are treated individually. Of special concern are retaining sufficient information to reflect the changes in the reactivity from exposure and tailoring the modeling to allow the desired information to be extracted from the results. Sophisticated methods allow interpreting the results for the original heterogeneous arrangement of materials.

Exposure effects are accountable for in a neutronics calculation with macroscopic cross sections associated with discrete volume elements. The average value of the neutron flux in each of the discrete energy groups is used, a spacial average, to calculate specific reactor rates, and a single-exposure calculation is done for each individual material associated with each discrete volume element. Often only one material is assigned to each elemental volume. What is the preferred discretization? There are a number of considerations. Two calculations are involved: neutronics and exposure. Discretization for each must be resolved.

There may be constraints to consider. A real constraint may be the amount of data that must be handled. Another may be computation cost, likely to some combination of processor time and data handling costs. Others may be the total computer resources that will be tied up and associated delay in turnaround of results.

Rather secondary modeling aspects may impose constraints. When refueling and repositioning of fuel assemblies are involved, requirements are imposed in that certain things must be adequately represented requiring a degree of discretization into distinct fuel elements. The available capability may have limitations regarding just what fuel movement can be modeled, and selection may be necessary from among alternative schemes to effect that most representative. Rotation or repositioning of a fuel element may cause the spatial differences in composition due to exposure to have increased importance, perhaps forcing discretization at a finer scale than at the fuel-element level. The geometric description presented to the neutronics code must be carefully discretized for modeling changes and exposure effects while satisfying the neutronics calculational requirements regarding adequate discretization to produce results of sufficient quality. The coarser the mesh intervals and the discretization of the volumes, the larger the error to be expected in the results. When the power-density distribution and peaking are of interest, the modeling may have to have finer intervals than would otherwise be needed and possibly attention must be paid to better resolution in certain locations of special interest or concern.

Primary modeling capability causes the effect of exposure to be calculated for the materials located in discrete volumes. A secondary capability may be available to treat a finer scale as an auxiliary calculation. The core must be discretized into a set of volumes. Thus the axial lengths are arbitrarily selected for subdivisions of the fuel elements to allow adequate accounting of exposure effects. The discretization is tailored to account for differences in the fuel loading, separating the old and the new material, and accounting for nuclide concentration variations. Thus burnable poison would be properly located as much as possible, rather than being distributed into adjacent materials, to properly account for the effect of its presence on the neutron flux distribution and local reaction rates. Control-rod modeling may impose a severe burden, even if only to admit evaluation of the insertion worth in a calculation that is adjunct to the core history problem. Explicit modeling of the cross-sectional area of control rods may be desirable to produce the most accurate results, but this is done only when necessary due to the computational burden. Note that desired axial-rod positioning may influence the axial discretization. Accurate modeling of the end of a control rod and local effects is usually beyond what is practical for core-history calculations, so a reasonable and convenient representation is usually chosen. The modeling is especially impacted by the separation of rods into several gangs positioned individually.

The reactivity swing over a 511-day exposure period between refuelings was calculated for a fast reactor with a set procedure. The results for the reactivity swing depend on the arrangement of the mesh points as shown below.

Meshpoints per Hex Assembly <sup>a</sup>	Exposure		Reactivity Swing	Apparent Relative Fractional Error
	Zones per Assembly	Computer Time (min)		
6	1	2.52	-0.0062120	0.57
24	1	8.65	-0.0047563	0.20
(Extrapolated)			-0.00427)	
3	1	0.92	-0.0032468	-0.18
12	6	2.15	-0.0037350	-0.054
48	6	8.48	-0.003784	-0.014
Extrapolated			-0.00395	

<sup>a</sup>The 6- and 24-point cases are meshpoint-centered locations while the others are mesh-cornered locations.

For estimating the relative error, the extrapolation of the results obtained with the most detailed modeling was used as the solution. Note that there is a significant variation in the result, although this may not be of much significance considering how small it is. It is not simple to establish adequate modeling requirements. A cost-benefit analysis is needed with importance assigned or bounds set on the accuracy of one or more of the results.

The nuclear data has an association with materials. Thus the cross sections for the moderator may vary from one location to another to account for differences in the local detail and in the position in the core. Softening of the neutron spectrum in the reflector causes the downscatter cross section to increase as one moves outward when weighted over a broad neutron-energy band. Thus the nuclide concentrations relate to locations and are associated with microscopic cross sections. This association can become somewhat involved with fueling changes and repositioning. When a fuel element is moved, do the associated cross sections go with it or are they associated with the location? Perhaps even new data applies with repositioning, requiring change in the association. The modeling capability that is available may be quite flexible, requiring careful selection from among the alternatives and special attention may have to be paid to the details of the input data descriptions to effect what is desired. What is desired may be done automatically without special instructions. On the other hand, the modeling capability may be severely limited, limiting what can be done or possibly forcing special action to be taken.

This section is concluded with the observation that the geometric modeling requirements for the core that has been operated, for the time history representation, are quite different than for the new core. Careful consideration is necessary of many aspects including the nature of the desired results and the factors that influence these and their reliability.

## THE NEUTRON ENERGY SPECTRUM

It is rather surprising that a very coarse representation of the energy dependence of the neutrons, the energy where reactions occur, is adequate. The fission neutrons start above 1 MeV, and significant resonance absorption occurs in the keV range, while over half of all reactions in a thermal reactor occur at thermal energy in the neighborhood of 0.04 eV. Even the large temperature variation across a reactor core does not have a major impact and may easily be accounted for. Careful cross-section weighting is, of course, essential. High-energy effects [enhanced fission and  $(n,2n)$ ], resonance shielding and the thermal cell flux suppression, and spectrum hardening are involved.

Calculations were done for a simple water-reactor problem. The dependence of the error in the results on the energy structure is shown below for an exposure period.

Energy Groups		Fractional Error in the Results at the end of the Exposure Period	
Thermal	Total	Fissile Inventory	k
1	2	0.027	0.0049
1	6	0.021	0.0025
4	14	0.0051	0.0031
12	32	0.0056	0.0019
30	60	0.027	0.0007

The fissile inventory is substantially the same calculated with two groups as with 60. Some improvement in the final multiplication factor may come from increasing the number of groups but not necessarily with the use of a few thermal groups. Compensation of the errors from the energy modeling and the time-history model make an intermediate energy-group structure attractive. (The error associated with the use of 60 groups would be eliminated by a better resolution of the spectrum changes with time.) These results illustrate the difficulty faced in reliability evaluation and in selecting the modeling details.

There is often a difficulty associated with the use of only a few thermal neutron groups. The scattering is sensitive to the shape of the flux spectrum within the groups. A specific situation may be tested elaborately and then accurately reproduced with a set of collapsed few group data. Application of this data to another situation, specifically to changed conditions, may produce a spectral approximation that is far from accurate. It may prove better to use only one thermal group or be necessary to use a correlation of the scattering data to accurately account for the effects of changes.

## MODELING NEUTRON TRANSPORT

Reactor-core analysis requires modeling the transport of neutrons. This is done with diffusion theory for most core calculations. Enhancement in higher-order modeling has always been a promise yet to be fulfilled. Experience has shown that the special data requirements are difficult to satisfy. Statistical variations in Monte Carlo results are hard to deal with, especially when low reaction rates are poorly sampled. It is a common practice to generate a neutronics result for a point in time applying a high-order transport model for benchmarking. Only when experimental results are available for the situation has the higher order result proven very useful. Poor modeling, discrepancies in the representation and in the data, and generally inferior solutions must be avoided. Bias factors are in common use, but generally these are not selected on the basis of a single higher order neutron transport solution, and of course biasing is to be avoided if possible using accurate modeling and tailored data.

Neutron transport across a reactor core is not the same thing as neutron transport within a cell model used for cross section collapse. The collapse of neutron transport cross sections for diffusion theory use is a rather complicated subject beyond this discussion; however, in order here is a caution regarding the need for and the importance of specific experience in this area.

## OTHER ASPECTS, AUXILIARY CALCULATIONS, AND GENERATING INFORMATION

Auxiliary calculations are needed to generate information essential for effective analysis. The edit of information from computer calculations is essential to support analysis. Of special importance is the need for some form of neutron accounting to convey to the analyst details about where the neutrons are going. General purpose computer codes do not satisfy the requirements for routine use in reactor analysis. Special action is necessary to reduce the burden of supplying input data and collecting the results. For example, average information may be desired about the fuel assemblies (power density, power-density peaking, burnup) while exposure is calculated at a finer scale.

The need for close-coupled engineering-type calculations should be obvious. Quite generally, results such as temperature distributions are to be optimized (not some intermediate information), requiring appropriate capability. This aspect is not addressed here.

Considering that only a few sums are required, it is practical to carry out the additional calculations to produce auxiliary results while the usual exposure calculation proceeds. The average power level is needed, for example. Inventory and average integral reaction rates by nuclide and by nuclide class support analysis, and such data are easily collected.

The average reaction rates over an exposure interval are the most representative of what is happening, and these can be approximated adequately for short intervals by using the average of the start and end nuclide densities. Perhaps the most confusing aspect of this generation of information for the average over the interval is that the accounting is often incomplete or not entirely accurate. The basis is the neutron flux used for the exposure calculations, and this would have been obtained at the start of the interval and not redetermined, although of course that was what was used for the calculation. Other contributions to the neutron accounting come from leakage and buckling loss that were determined by the neutronics calculation at the start of the interval. If control rods are being removed with time applying any of a number of possible models (smeared absorber, explicit modeling perhaps with an interval black absorber surface condition), then the data available at the start of the step is inaccurate for the average of the interval.

A complete and accurate accounting would require some interpolation of data over time, while the effort required to implement this is seldom dedicated. The assignment of the neutronics and exposure tasks is usually done in separate calculational modules for flexibility with simple data coupling. This causes the automated resolution of time-dependent accounting difficult to do. The analyst is often expected to make corrections to the reported results with little notification or documented help. Application experience is of much importance in any application when the results that are reported do not seem to be entirely consistent.

An important result that comes from an interval neutron accounting is the apparent multiplication, the ratio of the production rate from fission to the total loss rate that would normally be based on the average interval reaction rates. Since the neutron-flux distribution is correct only at the start of the interval (if then), an average  $k$  is an approximation subject to interpretation. However, this value of  $k$  is very useful, indicating the adequacy of such modeling variables as the length of an exposure interval and the provisions made to effect a critical system.

A neutron accounting is generated in a compact form by space, energy integration of reaction rates. For example, the total fission rate in one nuclide is given by

$$F_n = \int_V N_n(r) V(r) \int_E \sigma_{f,n}(r,E) \phi(r,E) dE dr . \quad (64)$$

Note the use here of volumes that do not enter the chain equations. With discretization this is often reduced to the form

$$F_n = \sum_z N_{n,z} V_z \sum_g \sigma_{f,n,x,g} \phi_{z,g} , \quad (65)$$

where association is provided between cross section set  $x$  and zone  $z$ . Given the specific reaction rates required in an exposure calculation for each location,

$$G_{n,f,z} = \sum_g \sigma_{f,n,x,g} \phi_{z,g} , \quad (66)$$

then

$$F_n = \sum_z N_{n,z} G_{n,f,z} V_z . \quad (67)$$

the total fission rate is given by the sum

$$Q = \sum_n F_n , \quad (68)$$

and with a simple representation the core power level is

$$P = \sum_n F_n W_n , \quad (69)$$

where  $W$  is thermal energy per fission. Impact comes to such a calculation from including other energy terms (a capture-gamma contribution), from including energy dependence in the power-per-fission values, and with modeling cross-section dependence on local conditions.

Reactor-core analysis involves the calculation of reaction rates and fissile-inventory accounting. A quantity often obtained, studied, and reported is the fissile conversion ratio called the breeding ratio if greater than unity. This ratio is formally defined as the ratio of the rate of fuel generation to the rate of fuel consumption,

$$C = \frac{\frac{dF^+}{dt}}{\frac{dF^-}{dt}} , \quad (70)$$

where the parts of the total derivative are shown. Both instantaneous and average time-integrated values are useful and used. A fissile-mass balance is given by

$$F(T) = F(O) + \int_{t=0}^T \left( \frac{dF^+}{dt} - \frac{dF^-}{dt} \right) dt , \quad (71)$$

where  $F$  stands for the fissile inventory. Combining these expressions and using  $Pdt = \eta dE$ ,

$$F(t) = F(O) \left[ 1 + \frac{P}{\eta} \left( \frac{\overline{dF}}{dE} \right) \int_{t=0}^T (\overline{C} - 1) dt \right] . \quad (72)$$

Several pieces of information are required to support the fissile mass accounting: the power level, the thermal efficiency, the rate of fissile consumption per unit thermal energy produced, and the fissile conversion ratio. The form of Eq. (72) is especially useful since the rate of fissile consumption per unit energy produced is relatively constant, although it does change as the fissioning nuclide concentrations change. Naturally  $^{235}\text{U}$  is consumed while  $^{239}\text{Pu}$  is generated by neutron capture in  $^{238}\text{U}$  and  $^{241}\text{Pu}$  also builds up. Typical specific consumption values for the fissile nuclides are shown below, the data taken from a gas-cooled, graphite-moderated core calculation.

Nuclide	$\frac{dF^-}{dE}$ (kg/W)
$^{233}\text{U}$	$1.39 \times 10^{-10}$
$^{235}\text{U}$	$1.52 \times 10^{-10}$
$^{239}\text{Pu}$	$1.96 \times 10^{-10}$
$^{241}\text{Pu}$	$1.64 \times 10^{-10}$

The relatively high value for  $^{239}\text{Pu}$  is due to its high unproductive capture cross section generating  $^{240}\text{Pu}$ . The fact that  $^{233}\text{U}$  is the preferred fissile nuclide in this type of reactor is evident from this data.

An effective fissile conversion ratio may be reported that allows for out-of-reactor fissile losses. Equation (72) may be recast for such interpretation from fissile inventories.

### CROSS-SECTION VARIATION

The high concentrations of certain nuclides such as  $^{238}\text{U}$ ,  $^{232}\text{Th}$ , and  $^{240}\text{Pu}$  cause the large resonances to be shielded, decreasing the reaction cross section with increasing concentration through flux suppression. A high concentration of burnable poison causes flux suppression, reducing its specific reaction rate and decreasing its consumption rate; thus some control over its time-dependent absorption rate is possible by varying its degree of concentration. The generation of the plutonium isotopes following  $^{238}\text{U}$  neutron capture introduces high cross sections in the thermal-energy range, especially at the elevated energies, causing flux suppression that affects the specific reaction rates in these nuclides as well as those in other nuclides. High cross section at low energy shifts the thermal spectrum upward in energy, affecting reaction rates. This may be caused by the presence of  $^{135}\text{Xe}$ , control-rod insertion, and burnable and soluble poison. Relatively quick changes, as due to control-rod insertion, or change in the  $^{135}\text{Xe}$  or the soluble boron cause shifts in the reactivity.

One way to account for effects in the thermal-energy range is to use several energy groups. Unfortunately poor modeling of changes has been found with a coarse group structure, likely due to a sensitivity of broad-group scattering data to the flux spectrum, forcing either the use of many groups or correlations, perhaps at the macroscopic level. The other difficulty is that the neutronics problems are very hard to solve unless tailored procedures are used to resolve the thermal flux distribution and spectrum, since up-scattering response is slow with a simple downward sweep in energy and the outer iteration error vectors take on a complicated form frustrating usual acceleration procedures.

A way to account for cross-section changes is by correlation. An adequate representation depends on the needs. For example, if the coolant density is to be fixed, then it need not be considered as a variable except as necessary to account for the local coolant-volume fraction and temperature differences and changes. Calculations that do not consider temperature effects, of course, do not need a temperature correlation. This leaves the exposure or the concentration of a nuclide as the key independent variable affecting the cross section of this nuclide. The influence of the concentrations of

the other nuclides that may be represented to first order with a macroscopic cross section dependence. In addition, both a  $1/v$  and a non  $1/v$  factor is likely needed for accurate modeling. Note that resonance shielding in a fixed geometry depends primarily on the nuclide temperature and concentration. Geometric variations are often of importance. For example, nuclides in the fuel pin next to the reflector experience less resonance shielding than in the interior pins. Fuel loadings may be varied to effect a preferred axial-power distribution. More than one fuel pin size may possibly be involved.

The amount of calculation that would be necessary and the amount of data that could be processed for a very accurate representation of microscopic cross sections and their changes is generally not justified. What is done is only to effect adequate approximations. Capability is implemented in the projects to satisfy the more important needs often using techniques developed for other applications where possible with but simple extensions. Generally the analyst must apply the procedures available to him to whatever situation is at hand. The specific modeling that is best used and options to be exercised must be established by testing. Establishing the adequacy is, unfortunately, quite difficult to do, especially without the capability for accurate reference modeling to benchmark against. Simple testing must be done. Calculations are often done that risk a relatively large uncertainty in the accuracy of the results. Still gross effects can readily be accounted for.

The best procedure of calculation to implement may well depend on the situation. The extension from treating two dimensions to treat three typically adds a considerable amount of data. For some calculations the nuclide concentrations need to be followed at only a few locations. In this case a somewhat elaborate cross-section generation scheme might be practical and less reliance placed on correlations. When many locations are involved, it is better to perform the necessary calculations initially and rely on a generalized representation that then requires little calculation and only a reasonable amount of data handling. Where the same conditions might exist at several locations, the same results are obtained from correlations, not from redoing elaborate calculations.

It is noted here that macroscopic cross sections can be correlated with exposure (cumulative fissions). This avoids solving the chain equations. The information content of such calculations may or may not be adequate for any specific application, depending on the needed results and the actual modeling available.

Note that data appropriate to an exposure step should be representative of conditions over the step, some average if nothing better. This is not the same as the requirements for a neutronics calculation if it is to be representative of the state at a point in time. As an example, there would not be any  $^{135}\text{Xe}$  in a clean or refueled core. If reactivity information for this state were desired, no  $^{135}\text{Xe}$  would be included. If, on the other hand, the primary objective is to initiate a core-exposure calculation, equilibrium  $^{135}\text{Xe}$  might be included representing a condition that could establish only after a few days of operation. Cross-section data representative of an average of the start and end of the exposure period nuclide concentrations are more appropriate for use during this period than data representative of either endpoint.

Here a simple example of a specific reaction rate that is linear in time will be used to study the effects of cross section variation and its modeling. Consider

$$\frac{dN(t)}{dt} = -a(t)N(t) \quad (73)$$

and let

$$a(t) = c_1 + c_2 t \quad (74)$$

Hoping for an explicit solution,

$$\int \frac{dN}{N} = - \int (c_1 + c_2 t) dt$$

$$- \ln \frac{N(\Delta)}{N(O)} = c_1 \Delta + c_2 \frac{\Delta^2}{2} . \quad (75)$$

If we approximate this with the form

$$\frac{dN(t)}{dt} = - bN(t) , \quad (76)$$

$$- \ln \frac{N(\Delta)}{N(O)} = b \Delta . \quad (77)$$

The preferred value of  $b$  to give the desired solution depends on  $\Delta$ ,

$$b = (c_1 + c_2 \Delta/2) . \quad (78)$$

If instead of  $b$ ,  $c_1$  were used, the relative error in the exponent of the solution is

$$\frac{c_2 \Delta}{2c_1} . \quad (79)$$

Note that this tends to zero with  $\Delta$  or  $c_1/c_2$  tending to zero, but for reasonable  $\Delta$ , this discrepancy may be significant. To keep the discrepancy less than some set amount  $\epsilon$ ,

$$\Delta < \frac{2c_1 \epsilon}{c_2} . \quad (80)$$

Results are shown below using data of  $c_1 = 0.1$ ,  $c_2 = 0.01$ .

$\Delta$	$c_1 \Delta$	$\exp(-c_1 \Delta)$	$\exp[-(c_1 \Delta + c_2 \Delta^2/2)]$	Fractional Relative Error in $N$
0.05	.005	0.995	0.995	.00001
0.1	.01	0.990	0.990	.00005
0.25	.025	0.9753	0.9750	.00031
0.5	.05	0.9512	0.9500	.00125
1.	.1	0.9048	0.9003	.00501
2.5	.25	0.7788	0.7548	.0317
5.	.5	0.6065	0.5353	1.13
10.	1.	0.3679	0.2231	1.65

## CROSS-SECTION DEPENDENCE ON TEMPERATURE

A linear correlation of the microscopic cross sections on the local temperature can use data at two reference temperatures,

$$\sigma(C) = \sigma(C_1) + x[\sigma(C_2) - \sigma(C_1)] , \quad (81)$$

$$\gamma = \left[ \frac{C - C_1}{C_2 - C_1} \right] ,$$

where  $x = \gamma$ ,  $C$  being the temperature of interest, and  $C_1$  and  $C_2$  being the temperatures at which the reference data applies (consistent subscript numbers). Note that the temperatures need not be absolute since only differences are involved. Mixing Centigrade and Kelvin values should be avoided. (Absolute temperature is often used, as for referencing scattering kernels, while the analyst may be used to using values in Centigrade, as for thermal hydraulic specifications such as the coolant inlet and outlet temperatures.) An evident advantage of this form of representation is that all controlled factors may be varied to produce data that is representative of two different situations; the actual correlating temperatures being nominal values, although some tie to real temperatures is necessary with a thermal hydraulics model to be very useful.

The tendency is for incremental increases in the temperature to have less effect on cross section as the temperature increases. Indeed some data may correlate better if divided by temperature. That is, assume cross section divided by absolute temperature is linear (or even constant in some applications).

An improvement to a linear dependence of cross section on temperature was desired. Note that a quadratic fit would increase the data requirements by 50%. Unwilling to impose this burden on the codes, an arctangent correlation was used, setting

$$x = \frac{\tan^{-1}(\alpha\gamma)}{\tan^{-1}(\alpha)} , \quad (82)$$

$\gamma$  being the ratio of temperature differences shown above. A set value of  $\alpha$  was used. (It would be possible to gain a more accurate representation by allowing  $\alpha$  to depend on the nuclide and possibly also on the reaction type and on energy). The use of the arctangent function has been found to give a reasonable curvature to the fit, although a simple correlation is subject to considerable error.

Application of the arctangent function led to an obvious difficulty. If some local temperature to be treated is higher than the upper reference temperature, the correlation may be poor. It may be desirable to assure that the reference temperatures span the full range. Otherwise a spot check may be essential to make sure that the correlation does not break down.

A less severe difficulty with the arctangent function is that it does not model the temperature variation of some cross sections very well.

Cross sections may, of course, be correlated at the macroscopic level. With a linear approximation to the temperature dependence and linear contributions of the microscopic cross sections to the macroscopic cross sections, the calculation is separable, so the correlation may be applied to either. (The diffusion coefficient being proportional to the reciprocal of the transport cross section makes it nonlinear and subject to a dependence on how it is calculated.) Note that application only to macroscopic data would not be consistent with the use of microscopic data for the calculation of exposure effects. Thus there may not be much incentive to implement macroscopic correlations.

## STRATEGY FOR MAINTAINING THE POWER LEVEL

Core-history calculations are usually done at full power to represent usual operation carrying base load. In the simplest and cheapest calculation, exposure for a time interval is carried out fixing the specific nuclide reaction rates, integral  $\phi\sigma$ . However, to effect a derived power level, the neutron-flux level must be increased with time to compensate for fuel consumption. Applying equations that assume that the neutron-flux level is constant over an interval of time invites the use of some technique for compensating for the drift.

One of the difficulties of the exposure problem is effecting a desired power level over a period while generating proof that such was maintained. A coarse estimate of what happened may or may not be adequate. For example, the end-point (start and end) power levels can be averaged to approximate what happened between them. However, the actual adjustment in the level of the flux that would be required to compensate for the change in the fissile-loading change tends to be linear only over a modest period of time. The generation of  $^{239}\text{Pu}$  tends to increase the power level due to its high-thermal fission cross section and may more than compensate for the consumption of  $^{235}\text{U}$ .

A first-level correction is to assume that the flux level is linear in time. If the slope were known prior to a calculation,

$$\phi(t) = a + bt, \quad (83)$$

then this information could be used.

The simplest way to compensate for this effect is to use an average for a reasonable period of time that is higher than required at the start. Over an interval  $(O, T)$ , the average is

$$\bar{\phi}(O, T) = a + \frac{bT}{2}, \quad \text{or} \quad (84)$$

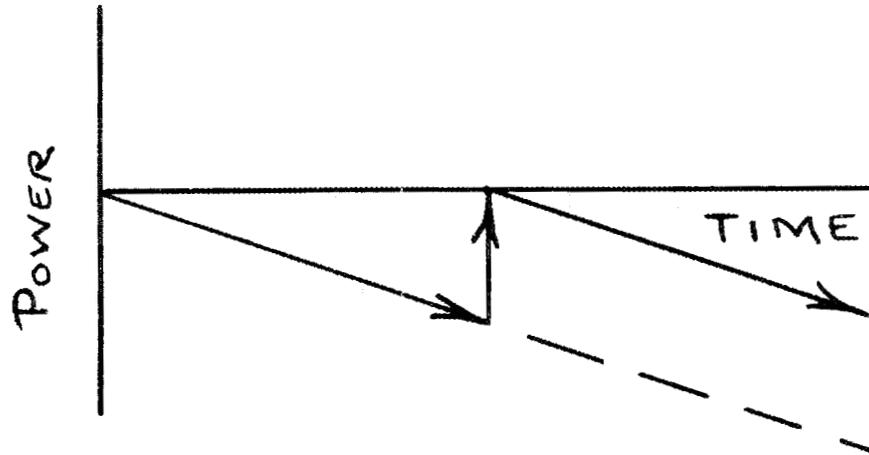
$$\frac{\bar{\phi}(O, T)}{\phi(O)} = 1 + \frac{bT}{2a}. \quad (85)$$

Thus if the flux level is established at  $\phi(O)$  at the start for the desired power level, it would be multiplied by this ratio to compensate for fuel consumption. A significant error is thereby reduced to an acceptable level for a reasonable time interval. The ratio  $b/a$ , relative slope, could be supplied, if known, adequately for any specific calculation.

Even though the technique noted above may be quite adequate, the flux slope may not be known or it may change with time and depend on the situation at hand. An alternative procedure could be used to account for the level change. The time interval can be divided into halves, and the power level determined after exposure for the first half interval. Adjusting the flux level then to effect the derived power level,

$$\phi(T/2) = \phi(O) \frac{P(O)}{P(T/2)}, \quad (86)$$

where  $P$  refers to the integrated power level. This leads to the power trace

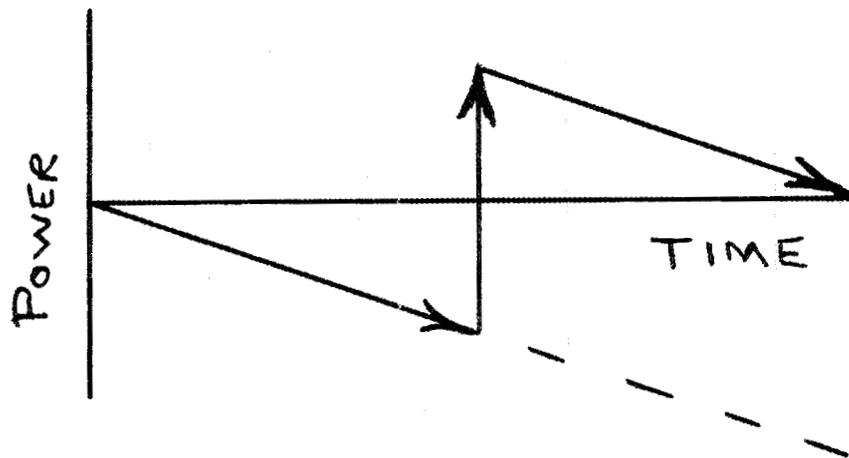


thus returning the power to the desired level half way through the interval roughly halves the error. That would result with no adjustment.

An improvement results if the requirements for a desired power level are effected on the average,

$$\phi(T/2) = \phi(O) \left[ 1 + 2 \frac{P(O)}{P(T/2)} \right], \quad (87)$$

giving the trace



Thus the discrepancy is effectively eliminated if the drift is linear. In the event of large flux-level changes, as may be associated with high fuel consumption, a more general scheme would allow the use of several subintervals, usually preselected. Consider a running average of the past history of the power level, estimated here as an average of the known values at discrete points at equal-time subintervals,

$$\bar{P}_n = \left( \frac{n-1}{n} \right) \bar{P}_{n-1} + \frac{1}{2n} \left[ P_{n-1} + P_n \right] .$$

Desiring  $\bar{P}_{n+1} = P_o$ , the power level for the interval  $(n, n+1)$  is needed,

$$P_o = \left( \frac{n}{n+1} \right) \bar{P}_n + \left( \frac{1}{n+1} \right) P_{n,n+1} ,$$

$$\frac{P_{n,n+1}}{P_o} = 1 + n \left( 1 - \frac{\bar{P}_n}{P_o} \right) . \quad (88)$$

Note that this is unity, if the ratio of the average to the initial power level is unity.

The adjustment of the flux level may be implemented as an adjustment in the specific reaction rates,

$$(x_n \phi) \sigma \big|_n = x_n (\phi \sigma) \big|_n \quad (89)$$

where  $x$  is the factor for adjusting the power level at the start of the interval in time. Note that one complication is that, if after interval  $n-1$  the specific reaction rates were adjusted, after interval  $n$  the appropriate factor is given by

$$X_n \phi \sigma \big|_n = Q_n X_{n-1} \phi \sigma \big|_n ,$$

$$Q_n = \frac{X_n}{X_{n-1}} . \quad (90)$$

Parallel data-processing procedures may be used that cause the reaction data to be resident in the computer in one case but on auxiliary storage in another. It is necessary to make the procedures consistent and correct. The data in auxiliary storage could be updated, or simply use  $Q_n$  when data are resident and  $X_n$  when the original data is accessed from auxiliary storage.

Additional calculations are required, as indicated above, to generate the information used to hold the power level constant by adjusting the specific reaction rates to account for the necessary change in the neutron-flux level. With no adjustments, calculations need not be done to indicate power levels. The analyst would, however, be left in the dark regarding the modeling and its reliability. An inferior calculation models a lower power level than desired; an error is introduced, and the fissile requirements underpredicted.

## LOCAL POWER DENSITY IMPORTANCE

Although operation is limited to temperatures well below where failure would be expected, design limits are pushed by economic considerations. Therefore, it is important to predict reasonable power-density distributions, especially peaks. In some analysis effort it is necessary to incorporate data that causes bounds to be applied. However, best estimates are usually desired with uncertainty applied to those. Of course, modeling is important so special attention must often be paid to the situation to

produce adequate results. Operation of a core at 5% below a reference power at which it should be operated increases power costs 5%.

### FISSILE MATERIAL ACCOUNTING

An essential result from core-exposure calculations is the accounting of fissile material. The fissile inventory in the core decreases with operation (except for a breeder). The amount of material, the refueled loading, the loading before refueling, and the refueling and discharge batch sizes to be handled is of interest. The consumption is easy to predict, so a discrepancy indicates the presence of a modeling error. The analyst becomes familiar with and anticipates the amount of fuel that should be in the core after refueling.

Mass-balance accounting is normally done by identifying an appropriate enclosing envelope and writing a balance equation that accounts for all changes,

$$V \frac{dN_i}{dt} = \text{Feed} - \text{Discharge} + \text{Generation} - \text{Loss} \quad (91)$$

The rate of change in the amount within the enclosed system equals the net of the rates of feed minus discharge plus generation minus loss.

### ECONOMIC IMPORTANCE

Economic aspects often dominate other considerations in decision making. Of some importance is the time of occurrence of cost and return. When return that pays costs lags the costs, indirect charges (interest) accumulate increasing the required return. Deferred costs have negative indirect charges. A simple way of accounting for these indirect charges is to use an effective discount rate, and continuous compounding is considered here for simplicity.

$$QR(t) = C(t - \Delta)e^{i\Delta} \quad (92)$$

where cost  $C$  occurs at time  $t$  while the return for sale of  $Q$  (amount of energy, etc.) that pays for it at rate  $R$  is not available until an interval of time  $\Delta$  later,  $i$  being the effective fractional annual discount factor. For small  $i\Delta$ ,  $e^{i\Delta} \approx 1 + i\Delta$ , so a year delay adds about  $i$  fractional costs. Cumulating returns and costs,

$$\sum_j [Q_j R_j(t) - C_j(t - \Delta_j)e^{i\Delta_j}] = 0 \quad (93)$$

Simply summing return does not, however, assign it a time importance. An improved form is

$$\sum_j [Q_j R(t_j) - C(t_j - \Delta_j)e^{i\Delta_j}] e^{-it_j} = 0 \quad (94)$$

This is a discount or present value form. Taking a fixed rate, and recasting the form to the general form

$$R = \frac{\sum_j C(t_j)e^{-it_j}}{\sum_n Q_n e^{-it_n}} \quad (95)$$

Thus the discount factor  $e^{it}$  is of relative economic importance. Costs that occur late in the life of a plant are of much smaller import than those occurring early. The effect of a year delay in initial plant operation is to increase the required return by  $i$  fraction. If there were no indirect charges, the direct contribution to the required return would be given with  $i = 0$  and constant  $Q$ ,

$$R_d = \frac{1}{NQ} \sum_j C(t_j) , \quad (96)$$

and the indirect contribution is the difference,

$$R_i = R - R_d . \quad (97)$$

The indirect charges tend to be proportional to the fissile inventory. Considering a plant or system of them, action is needed that reduces the fissile inventory and keeps the indirect charges under control. Thus the amount of new fuel on hand is kept down to what is needed.

### THE MULTIPLICATION FACTOR

Here the neutron multiplication factor is considered. To the neutronics specialist,  $k$  is the most positive eigenvalue of the regenerative neutronics problem involving mathematical modeling of transport and reaction processes. The core analyst finds an earthy definition more useful,

$$k = \frac{P}{A+L} , \quad (98)$$

where  $P$  is the neutron generation rate from fission,  $A$  is the neutron absorption rate, and  $L$  accounts for all other losses including core leakage. These terms are space energy integrals. Thus  $k$  is the ratio of the rate of neutron generation divided by the total rate of loss. For modeling the reactor history we desire  $k = 1$ . If  $k < 1$  likely there is a shortage of fissile material, and for  $k > 1$  an excess may be the case.

Many calculations are done using the approximation of allowing  $k$  to vary over a cycle between fuelings as an approximation to avoid the calculation of control losses. In effect, high-energy neutrons are lost rather than low-energy ones, and the approximation may or may not be acceptable depending on how much error is introduced. More accurate power-density distributions may be needed, the produced data being affected by the actual location of control absorptions.

Refueling may be indicated by  $k = 1.0$ . However, some excess reactivity may be deemed necessary for operation, and this is provided for with  $k > 1$ . Coast down with operation at a reduced power might be modeled with full-power calculations ending in  $k$  somewhat below unity.

### MODELING THE CRITICAL STATE

Of some concern in reactor-core calculations is an accurate modeling of the near critical state that must exist most of the time. The multiplication factor is very nearly unity all of the time. This is achieved by compensation for changes causing a shift in the state, altering not only the rate of fuel consumption but also affecting the poisoning effect of the products of fission that build up. Reactivity increase is possible, as in a core having a fissile breeding ratio higher than unity, and also possibly due to changes in the fuel material or poison consumption. However, the usual trend is loss in reactivity. Compensation is from consumption of burnable poison, decreasing the soluble boron content of the cooling water for a pressurized water-reactor core, or control-rod removal in most cores. Certain small reactors use enhanced reflection for compensation. These aspects are considered in setting up an

acceptable model for the calculation; and, of course, primary attention is focused on those contributing factors that are known to have the most influence on the results.

It is relatively obvious that an exposure calculation modeling the behavior of a reactor core should indicate that  $k$  is unity at startup initially or after refueling, and  $k$  is also unity when shutdown for refueling. What may not be so obvious is how the details that affect  $k$  are best modeled over the history between refuelings. Actually the preferred modeling may depend on how reactivity is maintained.

Consider the core that has explicit fuel and fertile zones that would be continuously repositioned to effect the critical state. The loss in reactivity is compensated, primarily by decreasing the integral reaction rate in fertile material.

A neutron accounting using integral reaction rates at any point in time yields

$$L = A + B + O , \quad (99)$$

$$k = \frac{P}{L} \quad (100)$$

where  $L$  is the total loss rate,  
 $A$  is the absorption rate in fuel,  
 $B$  is the capture rate in fertile,  
 $O$  is all other loss rate,  
 $P$  is the neutron production rate.

With effective macroscopic data,

$$P = \nu F , \quad (101)$$

where  $F$  is the fission rate, and

$$A = \nu F / \eta$$

$$\nu \frac{F}{k} = \nu \frac{F}{\eta} + B + O ;$$

so the capture rate in fertile material is given by

$$B = \nu F \left[ \frac{1}{k} - \frac{1}{\eta} \right] - O \quad (102)$$

and the conversion ratio is given by the approximation

$$C = \frac{B}{A} , \text{ or} \quad (103)$$

$$C = \frac{\eta}{k} - \frac{O}{A} - 1$$

Assuming that the reference and desired state is  $k = 1$ , then if  $k > 1$ ,  $C$  is low; and if  $k < 1$ ,  $C$  is high. That is, a high value of  $k$  represents a state where there are excess neutrons not being put to good use. A low value of  $k$  indicates a state where the utilization is being overestimated, there are not enough neutrons to support the estimated fissile generation rate.

We expect  $k$  to be unity on the average. If the effect of fissile consumption, reducing  $k$ , were ignored, the generation of fuel would be overestimated. The direct consequence of a calculation done at  $k < 1$  is overestimating fissile production and overestimating the length of time between reactor refuelings.

The effect can be quantified. Consider that an exposure history is done between refuelings in intervals and the reactivity swing that must be compensated over the cycle is  $\Delta k$ . That is, the conversion ratio decreases from an initial value of  $C_0$  to a lower final value,  $C_T$ . Since  $\Delta k$  fewer neutrons are available for fissile conversion relative to  $B$  available initially,

$$\frac{C_T}{C_0} = 1 - \frac{\Delta k}{B} .$$

The average value of the conversion ratio is

$$\begin{aligned} \bar{C} &= \frac{1}{2} (C_0 + C_T) , \\ \bar{C} &= \left[ 1 - \frac{\Delta k}{2B} \right] C_0 . \end{aligned} \quad (104)$$

If the calculation were done in one step using initial reaction rates, the amount of fissile material at the end of time,  $T$ , would be estimated as

$$\frac{F(T)}{F(O)} = XT(C_0 - 1) , \quad (105)$$

where  $X$  is a conversion factor when it should be

$$\frac{F(T)}{F(O)} = XT(\bar{C} - 1) = XT \left[ \left[ 1 - \frac{\Delta k}{2B} \right] C_0 - 1 \right] . \quad (106)$$

The relative error in  $\frac{F(T)}{F(O)}$  is

$$\text{Error} = \left[ 1 - \frac{1}{\frac{\Delta k}{2B}} \right] - 1 \approx \frac{\Delta k}{2B} . \quad (107)$$

Carrying out the exposure over some interval in  $m$  steps reduces this relative error to

$$\text{Error} = \frac{\Delta k}{2mB} . \quad (108)$$

Thus the error is proportional to the reactivity decrease over the period. A linear rate of error reduction is rather slow, and many steps could be necessary to generate an accurate answer.

More accurate modeling is possible. A simple technique is to require  $k > 1$  at the start of each interval to compensate for its subsequent decrease.

### FUEL MANAGEMENT CAPABILITY

All that is needed is the capability to model the problems to be solved. Direct support of application by methods development should cause the requirements to be satisfied. However, future requirements are not simple to predict; available methods impose limitations and restrictions, and problems involving fuel management tend to be complicated and not easily solved with simple methods. It is not easy for an analyst to understand the unfamiliar schemes and to become expert in specifying their details, especially when the documentation may leave much unsaid. A change in what is done one cycle affects future cycles. Poor resolution of the fueling requirement at one time disrupts a calculation. Fueling requirements are not simply determined when later conditions (end-of-cycle) are to be satisfied and when significant changes occur as with fuel repositioning and recycle.

Simple fuel-assembly repositioning is complicated by the need to carry along cross-section association (or not leaving it position dependent). Recycle involves conservation, as of partial  $^{233}\text{Pa} \rightarrow ^{233}\text{U}$ , while repositioning involves retaining material that has been generated.

A major challenge in implementing fuel-management capability is making the association between the atom densities of the nuclides required by the neutronics and exposure codes and the mass contents of the fuel assemblies needed for accounting. The complication of this association needs somehow to be hidden from the analyst so that straightforward instructions are prepared for a calculation. Typically atom densities must be specified, cross-section associations made and maintained, refueling and repositioning done with other specifications, and results then reported at the pleasure of the code developer. Approaching the requirements from the viewpoint of reducing the user burden and reducing the likelihood of discrepancies, a more satisfactory input description would start with identifying fuel assemblies and how they are to be broken down for carrying nuclide densities on a subscale along with cross-section association for calculation macroscopic cross sections and accounting for exposure. Then fuel-assembly handling may be described directly with provision for repositioning, rotation, refueling, etc. The system of codes that result when usual neutronics-code data-input requirements are retained without change cannot be considered adequate for much analysis effort. Satisfying basic user needs must be considered to be important and essential coding justified to allow reliable routine application. Too often the requirements of an available neutronics code have been retained thwarting the development of the most useful capability and limiting the utility of what is implemented. In this area there may be difficulty justifying the necessary coding and perhaps in interesting the developers in relatively uninteresting work considering that there are never-ending needs to enhance available methods. A careful look at the data input requirements should show that the probability of error in a problem description increases directly with the complexity, amount of data, and redundancy. Reducing error and analyst time required to prepare quality data justify considerable effort.

### ACCURACY, IMPORTANCE AND UNCERTAINTY

How accurate is a calculated result? It may take more effort to assign a reasonable uncertainty to a result than to calculate it. Note that assigning a large uncertainty may so discredit a result as to make it useless. Accuracy in an absolute sense is, of course, harder to evaluate than the accuracy regarding results to be compared in a relative sense. Generally one expects the reactivity swing over a cycle to have a larger relative uncertainty the smaller it is; hence there may be a strong dependence on the situation.

Evaluating uncertainty involves establishing the effects of all contributions from the data through the modeling. Whereas interest is in a collective effect, most evaluation must be done at the individual contribution level. Thus calculations are done to quantify effects, and a store of experience is accumulated that is not available at the start of a project.

How should uncertainty in results be reported? Likely a percentage is the most practical with the meaning of one standard deviation ( $1\sigma$ ) unless specified differently. (It is common to misunderstand the possible magnitude of the error from such data.) Weighting of independent contributions in a usual statistical sense (mean of the square root of the sum of the squares) is in order. Note, however results obtained from an uncertainty calculation and others obtained otherwise, as by perturbation, may not be simple to combine; both independent and related contributions may be involved.

An analyst establishes the accuracy needed in any results to be obtained. An analysis to be done is likely influenced by the required accuracy, the choice of calculational methods being one option to be resolved. Preliminary calculations may be in order to support decision making. It may not seem very scientific, but it is often quite proper to produce a preliminary result, when possible, by a coarse method and refine it by adding sophistication to the calculation. A result produced by a coarse method often proves to be so useful that consideration should be given to starting this way. The most useful analysis capability allows a coarse modeling.

Here the generation of auxiliary information is addressed that requires considerable computational capability to be implemented. It may be most usual for calculations in this area to be done with less than the elaborate capability in use to treat the reactor-core history. Simple modeling may be used to hold down the cost of calculations. For example, useful information may be generated with calculations that assume that the same number of fuel elements are replaced and the same number repositioned each time of refueling so that a truly repeating history occurs, rather than modeling actual conditions that cause variations between successive cycles. Still the most useful information would come from application of the full modeling capability in use for base reactor-history calculations.

Importance information supports core-performance analysis. Reaction-rate integrals are a form of importance; they show neutron economy, and a study of them is done to seek improvements. Treating time as a variable in importance analysis is a severe complication. Importance data allows assessment of the effect of changes, and the reliability of such assessment is increased by increasing both the accuracy of the importance data and the sophistication of modeling of importance. Sensitivity data indicates the importance of contributing factors on specific results. Generalized results span the range of interest and contain far more information than can be generated with discrete perturbations. First-order approximations are used because higher-order calculations seem uneconomical, so application may be somewhat limited. For example, first-order perturbation theory is seldom adequate for quantifying control rod worth.

In reactor core design and operation support it is important to understand aspects that have a strong influence on the performance. Thus any tendency for the power density to shift from a favorable distribution to an unfavorable one is evidently to be avoided. It is also important to identify aspects that have a small influence on the results, removing them from consideration when improvement is undertaken.

Generally the reactor-core history problem involves so many variables and is so complicated that often the analyst needs more information than he has available. What is the preferred burnable poison distribution and control-rod positioning schedule to optimize core material temperatures? This question is not now answered by solving a single problem. Importance information helps.

Sophisticated uncertainty analysis is a rather different subject. In a sense project success can be predicted, and, likely of more direct interest, individual aspects of a project evaluated. Can a system go critical? How much additional fuel might be needed? If cross-section data improvements are needed, new measurement effort can be directed at an area where most needed or where the most improvement can be effected by reducing the uncertainty in the results through data uncertainty reduction.

It may or may not be difficult to determine what aspects or independent variables or the data are the most important in a calculation. Considering reactivity effects to be paramount, then those things that affect the fissile inventory are quite generally important. Underestimating the amount of fuel that must be consumed to generate a certain amount of energy causes fueling requirements to be underestimated.

The reactivity importance of fuel tends to decrease when moving away from the center of the reactor. The neutron-flux level also tends to decrease when moving away from the center. This results in a decreasing power density and a high-power density peak with a uniform loading. Loading the core with more fuel toward the edge to increase the power density there while reducing the peaking increases the fissile loading. Failure to consume all of the burnable poison that is used increases the fissile loading. Any positive reactivity requirement, such as for  $^{135}\text{Xe}$  override, increases the fissile loading.

Whereas the scattering cross section of  $^{238}\text{U}$  can play but a small role in the neutron distribution, the total cross section does significantly affect the neutron accounting at a point in time. Considering the time variable, the  $^{238}\text{U}$  capture cross section causes  $^{239}\text{Pu}$  generation affecting the fuel inventory and, therefore, is a very significant consideration in fuel accounting. In a thorium-loaded core these comments apply to  $^{232}\text{Th}$ .

The consequence of uncertainty in nuclear data depends very much on the situation. Uncertainty in the  $^{232}\text{Th}$  cross section seems rather unimportant in thorium-utilization calculations assuming there would be no physical loading constraint. If the  $^{232}\text{Th}$  absorption cross section is higher than assumed, the calculated results would be effected with a higher loading. If the cross section is too high, a lower loading produces essentially the desired results. Of course there would be small changes, and the situation becomes complicated by variation in the loading, the use of larger fertile loaded pins than fuel pins, etc.

A lot of data is required for uncertainty analysis. It must be evaluated, made available, and be processed.

Interesting uncertainty and importance results, however, can be obtained with the simple assumption that the relative uncertainties in all of the cross sections are approximately the same. The change in the multiplication factor for a fixed relative difference,  $g$ , in the cross sections is given by

$$\Delta k = \sum_i \frac{\partial k}{\partial \Sigma_i} (g \Sigma_i) ,$$

or

$$\Delta k = g \sum_i \Sigma_i \frac{\partial k}{\partial \Sigma_i} . \quad (109)$$

The importance data,  $\partial k / \partial \Sigma$ , are usually approximated by first-order perturbation theory requiring the regular flux and the adjoint solutions and usual importance integrals over space and energy.

Assume a fixed uncertainty in each cross section, positive or negative, in the relative probabilistic sense. With effects acting independently, uncorrelated uncertainties, the result for uncertainty in the multiplication factor is

$$\delta k = \left\{ \sum_i \left[ f \Sigma_i \frac{\partial k}{\partial \Sigma_i} \right]^2 \right\}^{1/2},$$

$$\delta k = f \left\{ \sum_i \left[ \Sigma_i \frac{\partial k}{\partial \Sigma_i} \right]^2 \right\}^{1/2}. \quad (110)$$

Thus  $\Delta k$  is proportional to  $g$  and  $\delta k$  is proportional to  $f$ . A 50% reduction in  $f$  would reduce  $\delta k$  50%.

It does seem that often the cross-section uncertainties are not well known, and they may tend to be underestimated. Arguments can be made that these uncertainties should be similar. The results that are generated with the simple approximation above are considered to be very useful, and no severe data processing burden is involved.

The uncertainty in  $k$  was found to have the contributions shown in Table 2 for a high-temperature, gas-cooled, graphite-moderated core. The dominating contributions from the thermal neutron-energy range (group 4) are evident.

**Table 2. Thermal high-temperature reactor reactivity uncertainty**

Energy Group	Upper Energy (eV)	Average Flux		Neutron Absorption Rate (Integral)	Fertile Capture Rate (Integral)	Fissile Absorption Rate (Integral)	Core Reactivity Importance		Uncertainty in $k$ Due to 100% $\Sigma$ Uncertainty (Uncorrected)
		Regular $\phi$ (n/cm <sup>2</sup> ·s)	Adjoint $\phi^*$ (Relative)				$\frac{\partial k}{k \partial \Sigma a}$	$\frac{\partial k}{k \partial v \Sigma f}$	
1	1.5+7	2.058+13	4.404	0.058+19	0.024+19	0.013+19	-99.4	99.5	0.0132
2	1.8+5	3.219+13	4.450	0.415+19	0.303+19	0.077+19	-157.3	155.8	0.0463
3	5.8+2	2.629+13	4.594	2.925+19	1.573+19	0.708+19	-132.6	127.2	0.2975
4	1.8	5.582+13	5.582	8.995+19	1.612+19	5.615+19	-342.4	270.3	1.2620
Total		13.488+13	19.030	12.393+19	3.512+19	6.413+19			1.2975

Other analytical results are often of more interest than  $k$ . Consider the fissile conversion ratio and its uncertainty. The primitive fissile conversion ratio is given by the rate of fuel generation divided by the rate of fuel consumption,

$$B = \frac{C}{A}, \quad (111)$$

where  $C$  is the integral neutron-capture rate in fertile material and  $A$  is the integral neutron-absorption rate in fissile material. (Various techniques are used to account for other contributing factors, including the loss in fuel production from absorption in intermediate nuclides like <sup>233</sup>Pa and variation in

importance of the individual nuclides to make calculated values of the conversion ratio most representative and hence useful in analysis. Of course, inconsistencies are to be avoided.) A simple perturbation yields

$$\frac{\Delta B}{B} = \frac{\Delta C}{C} - \frac{\Delta A}{A} \quad (112)$$

This leads to the uncertainty estimate of

$$\frac{\delta B}{B} = \{ f_C^2 + f_A^2 \}^{1/2}, \quad (113)$$

where the individual contributions from fertile capture and fissile absorption are shown.

Uncertainty results are shown in Table 3 for a high-temperature reactor core. The direct contribution comes from the reaction rate changes from the reference state while the indirect contributions are obtained with a fissile conversion ratio importance solution specific to the situation.

The above techniques must be extended to consider the somewhat more interesting and important situation at the nuclide and microscopic cross-section level. Here we are also interested in considering the effect of time.

**Table 3. Thermal high-temperature reactor uncertainty conversion ratio**

Energy Group	Importance Source $S^*$	$\phi_1^*$ (Space average)	$\phi\phi_1^*$ (Integral)	Uncertainty Due to 100% $\Sigma$ Uncertainty (Uncorrelated)				
				Direct Fertile Capture	Direct Fissile Absorption	Overall Direct	Indirect	Overall
1	0.236-15	0.514-21	+0.026	0.0069	0.0021	0.0072	0.0049	0.0087
2	2.305-15	0.52-21	-0.771	0.0863	0.0121	0.0871	0.0744	0.1145
3	12.84-15	0.043-21	-10.647	0.4479	0.1103	0.4613	0.3576	0.5836
4	-7.46-15	-3.576-21	-158.343	0.4589	0.8755	0.9885	0.4088	1.0697
Total		-2.477-21	-169.735	0.6471	0.8825	1.0943	0.5482	1.2239

Not much use has been made of importance and uncertainty techniques that include time as a variable. A reason for this is that generally a reference solution over time is always needed for any calculation, and the generation of importance information doubles the amount of calculation as well as requires that special capability be implemented for solving the equations. Note that a simple auxiliary analysis does not change the result of the reference calculation done with the best estimate data. (Distorted results from biased data would not be easy to work with.)

Time-dependent importance theory is beyond the scope of this discussion. It is noted, however, that a variational technique is used to minimize an appropriate integral. The result generally takes the form

$$\Delta R \approx \sum_i \frac{\partial R}{\partial X_i} \Delta X_i, \quad (114)$$

and

$$\frac{\partial R}{\partial X_i} = \int L^* dv , \quad (115)$$

where  $R$  is a response function,  $X_i$  is a dependent variable,  $\Delta X_i$  its change, and the appropriate Lagrange multiplier (importance)  $L^*$  is integrated over phase space. A particular advantage of such an approach is that general importance data can be generated for a problem not specific to a particular perturbation and these are then used for elaborate analysis. Restrictions come in the limitation of the importance to a specific response, complexity in the situation of interest often involving several responses, and the limited accuracy of first order methods in some applications.

### EXAMPLE OF IMPLEMENTED CAPABILITY

In a system for reactor-core analysis, an exposure code is supplied nuclear data, neutron-flux data, and nuclide concentrations for the start of an interval. It is also given certain task assignment instructions. A common-task assignment is to return nuclide concentrations predicted for the end of an exposure period. Typically defaults are implemented for coded options that are representative of usual application, and repeated application of the same instructions is common for successive task assignments (typically alternating with the use of a neutronics code to generate current neutron flux data).

A calculational procedure was implemented to support core analysis in the breeder-reactor development program. The code BURNER<sup>14</sup> is a module used to treat an exposure period given only information (neutron flux and nuclide densities) at the start. Shown in Fig. 1 is the exposure calculational procedure. Certain key points are noted here about this procedure. A reactor-core problem is modeled with zones of material, each zone being considered to be homogeneous for the purpose of the calculation wherein the nuclides have distinct nuclear properties. A multigroup neutron-flux spectrum is provided for each zone, generally a simple sparial averaging over the volume associated with each zone. A second level of representation is allowed in the form of subzones, each subzone being assigned to a zone. Thus several different compositions may be associated with a single zone, and to be exposed to its neutron flux the effects of exposure to be treated individually. Thus as a simple example, the situation of countercurrent fueling may be modeled directly with two sets of nuclide concentrations assigned to each zone. In the case of moving fuel, the multipass of pebble-fuel elements may be modeled directly. Treatment of an exposure period may be followed by a shutdown period. The capability to break the exposure step into substeps is indicated, allowing the flux level to be renormalized to effect a desired power level on the average over the interval. After the primary calculation has been done, a fine-scale calculation may be done to generate detailed results for one or at most a few selected locations.

The available procedures for solving the chain equations are briefly

1. the matrix exponential,
2. the average generation rate, or
3. the explicit solution.

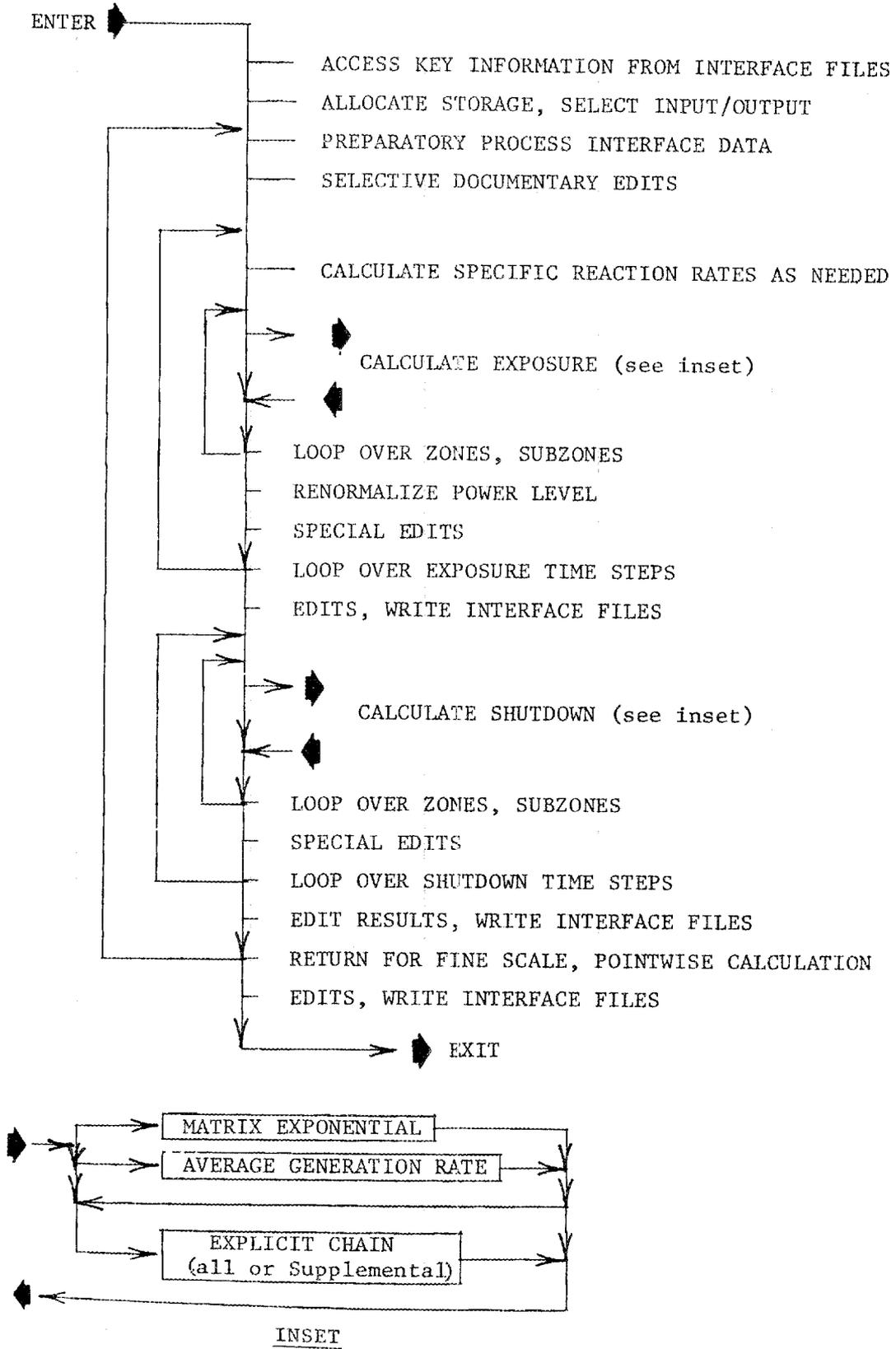


Fig. 1. The exposure calculational procedure of the BURNER code.

Any one of these may be applied individually, or either 1 or 2 may be used with 3. Thus, the instructions select a solution procedure. Not indicated are options on the matrix-exponential method to use the detailed scheme or to drop out the short-lived nuclides for the equilibrium approximation.

Additional options not shown include

1. weighting neutron flux data (recalculation of exposure) and
2. the application of a continuous fueling model that allows following fuel movement through the core.

### TASK ASSIGNMENTS TO CODE MODULES

Clean data-interfacing lines must be drawn between the code modules. These become clear once task assignments have been made to the codes, problem-solving capability has been specified, and data requirements are identified. Unfortunately, with further developments come new requirements that were not foreseen and that can seriously impact the development process.

Given the circumstances and based on our experience regarding needs, it was decided to construct a true modular-code system. Each code would carry out a major task assignment in a prescribable calculational process. All data communication was from external files (data not contained in memory). Each code was to be a major one having extensive capability (coarse rather than fine blocking minimizing data communication).

Task assignments are of interest. Consider that in a complicated problem there may be one or more data files available. The primary task assignment to the neutronics code would be to solve the neutronics problem for the current reactor-core state. The code would be expected to selectively use the latest version of the nuclide concentrations, appropriate cross sections, and recover a point-wise flux distribution as the best starting place to generate a new neutron-flux solution. Such basic information as the geometric description and cross-section association would be available. For the exposure calculation, the neutronics code must produce zone-averaged group flux values. It would also need to write a new nuclide concentration file if these were changed, a point-wise flux file for later recovery, and a power-density file if a thermal hydraulics calculation is to be done, and it may also need to save iteration solution data for recovery. Optional instructions to the neutronics code might include solving the equilibrium  $^{135}\text{Xe}$  concentrations that affect the flux distribution, and procedure and edit choices.

The primary task assignment to an exposure code would be to carry out the exposure calculation or not, a possible alternative being to include shutdown calculation (only decay) or do exposure followed by shutdown. The instructions to the code would include the following

1. Exposure time interval
2. Shutdown time interval
3. Solution method option
4. Solution method detail option
5. Number of subintervals (for flux level renormalization)
6. Power level (likely relative)
7. Flux level normalization option

8. Edit option
9. Debug edit option
10. Cross section option
11. Neutron flux option
12. Auxiliary results option
13. Nuclide concentration file writing option
14. Auxiliary results file writing option
15. Localized point exposure option
16. Special modeling data
17. Override coded abort rules
18. Parallel data handling/procedure option
19. Accuracy, reliability data
20. Constraint data
21. Data for auxiliary calculations

A task assigned to the neutronics code in this system, rather than to the exposure code, was proper normalization of the neutron-flux level to effect a desired power level. A reason for this is that exposure calculations can be done without the detailed geometry data needed for flux normalization. Zone volumes are derived from the basic data describing the geometry. (They might be inconsistent with it.) Requiring proper normalization of the flux by the neutronics code is not really a burden here; it should have such capability to produce results that are user friendly, and calculation of the equilibrium  $^{135}\text{Xe}$  imposes the requirement of proper flux-level normalization.

A neutronics code solves the neutron-flux problem using macroscopic cross sections. Association of a set of these data is made with a discrete volume in three dimensions. Data used by the neutronics code associates nuclide concentrations with microscopic cross sections for calculation of macroscopic cross sections. Naturally an exposure calculation used with a neutronics code would have to be entirely consistent regarding data association, details of the modeling, and instruction interpretation. Typically fine-scale details, such as of fuel plates and pins, have been eliminated by homogenization. A second level of representation is, however, often allowed, and this is called a subzone representation here. That is, there may be nuclides assigned directly to zones along with a volume fraction, and there also may be one or more subzones contained in each zone having associated volume fractions. The neutronics code sums all contributions when macroscopic cross sections are generated and then does not use the finer detail in solving a neutronics problem. Exposure must, however, be done at both the zone and the subzone levels when the latter modeling is used.

The "subzone" modeling bears explanation. Consider a pebble-bed reactor, the fuel embedded in a 2.5-cm-radius sphere with a 0.5-cm graphite shell. With multiple pebble passes, the history of the traverse of a pebble involves a first pass, a second pass, etc. Thus at any location on a relatively fine scale, for  $N$  passes there are  $N$  pebbles of different ages, different times of exposure. It would be impractical to represent the flux spectrum in each pebble for more than two million pebbles. Also the randomness of pebble locations makes explicit representation impractical. Instead, the appropriate nuclide data are volume weighted over discrete zones for the neutronics calculation. The exposure calculation, however, follows the history of representative pebbles through the reactor, one for each pass for each discrete zone, thereby accounting directly for the effects of exposure.

Alternatively the "subzone" modeling capability may be used to associate a single set of nuclide concentrations with a zone location. Then repositioning and refueling is done on this subzone basis, and cross-section association may be with the material (subzone) rather than with the position (zone).

## NUCLIDE CHAINS FOR REACTOR CORE ANALYSIS AND NUCLIDE IMPORTANCE

Only a few nuclides play a significant role in the performance of a reactor core in the sense of having much effect on the gross neutron accounting. Here the actinides and fission products will be considered but not the structure, moderator, coolant, reflector, control, or poisons requiring specific attention to the situation at hand. Note that if fuel were used in the form of enriched  $\text{UO}_2$  or fissile material mixed in ThC, or if there is contamination, other nuclides would be involved.

The key actinide chain relationships are shown in Fig. 2. Often  $^{238}\text{Np}$ ,  $^{238}\text{Pu}$ ,  $^{230}\text{Th}$ ,  $^{231}\text{Pa}$ ,  $^{232}\text{U}$ , and  $^{228}\text{Th}$  nuclides would not be included since they are needed only for special purposes. Dropping these reduces the number in the set from 22 to 16, and if no thorium is involved there would be only 13 including  $^{234}\text{U}$ . With plutonium recycle, a few higher actinides could be of interest. The decay of  $^{241}\text{Pu}$  is a small effect, while holdup of fuel as  $^{233}\text{Pa}$  is a significant effect. Short half-life intermediates are ignored. The fact that a neutron capture in  $^{238}\text{U}$  produces  $^{239}\text{U}$  is of no interest even though a large fraction of the neutrons in a reactor core are captured in  $^{238}\text{U}$  producing  $^{239}\text{U}$ . Since the half-life of  $^{239}\text{U}$  is relatively short and the cross section for nuclear reaction is relatively small, its production may be ignored. The decay product  $^{239}\text{Pu}$  is another matter, however, as its role as nuclear fuel is quite important.

The fraction neutron absorptions at the end of cycle before refueling are shown in Table 4 for a water reactor. The absorption rate indicates reactivity importance with consideration of the amount of the material calculated with the ORIGEN-S code.<sup>13</sup> The fraction absorption drops below 1% for the seventh nuclide (in order of absorption importance), below 0.1% for the twelfth one, and below 0.01% for the sixteenth.

The use of first-order perturbation theory allows reactivity importance to be calculated with regular flux, adjoint weighting. Data are shown in Table 5 for a high-temperature thermal gas-cooled core with fully enriched fuel. The basis is a concentration increase of 1 atom/barn-cm. It may be noted that a fertile nuclide has a large negative reactivity importance. Increasing its concentration decreases the multiplication. However, fertile material is needed to generate fissile material and hence has a worth. More comprehensive importance data would consider the time effects and show relative merits of altering controllables such as the feed composition and the exposure time. Accounting for all of the contributions to some figure of merit is a challenge. Shown are the reactivity worths of the fissile nuclides in decreasing the order of  $^{241}\text{Pu}$ ,  $^{239}\text{Pu}$ ,  $^{233}\text{U}$  and  $^{235}\text{U}$ , the large thermal cross sections of the fissile plutonium nuclides enhancing importance. Shown also are effective (one group) values of  $\eta = \nu\sigma_f/\sigma_a$  appropriately weighted over the energy spectrum indicating the importance of an absorption to the neutron economy. The preference for  $^{233}\text{U}$  fuel is indicated by the eta data.

A reasonable representation of the fission products is shown in Fig. 3 using 29 nuclides including two lumped ones to account for the effects of all others (more than 2000) not treated.  $^{135}\text{I}$  is included to allow treatment of the period after a shutdown (xenon override and long-time reactivity gain), even though the local equilibrium  $^{135}\text{Xe}$  concentration may be calculated. Some elaboration of the source to  $^{149}\text{Sn}$  is also included since it accumulates after a shutdown and requires override. A very simple modeling of the fission products may, however, prove adequate in a specific application using appropriately evaluated data.

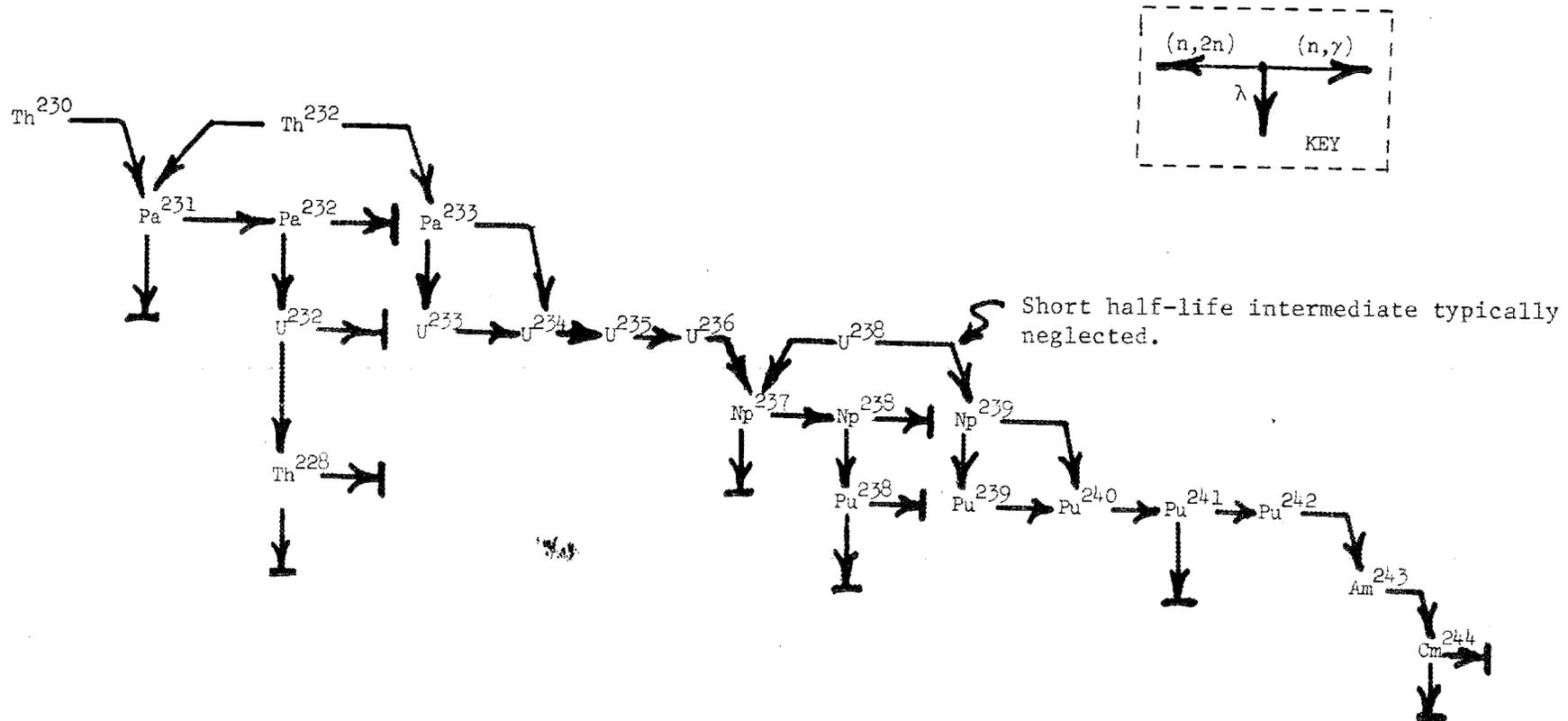


Fig. 2. Actinide nuclide chains.

**Table 4. Importance of the actinides**

Nuclide	Fraction neutron absorptions
<sup>238</sup> U	.288
<sup>239</sup> Pu	.264
<sup>235</sup> U	.145
<sup>240</sup> Pu	.0651
<sup>241</sup> Pu	.0513
<sup>236</sup> U	.0119
<sup>237</sup> Np	.0057
<sup>242</sup> Pu	.00498
<sup>238</sup> Pu	.00203
<sup>243</sup> Am	.00168
<sup>234</sup> U	.0011
<sup>239</sup> Np	.000456
<sup>244</sup> Cm	.000209
<sup>242m</sup> Am	.000159
<sup>243</sup> Cm	.0001
<sup>238</sup> Np	.0000492
<sup>242</sup> Cm	.000072
<sup>242</sup> Am	.0000463
<sup>243</sup> Cm	.0000328
<sup>237</sup> U	.000013
<sup>246</sup> Cm	.00000265
<sup>244</sup> Am	.00000181
<sup>233</sup> U	.00000111
<sup>247</sup> Cm	.000000515
<sup>230</sup> Th	.000000114
<sup>243</sup> Pu	.00000011
<sup>231</sup> Pa	.0000000515
<sup>232</sup> U	.0000000286
<sup>236</sup> Pu	.0000000231
<sup>248</sup> Cm	.00000000314
<sup>232</sup> Th	.00000000263
<sup>233</sup> Pa	.00000000179
<sup>249</sup> Bk	.00000000077
<sup>250</sup> Cf	.000000000464
<sup>251</sup> Cf	.000000000296
<sup>249</sup> Cf	.000000000177
<sup>228</sup> Th	.000000000048
<sup>236</sup> Np	.00000000000548
<sup>252</sup> Cf	.00000000000202
<sup>229</sup> Th	.00000000000107
<sup>250</sup> Bk	.000000000000901
<sup>233</sup> Th	.000000000000179
<sup>253</sup> Cf	.0000000000000291
<sup>224</sup> Ra	.0000000000000251
<sup>249</sup> Cm	.0000000000000192
<sup>253</sup> Es	.0000000000000064
<sup>244</sup> Pu	.00000000000000273
<sup>254</sup> Cf	.0000000000000018

**Table 5. Nuclide reactivity importance in a high-temperature gas-cooled reactor**

Nuclide	Reactivity importance	Effective $\eta$
$^{232}\text{Th}$	-1,501	0.0057
$^{233}\text{Pa}$	-19,500	0.0068
$^{233}\text{U}$	109,000	2.290
$^{234}\text{U}$	-19,300	0.011
$^{235}\text{U}$	83,000	1.992
$^{236}\text{U}$	-6,550	0.013
$^{238}\text{U}$	-2,550	0.016
$^{239}\text{Np}$	-14,000	0.017
$^{239}\text{Pu}$	153,000	1.785
$^{240}\text{Pu}$	-144,000	0.0032
$^{241}\text{Pu}$	201,000	2.171
$^{242}\text{Pu}$	-22,900	0.011
$^{243}\text{Am}$	-31,500	0.0056
$^{135}\text{Xe}$	$-2.2 \times 10^8$	
$^{147}\text{Pm}$	-62,900	
$^{148}\text{Pm}$	$-1.2 \times 10^6$	
$^{148\text{m}}\text{Pm}$	$-2.9 \times 10^6$	
$^{149}\text{Sm}$	$-7.0 \times 10^6$	
$^{143}\text{Nd}$	-28,000	
Slowly saturating FP	-2,720	
Non-saturating FP	-258	

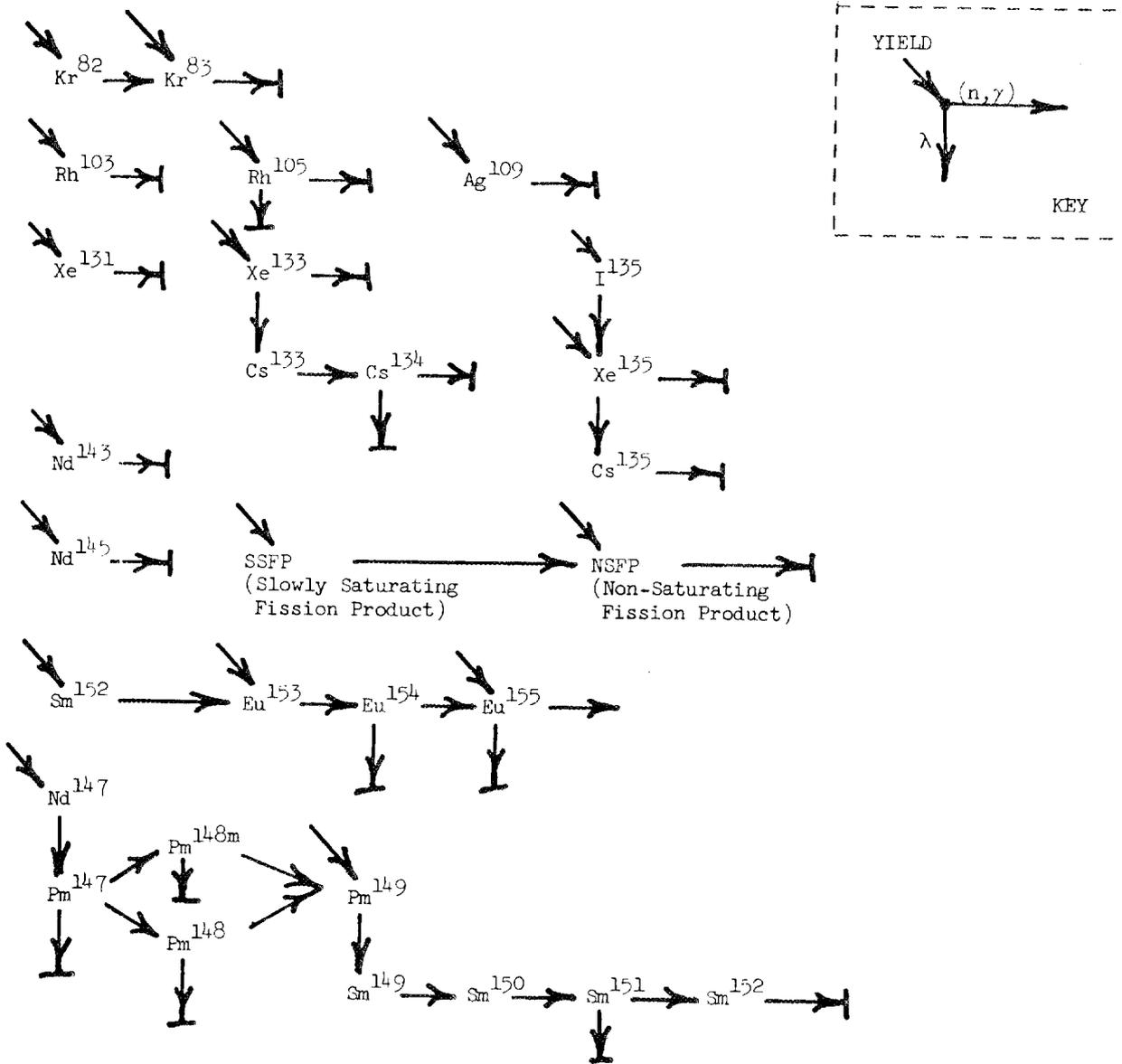


Fig. 3. Fission product nuclide chains.

Table 6 shows the importance of many of the fission products at refueling time for a pressurized water reactor core.

Table 6. Fission product importance

Nuclide	Fraction absorption rate	Nuclide	Fraction absorption rate
<sup>135</sup> Xe	.01815	<sup>97</sup> Mo	3.73-4
<sup>103</sup> Rh	.01045	<sup>107</sup> Pd	3.44-4
<sup>143</sup> Nd	.00906	<sup>157</sup> Gd	3.28-4
<sup>149</sup> Sm	.00703	<sup>106</sup> Pd	2.12-4
<sup>133</sup> Cs	.0064	<sup>113</sup> Cd	1.86-4
<sup>131</sup> Xe	.00582	<sup>144</sup> Nd	1.77-4
<sup>99</sup> Tc	.00515	<sup>148</sup> Nd	1.39-4
<sup>147</sup> Pm	.00506	<sup>98</sup> Mo	1.36-4
<sup>152</sup> Sm	.00420	<sup>102</sup> Ru	1.24-4
<sup>151</sup> Sm	.00412	<sup>127</sup> I	1.17-4
<sup>153</sup> Eu	.00309	<sup>91</sup> Zr	1.07-4
<sup>145</sup> Nd	.00265	<sup>133</sup> Xe	1.01-4
<sup>148m</sup> Pm	.00201	<sup>155</sup> Gd	1.00-4
<sup>150</sup> Sm	.00195	<sup>96</sup> Zr	1.00-4
<sup>95</sup> Mo	.00195	<sup>143</sup> Pr	9.78-5
<sup>154</sup> Eu	.00187	<sup>100</sup> Mo	9.40-5
<sup>155</sup> Eu	.00184	<sup>104</sup> Ru	8.97-5
<sup>109</sup> Ag	.00160	<sup>115</sup> In	8.71-5
<sup>129</sup> I	.00156	<sup>104</sup> Pd	8.65-5
<sup>101</sup> Ru	.0015	<sup>156</sup> Gd	8.55-5
<sup>147</sup> Sm	.00109	<sup>103</sup> Ru	7.90-5
<sup>105</sup> Pd	.00905	<sup>156</sup> Eu	7.85-5
<sup>134</sup> Cs	.00829	<sup>146</sup> Nd	6.94-5
<sup>93</sup> Zr	.000708	<sup>151</sup> Pm	6.63-5
<sup>105</sup> Rh	.00069	<sup>149</sup> Pm	6.63-5
<sup>141</sup> Pr	.000672	<sup>147</sup> Nd	6.53-5
<sup>83</sup> Kr	.000594	<sup>141</sup> Ce	6.12-5
<sup>108</sup> Pd	.000584	<sup>148</sup> Sm	6.08-5
<sup>148</sup> Pm	.000542	<sup>132</sup> Xe	5.17-5
<sup>139</sup> La	.000527	<sup>150</sup> Nd	4.90-5
<sup>135</sup> Cs	.000448	<sup>142</sup> Ce	4.87-5
		<sup>100</sup> Ru	4.62-5
		Total (all fp)	0.1083

## RESULTS OF CALCULATIONS

Results of a few calculations are presented here to support continuing discussion on methods. The microscopic nuclear data was fixed and not dependent on nuclide concentrations. The methods that have been discussed were used. The BOLD VENTURE system of codes that implement these methods was run on the ORNL IBM-3033 computers.

### A URANIUM FUEL BENCHMARK EXPOSURE PROBLEM WITH FEEDBACK

A reference problem was described by M. V. Gregory of SRL in a contribution to the ANS, Mathematics and Computation Division benchmark problem effort reference no. 15-A2. Given initial concentrations (Atoms/barn-cm) of  $^{235}\text{U}$  7.4003-05 and  $^{238}\text{U}$  6.936-03, 25 actinides plus an intermediate excited state are modeled, and 10 fission products also plus an intermediate are considered for an exposure of 50 days to a fixed fast flux of  $6.1 \times 10^{14}$  and a thermal flux of  $2.5 \times 10^{14}$  n/cm<sup>2</sup>-sec. The chain relationships are shown in Fig. 4. Note that as described there are a number of couplings which cause feedback in the problem.

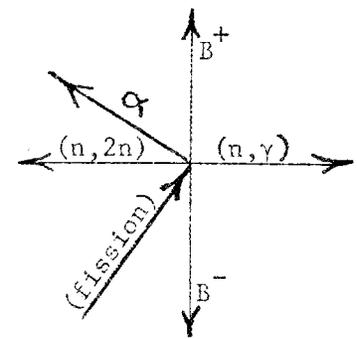
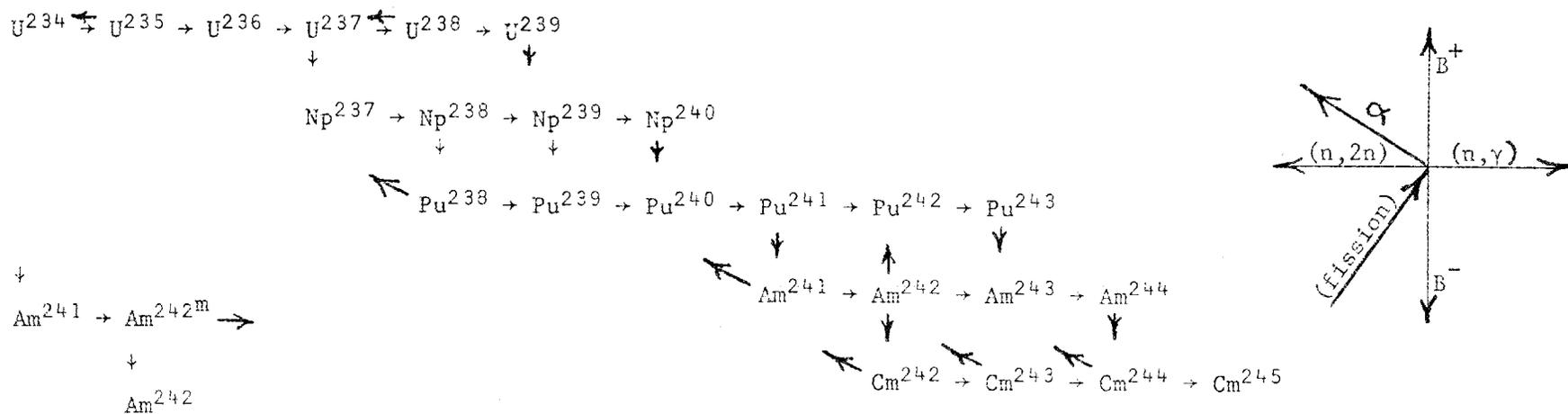
Results are shown for the matrix exponential, the average generation rate, and the explicit methods of solution in Table 7. The generation rate of fission products is taken as the average between start and end step values with the explicit chain method, which is often quite good for usual reactor evaluations but rather poor when a desired power level is not maintained, as was the case in this problem (constant flux). The error caused by this approximation is shown to decrease when the exposure period is divided into substeps. The explicit chain treatments include an elaborate representation involving 33 chains (799 chain entries) which includes the  $B^+$  decay of  $^{242}\text{Am}$  and only one  $\alpha$  decay, the feedback of  $^{238}\text{Pu} \rightarrow ^{234}\text{U}$ . A primary chain representation was also used that requires 15 chains (229 chain entries) of which four are required to treat the fission products and no  $\alpha$  decay feedback. Matrix exponential method results were also obtained by setting the nuclide concentrations equal to equilibrium values at end of step for those nuclides having high specific loss rates.

Processor times shown are totals for the exposure module use. Note that the average generation-rate method of solution is quite inefficient, and the full matrix exponential method is costly as coded. If this calculation must be done at 1,000 locations to treat a reactor core, 3.6 seconds translates into one hour computer time for a single step, generally unacceptable.

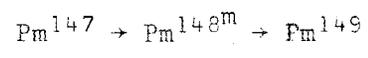
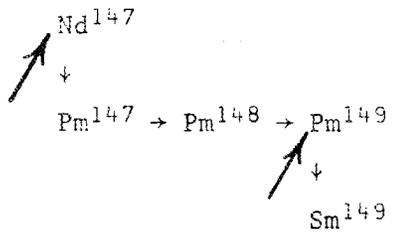
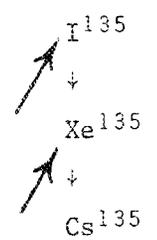
Selection of a method for general use from the data given would reduce to a choice between the explicit chain or the matrix exponential with special treatment of a few nuclides.

### A FAST REACTOR BENCHMARK CORE HISTORY PROBLEM

A reference fast-breeder reactor benchmark core-history problem was set up in an interinstallation cooperative effort sponsored by the USDOE Division of Reactor Research and Technology. A two-dimensional core sector containing a heterogeneous arrangement of hexagonal fuel and blanket elements with 30° symmetry was described in detail and four-energy-group cross sections were provided. Except for minor differences, results obtained for a 511-day exposure period by the participating installations were in substantial agreement. Of interest here are the effects of discretization on the results. Key results are shown in Table 8 using both mesh-centered and mesh-cornered meshpoint arrangements on a triangular grid. The number of meshpoints, number of time steps, and the number of substeps were increased to reduce the modeling error. Also schemes of recalculating the exposure period to improve the accounting of the charge in the neutron-flux distribution were applied, and the reported results indicate that this approach has merit.



INSET



INSET



Fig. 4. Nuclide chains for a test-sample problem.

**Table 7. End-of-step nuclide concentration obtained for the uranium fuel benchmark exposure problem**

Nuclide	Explicit chain			Matrix exponential assuming equilibrium		Matrix exponential: (570 steps)	Average generation rate			
	Elaborate chains (33) (1 step)	Primary chains (15)		(Less 8 nuclides) (2 steps)	(Less 6 nuclides) (5 steps)		(24 steps)	(100 steps)	(768 steps)	(1536 steps)
		(1 step)	(4 steps)							
<sup>238</sup> U	0.428821-09	0.428821-09	0.428820-09	0.428822-09	0.428822-09	0.428821-09	0.432797-09	0.429788-09	0.428948-09	0.428885-09
<sup>235</sup> U	0.583389-04	0.583389-04	0.583388-04	0.583390-04	0.583390-04	0.583390-04	0.583390-04	0.583390-04	0.583390-04	0.583390-04
<sup>238</sup> U	0.286057-05	0.286057-05	0.286056-05	0.286057-05	0.286057-05	0.286057-05	0.286060-05	0.286057-05	0.286057-05	0.286057-05
<sup>237</sup> U	0.356780-07	0.356780-07	0.356780-07	0.356780-07	0.356780-07	0.356780-07	0.356615-07	0.356773-07	0.356780-07	0.356780-07
<sup>236</sup> U	0.691915-02	0.691915-02	0.691914-02	0.691915-02	0.691915-02	0.691915-02	0.691915-02	0.691915-02	0.691915-02	0.691915-02
<sup>239</sup> U	0.718360-08	0.718360-08	0.718359-08	0.718359-08	0.718359-08	0.718360-08	0.718396-08	0.718368-08	0.718361-08	0.718360-08
<sup>237</sup> Np	0.104739-06	0.104739-06	0.104739-06	0.104739-06	0.104739-06	0.104739-06	0.104623-06	0.104733-06	0.104739-06	0.104739-06
<sup>238</sup> Np	0.780515-09	0.780515-09	0.780515-09	0.780515-09	0.780515-09	0.780515-09	0.776410-09	0.780286-09	0.780513-09	0.780515-09
<sup>239</sup> Np	0.102944-05	0.102944-05	0.102944-05	0.102944-05	0.102944-05	0.102944-05	0.102944-05	0.102944-05	0.102944-05	0.102944-05
<sup>240</sup> Np	0.132292-10	0.132292-10	0.132292-10	0.132292-10	0.132292-10	0.132292-10	0.132300-10	0.132294-10	0.132293-10	0.132293-10
<sup>238</sup> Pu	0.441710-08	0.441710-08	0.441710-08	0.441888-08	0.441870-08	0.441869-08	0.438590-08	0.441678-08	0.441867-08	0.441869-08
<sup>239</sup> Pu	0.105746-04	0.105746-04	0.105747-04	0.105786-04	0.105786-04	0.105747-04	0.105603-04	0.105775-04	0.105779-04	0.105741-04
<sup>240</sup> Pu	0.995920-06	0.995919-06	0.995924-06	0.996660-06	0.996660-06	0.995925-06	0.993025-06	0.996450-06	0.996522-06	0.995817-06
<sup>241</sup> Pu	0.334203-06	0.334203-06	0.334204-06	0.334611-06	0.334611-06	0.334204-06	0.332829-06	0.334508-06	0.334535-06	0.334147-06
<sup>242</sup> Pu	0.163743-07	0.163650-07	0.163650-07	0.164041-07	0.164032-07	0.163743-07	0.163166-07	0.163978-07	0.163978-07	0.163706-07
<sup>243</sup> Pu	0.136356-10	0.136279-10	0.136279-10	0.139598-10	0.139591-10	0.136356-10	0.128797-10	0.135892-10	0.136541-10	0.136321-10
<sup>241</sup> Am	0.586403-09	0.586403-09	0.586404-09	0.587413-09	0.587413-09	0.586404-09	0.584223-09	0.587227-09	0.587227-09	0.586273-09
<sup>242</sup> Am	0.520998-11	0.520998-11	0.520998-11	0.558162-11	0.521915-11	0.520998-11	0.506562-11	0.520959-11	0.521732-11	0.520876-11
<sup>243</sup> Am	0.504831-11	0.448086-11	0.503844-11	0.505884-11	0.505884-11	0.504831-11	0.503334-11	0.505735-11	0.505691-11	0.504700-11
<sup>244</sup> Am	0.457063-09	0.456782-09	0.456844-09	0.471053-09	0.471028-09	0.457063-09	0.469838-09	0.455217-09	0.457874-09	0.456923-09
<sup>244</sup> Am	0.638028-13	0.637637-13	0.637722-13	0.659185-13	0.659150-13	0.638029-13	0.597730-13	0.622171-13	0.638416-13	0.637633-13
<sup>242</sup> Cm	0.449681-10	0.449681-10	0.449681-10	0.491413-10	0.450717-10	0.449681-10	0.435962-10	0.449784-10	0.450514-10	0.449552-10
<sup>243</sup> Cm	0.950979-13	0.950979-13	0.950979-13	0.105839-12	0.953659-13	0.950978-13	0.922981-13	0.951678-13	0.953147-13	0.950664-13
<sup>244</sup> Cm	0.206748-10	0.206635-10	0.206663-10	0.215165-10	0.215151-10	0.206748-10	0.216066-10	0.206454-10	0.207691-10	0.206595-10
<sup>245</sup> Cm	0.243334-12	0.243213-12	0.243223-12	0.254910-12	0.254894-12	0.243333-12	0.258532-12	0.243081-12	0.244637-12	0.243128-12
<sup>135</sup> I	0.832002-08	0.832002-08	0.872511-08	0.883481-08	0.883481-08	0.882752-08	0.881344-08	0.882746-08	0.882832-08	0.882737-08
<sup>135</sup> Xe	0.862199-09	0.862199-09	0.904186-09	0.915555-09	0.915555-09	0.914759-09	0.913341-09	0.914414-09	0.914828-09	0.914740-09
<sup>137</sup> Cs	0.772908-07	0.772908-07	0.772677-07	0.778882-07	0.778882-07	0.771693-07	0.778205-07	0.771638-07	0.771630-07	0.771637-07
<sup>147</sup> Nd	0.119566-06	0.119566-06	0.121042-06	0.121169-06	0.121169-06	0.121156-06	0.121106-06	0.121166-06	0.121167-06	0.121155-06
<sup>147</sup> Pm	0.203043-06	0.203043-06	0.202102-06	0.201837-06	0.201837-06	0.201814-06	0.201612-06	0.201824-06	0.201833-06	0.201810-06
<sup>148</sup> Pm	0.460801-08	0.460801-08	0.457801-08	0.457096-08	0.457096-08	0.457042-08	0.455253-08	0.456989-08	0.457084-08	0.457034-08
<sup>149</sup> Pm	0.389858-08	0.389858-08	0.387359-08	0.386767-08	0.386767-08	0.386722-08	0.385151-08	0.386674-08	0.386757-08	0.386715-08
<sup>149</sup> Pm	0.193223-07	0.193223-07	0.198854-07	0.199704-07	0.199704-07	0.199682-07	0.199135-07	0.199671-07	0.199700-07	0.199678-07
<sup>149</sup> Sm	0.116169-07	0.116169-07	0.119519-07	0.122111-07	0.119790-07	0.119776-07	0.119219-07	0.119757-07	0.119787-07	0.119774-07
FP	0.145394-04	0.145394-04	0.145376-04	0.145246-04	0.145246-04	0.145227-04	0.145164-04	0.145241-04	0.145243-04	0.145224-04
IBM 360/91 cpu time (sec)	2.52	1.38	1.62	1.08	1.14	13.5	0.96	1.62	6.48	12.1

Table 8. Results for a fast-reactor core history problem

ORNL code	Points/hex (meshpoints)	Depletion zones (zones/Hex)	Neutronics time steps	Depletion substeps (flux renormalized)	k(0)	k(T) - k(0) (T = 511 days)	Fissile breeding ratio <sup>a</sup>	IBM-3033 CPU time (min)		Peak power density (Wth/cc @T = 511)	
								Base <sup>b</sup>	Total		
VALE <sup>c</sup>	Usual mesh centered finite difference										
	3 (240)	7	1	1	1.006879	-0.0043829	1.24468	0.31		416.80	
				2 <sub>g</sub>		-0.0043916	1.24476			416.89	
				10 <sub>g</sub>		-0.0043982	1.24471			416.94	
				2		-0.0044002	1.24482	0.31		416.95	
				10		-0.0043994	1.24462	0.31	0.70	416.94	
			2	2		-0.0036944	1.24764	0.48	0.83	412.34	
			6	2		-0.0032468	1.24960	0.92	1.67	409.90	
			1R <sup>e</sup>	1		-0.0030999	1.25066	0.42		408.86	
			1R <sup>f</sup>	10		-0.0031130	1.25060	0.41		409.46	
		Constrained linear finite element									
				1	10	1.005481	-0.0034419	1.25022	0.32		415.90
				1R <sup>e</sup>	1		-0.0021573	1.25576	0.44		407.41
		Usual mesh centered finite difference									
		274 (6)		1	1		-0.0040678	1.24196	0.36	1.72	404.38
				2		-0.0040854	1.24214	0.37	1.73	404.70	
				3		-0.0040836	1.24168	0.38	1.74	404.70	
				10		-0.0040849	1.24191	0.46	1.82	404.67	
				25		-0.0040839	1.24196	0.62	1.98	404.70	
				50		-0.0040851	1.24197	0.88	2.24	404.68	
				100		-0.0040863	1.24195	1.39	2.75	404.68	
VENTURE <sup>d</sup>	Usual mesh centered finite difference										
	6 (1250)	7	1	1	1.013126	-0.0073966	1.24410	0.70		414.25	
				2 <sup>g</sup>		-0.0073929	1.24415			414.40	
				10 <sup>g</sup>		-0.0073913	1.24411			414.45	
				2		-0.0073945	1.24420	0.70		414.37	
				10		-0.0073945	1.24404	0.70	1.05	414.36	
									Base <sup>b</sup>	Total	
			2	2			-0.0066709	1.24694	0.99	1.32	408.80
		6	2			-0.0062120	1.24887	1.92	2.52	405.91	

Table 8. Continued

ORNL code	Points/hex (meshpoints)	Depletion zones (zones/Hex)	Neutronics time steps	Depletion substeps (flux renormalized)	k(0)	k(T) - k(0) (T = 511 days)	Fissile breeding ratio <sup>a</sup>	IBM-3033 CPU time (min)		Peak power density (Wth/cc @T = 511)
								Base <sup>b</sup>	Total	
VALE		12 (900)		7	1	1	1.008753	-0.0051737	1.24672	
				2		-0.0051844	1.24686			415.85
				10		-0.0051841	1.24666	0.71	1.19	415.83
		52 (1)	1	2		-0.0048691	1.24458	0.74	1.20	405.74
		274 (6)	1	2		-0.0048117	1.24401	0.79	1.88	401.91
		274 (6)	6	2		-0.0037350	1.24981	2.15	5.80	396.28
VENTURE	24 (5000)	7	1	1	1.010336	-0.0059253	1.24651			415.04
				2		-0.0059306	1.24663			415.18
				10		-0.0059302	1.24644	3.40	3.82	415.18
			2	2		-0.0052115	1.24926	4.59	5.00	409.84
			6	2		-0.0047563	1.25109	8.65	9.67	407.08
VALE	48 (3481)	7	1	1	1.009221	-0.0053596	1.24739			415.20
				2		-0.0053674	1.24752			415.38
				10		-0.0053671	1.24732	3.60	4.40	415.37
		274 (6)	1	2		-0.0049692	1.24460	3.38	4.75	
		274 (6)	6	2		-0.0038974	1.25032	8.48	10.15	395.83
EXTRAPOLATIONS:										
	(∞)	7	1	2	1.00938	-0.00543	1.248			415.
	(∞)	7	(∞)	(-)		-0.00319	1.250			405.
	(∞)	274 (6)	6	2		-0.00395	1.250			396.
	(∞)	(∞)	(∞)	(∞)		-0.00374	1.252			394.

<sup>a</sup>Primitive based on mass balances requiring an estimate of the fissile consumption rate, excludes axial blanket time average value used when more than one neutronics problem was solved (note single precision).

<sup>b</sup>Base processor time for neutronics and exposure solutions only.

<sup>c</sup>30° symmetry, 1/12 of core cross-section; Δk results accurate to not more than five digits after the decimal.

<sup>d</sup>60° symmetry, parallelogram 1/6 core cross-section (less than half of the points are active and actual problem treated was 1.346 times as large as necessary, but inactive points have little cost penalty).

<sup>e</sup>Exposure for the full period done in one step, then redepletion done in one step using the average of the start and end flux data.

<sup>f</sup>Same as *e* except that the final redepletion was done in ten steps using a linear interpolation of the flux in time.

<sup>g</sup>Renormalization of the flux at the end of each step to effect the desired power (no anticipation of the need for further compensation).

It is noted that modeling of a fast breeder core usually presents no major challenge. The neutronics problems are easier to solve than for thermal-reactor problems, and even the heterogeneous arrangement of fuel and fertile elements presented no major challenge. Considerable dependence is, however, shown of the swing in reactivity over the exposure period on the modeling. Only modest differences in the peak-power density and the fissile breeding ratio are noted, generally even the coarsest results for these would be adequate for most purposes, especially if an estimated bias from fact were known. Such data as shown is of considerable utility in guiding the effort that goes into setting up an adequate model for core analysis. However, the data must be applicable to the situation at hand to be of much utility.

High-temperature core-modeling calculations were done for a thermal gas-cooled, graphite-moderated high-temperature core illustrated in Fig. 5. The core considered has hexagonal fuel assemblies arranged in patches of seven for common coolant orificing and removal and stacked eight high. With one-quarter annual core refueling, at any time there would be batches of material that have been resident  $n$ ,  $n + 1$ ,  $n + 2$  and  $n + 3$  years where  $n$  starts at 0 after refueling and becomes 1 just before refueling. Full-core calculations could not be justified, but a full axial traverse was needed to study heat removal and temperatures, and the individual batches of fuel would have to be modeled. A cut through the patches of four patches of assemblies is shown in Fig. 6. Note that such a cut will not model the situation very well because

1. Geometric boundaries are not regular when references from a coordinate system connecting patch centers,
2. Isolation of these pieces of patches requires the application of reflecting boundaries not quite precise,
3. The full core is not treated sacrificing modeling accuracy, and
4. Variations in fueling from one cycle to the next are ignored.

Still this is a good model for parametric studies of heat removal.

A calculation was carried out for several cycles to establish a repeating condition. Then variations were done to assess effects on the results for the next cycle. Special modeling was used for the burnable poison using two nuclides to simulate the effect of cross-section shielding (local flux suppression in lumped material) that would be realistic only if the exposure interval was subdivided into at least a few exposure periods. Results shown in Table 9 are self explanatory. The importance of effecting the desired power level (or correcting the results for the effective power level) is indicated. The problem is well behaved so that reasonably good results are obtained with a relatively coarse modeling of time. Somewhat fortuitous results are obtained with a single recalculation calculation, another repeat not showing much improvement if any. The interval is rather long and the model somewhat complicated with burnable poison and two fuel enrichment zones for a single exposure step, even with the recalculation the results indicate that redepletion can be used to advantage, although some sophistication is necessary to break up long exposure steps.

#### **PRESSURIZED WATER-REACTOR DEPLETION BENCHMARK**

A reference, pressurized-water reactor depletion problem was described by M. R. Wagner and associates.<sup>16</sup> The calculation involves two exposure cycles with refueling and repositioning of fuel assemblies. Simple two-group nuclear data were specified, cross-section changes being ignored. The initial fuel loading and refueling were specified for one-eighth core symmetry. The calculation involves the determination of the critical soluble boron concentration over the cycles with equilibrium <sup>135</sup>Xe.

ORNL-DWG 83C-19536A

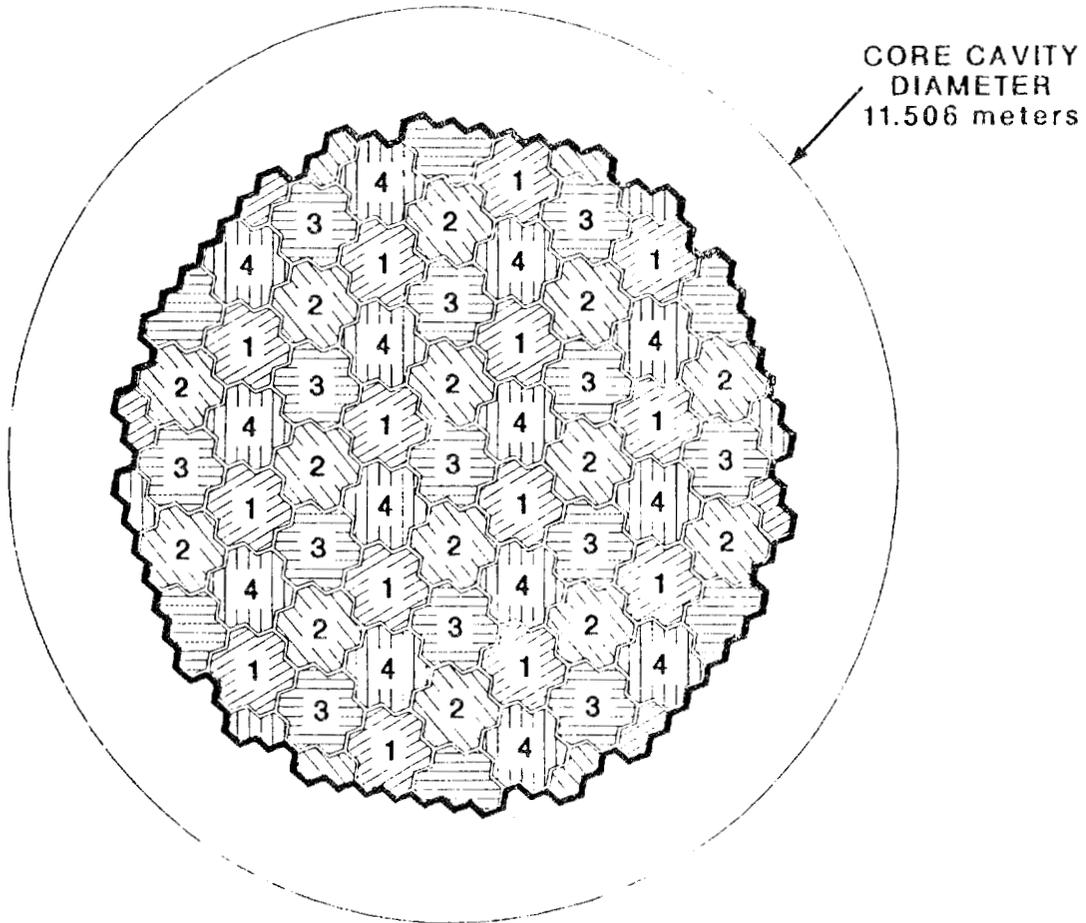


Fig. 5. Layout of patches of fuel assemblies for a high-temperature reactor core.

ORNL-DWG 83C-19866

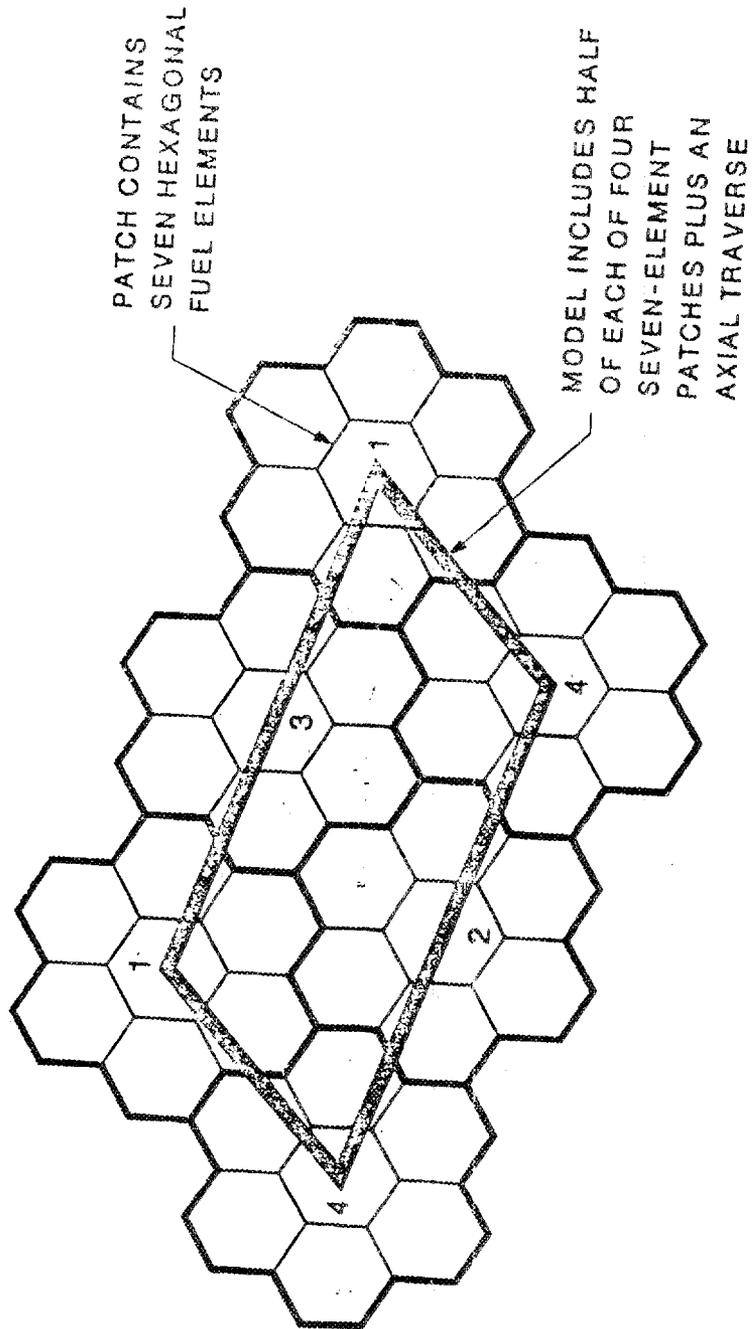


Fig. 6. Section through four patches for core modeling.

**Table 9. Calculated end-of-depletion conditions for a high-temperature gas-cooled core**

Method	Straight marchout						Re-deplete				
	1						1				
Depletion steps											
Exposure subintervals	1	2	5	6	18	36	1	5	5	5	
Count of problem sweeps	1	1	1	1	1	1	2	2	3	5	
Neutronics problems solved	2	2	2	7	7	13	3	3	4	6	
$k^a$	1.00574	1.001603	1.00191	1.00236	1.00149	1.00137	1.00133	1.00307	1.00125	1.00076	1.00074
Peak power density (W/cm <sup>3</sup> )	8.341	8.293	8.293	8.405	8.377	8.388	8.392	8.519	8.596	8.201	8.225
Fissile inventory (kg)	1885.6	18868.9	1867.9	1842.8	1838.6	1835.7	1834.7	1845.3	1839.6	1836.1	1835.8
Peak fuel temperature (°C)	913.9	918.3	918.4	915.5	916.7	917.4	917.6	913.0	913.1	917.7	917.2
Relative energy extracted <sup>b</sup>	0.94603	0.99931	1.00004	0.98876	1.00000	1.00001	0.99403	1.00014	1.00016	1.00016	1.00016
Computer processor time (min)	5.3	4.6	5.5	13.7	10.2	14.5	6.0	6.2	7.6	11.6	
Local cost (\$)	13.9	11.8	14.3	36.2	27.0	39.4	15.3	15.7	19.3	29.0	

<sup>a</sup>The answer for  $k$  to this problem is not known; it is unlikely to be unity.

<sup>b</sup>To Calculate this apparent value, the end-point values of the substeps are simply averaged; this would be precise only if the power level varied linearly within each substep. Note that a high fissile inventory usually indicates inadequate energy extraction and produces a high value of  $k$ .

The end-of-cycle is defined as that time when the soluble boron concentration goes to zero. Results of quarter-core, two-dimensional calculations are shown in Table 10. Care was taken in these calculations to effect the desired power level by adjusting the flux level during the exposure periods. Of special interest is the effect of discretization on the results. (Of interest is the trend in such analysis toward the use of nodal neutronics methods and the impact from the need to account for spatial variation in the effect of exposure to model the consequence of reorientation of fuel assemblies on the power density distribution.)

### CONTINUOUS FUELING CALCULATION

Continuous fueling of a nuclear-reactor core is attractive to achieve the best possible neutron economy and to effect a high availability maximizing the energy output. Special capability is needed for effective analysis of the effects of the variables on the performance. Information is presented here about calculations for a 1170-MWth pebble-bed core utilizing thorium. The annular core with a central concrete plug and reflector stands 7.5 meters high and contains over  $10^6$  fueled pebbles of 6 cm diameter packed randomly and recycled for five passes before being discarded. The steady state associated with continuous operation and continuous feed of a set composition is resolved by a direct iteration process. The necessary feed composition of fully enriched uranium, the distribution of materials in the core, and the neutron flux distribution are resolved for the critical equilibrium state. The exposure of materials is calculated by following representative paths of the pebbles.

Results of two-dimensional calculations are shown in Table 11 for a coarse model and also for a more detailed model. For the more detailed model, the meshspacing was halved (four times as many meshpoints) and the number of exposure zones was doubled. The discretization errors are not large but yet are significant.

A point to be made here is that the analyst always works with data that is less than ideal. Some results may be accurate while others are quite inaccurate. Modeling effects cannot be ignored. Error extraction is complicated and quite generally special calculations are necessary to guide effort. But, for most effort, we rely on the best estimate possible at a reasonable investment considering the situation and the importance of the information to be generated. Some cancellation of error is anticipated from the various sources.

Given the results in Table 11, what is the best estimate of the required fissile feed rate? Simple extrapolation changes the reference best calculation result from 1.0895-kg-per-full-power day to 1.0858, a modest change. For most purposes, the result obtained with the coarse model, only 1.4% higher, would be quite adequate. However in comparative evaluation the effects of changes may be of more importance than absolute values, for example, effects of parameter changes. The modeling needs to be tailored to effect accurate differences.

A calculation that involves the influence of time requires modeling the exposure effects. Typically, volumes of selected size are represented wherein the contents are assumed to be homogeneous, and the time effects are calculated on the basis of these average conditions. The analyst must choose a discretization, and the tendency is often to use a fine instead of a coarse representation (within cost constraints), unless definitive information about the situation under study is readily available. There is the penalty of increasing cost with increasing fineness (used to effect increasing accuracy of such generated information as the peak power density).

Table 10. PWR core benchmark problem results (quarter core)

Case	101	103	162	204	304	315	404	473	415
Exposure zones	31	31	31	102	397	397	1,566	1,566	1,566
Meshpoints	81	1,156	1,156	4,624	4,624	18,496	4,624	4,624	18,496
Points/exposure zone	1.16	16	16	16	4	16	1	1	16
Points/fuel assembly	1.16	16	16	64	64	256	64	64	256
Model in time	Marchout	Marchout	Redeplete	Marchout	Marchout	Marchout	Marchout	Redeplete	Marchout
Steps in time	(4,3)	(4,3)	2(2,2)	(4,3)	(4,3)	(8,6)	(4,3)	2(3,3)	(8,6)
Neutronics problems solved	16	16	12	16	16	23	16	16	23
First cycle time (days)	420.41	390.57	390.44	383.35	382.12	382.01	381.80	382.23	381.65
Second cycle time (days)	271.50	265.99	263.64	264.53	264.31	263.06	264.25	261.79	263.02
Peak power density (W/cm <sup>3</sup> ), average 93									
First cycle start	148.82	118.95	119.34	117.76	122.29	126.10	122.36	122.44	126.11
First cycle end	103.22	115.46	113.50	116.08	114.74	117.51	113.64	112.62	116.19
Second cycle start	229.22	165.19	170.07	149.56	147.72	145.08	147.42	149.09	144.72
Second cycle end	128.86	125.03	137.32	125.00	124.30	124.52	124.27	124.36	124.36
Fissile Loading (kg), initial 1.68746; 0.77200 added on refueling									
First cycle end	1.14725	1.18692	1.18988	1.19634	1.19941	1.19979	1.19806	1.19770	1.19997
Second cycle start	1.58461	1.62321	1.61987	1.63082	1.63210	1.63293	1.63232	1.63109	1.63320
Second cycle end	1.22998	1.28126	1.28036	1.29146	1.29298	1.29506	1.29333	1.29402	1.29540
Initial soluble boron (ppm)									
Rods in, no Xe	1021.2	554.1		537.6	537.5	531.9	537.5		532.2
Rods out, no Xe	1419.7	1287.6		1280.7	1280.7	1278.6	1280.8		1278.6
Rods out, with Xe	1155.8	1038.9	1048.6	1041.6	1041.4	1039.4	1041.4	1041.3	1039.4
Conditions at the end of the first cycle before refueling, no Xe									
Soluble boron (ppm)	248.2	248.1		247.5	247.7	247.9	247.7		248.0
k, rods in	0.94903	0.92891		0.92645	0.92637	0.92562	0.92637		0.92561
Conditions after refueling, soluble boron (ppm)									
Rods in, no Xe	1268.4	598.8		548.5	550.5	532.8	551.0		533.6
Rods out, no Xe	1560.7	1268.0		1253.5	1266.2	1262.1	1267.0		1262.9
Rods out, with Xe	1232.1	979.4	972.4	977.8	980.3	976.8	980.9	976.7	977.6
Computer time (min)	1.2	3.8	2.8	12.8	13.7	99.8	16.2	18.8	99.1

**Table 11. Effect of modeling on the calculated performance of a continuously fueled reactor core**

Meshpoints	3,294	13,176
Depletion zones	60	120
Fissile loading (kg)	979.5	968.7
Fissile feed (kg/FD Day)	1.1007	1.0895
Fissile discharge (kg/FP Day)	0.4746	0.4699
Fissile conversion ratio	0.591	0.592
Peak power density (W/cm <sup>2</sup> )	10.54	11.04
Peak reflector flux (n/cm <sup>2</sup> -sec > 0.18 MeV)	3.16 + 13	3.47 + 13
Coolant pressure drop (atm)	0.462	0.462
Temperatures (°C)		
Peak coolant outlet	834	842
Peak pebble surface	838	846
Average fuel	632	631
Effective fuel	582	584
Peak fuel	856	869
Fraction fuel > 800°C	0.0561	0.0648

The continuously fueled core without external recycle is interesting to study regarding the fineness of the degree of modeling exposure effects. Affects that would enter most problems are avoided here by solving directly for only the steady state, continuously fueled equilibrium core condition. Thus, there is a single problem to be solved for each set of specifications, albeit a rather complicated one since core conditions depend on exposure effects that are accurately resolved only when the core neutron flux distribution has been solved. An iteration process is used to determine the feed composition that effects a steady state neutron flux distribution, involving successive neutronics (based on the current estimate of nuclide densities) and exposure (based on the current estimates of the feed and neutron flux distribution). The approximate solution does depend to some extent on the method and the approach to the result. Well converged solutions are needed to show the effects of interest. The dependence of the results on the number of exposure zones is to be established. It is noted that the average nuclide densities in a zone are calculated by the method in use simply as the average of the material entering and that leaving, and this loses accuracy with large changes. An independent variable of interest is the number of pebble passes; the pebbles are recycled an arbitrarily specified number of times (treated ideally) before discharge. One effect of increased recycle is to shift the low-exposed fuel away from the inlet effecting a more homogeneous core. Thus, one might expect fewer axial zones to be required as the number of pebble passes is increased. To allow following the nuclide concentrations the number of different sets of these carried is the product of the number of axial zones with the number of pebble passes. These problems are one-dimensional rather than the two or three typical of usual analysis for simplicity and to hold down costs. The number of meshpoints was fixed with 64 in the fueled core.

Results of calculations are shown in Table 12. The effect of the number of axial zones on the results is displayed for a variety of pebble passes. The neutronics and the thermal hydraulics calculations use the same mesh, and for the latter the pointwise heat source was made available as calculated without any mesh changes. A value for the multiplication factor,  $k$ , is reported that required a special neutronics calculation done at the end (a composition adjustment is involved in the global solution iteration process); this  $k$  should be unity, so variation from unity indicates some inaccuracy in the results. Only a reasonable number of digits are shown in the results somewhat constraining what can be done in the way of numerical analysis, yet what is shown should, of course, be significant.

**Table 12. The effect on the calculated performance of a pebble bed reactor core of the number of axial exposure zones**

Pebble passes <sup>a</sup>	1	1	1	1	1	1	2	2	4	4	4	8	8	16	16	16	16
Axial zones	1	2	4	8	16	32	4	16	2	8	16	4	16	1	2	4	16
Exposure compositions <sup>b</sup>	1	2	4	8	16	32	8	32	8	32	64	32	128	16	32	64	256
<i>k</i>	1.0003	1.0006	1.0000	1.0002	0.9999	0.9999	1.0007	1.0001	1.0001	1.0011	0.9994	0.9998	0.9999	—	0.9998	1.0003	1.0005
Fissile feed (kg/D)	0.704	0.759	0.837	0.875	0.885	0.886	0.854	0.867	0.834	0.856	0.856	0.847	0.850	0.842	0.843	0.847	0.848
Fissile inventory (kg)	437.4	432.1	442.1	451.0	452.8	453.0	457.7	462.1	456.5	464.2	463.0	461.7	462.9	461.2	461.0	462.4	463.1
Peak power density (W/cm <sup>3</sup> )																	
Zone level	5.159	7.471	9.594	9.767	9.507	9.265	7.244	6.624	5.887	5.817	5.772	5.370	5.400	5.154	5.266	5.209	5.239
Pebble (zone) level	6.691	10.65	14.66	15.37	15.14	15.11	12.33	11.97	10.16	11.30	11.33	10.58	11.04	8.635	9.411	10.79	10.04
Fissile conversion ratio	0.765	0.753	0.732	0.727	0.725	0.724	0.740	0.736	0.750	0.742	0.741	0.746	0.745	0.748	0.748	0.747	0.746
Core pressure drop (atm)	0.459	0.509	0.523	0.518	0.516	0.515	0.500	0.495	0.481	0.485	0.485	0.475	0.477	0.459	0.465	0.468	0.470
Temperatures (°C), coolant downflow, 300°C inlet, 850°C outlet																	
Peak fuel	659.8	885.4	860.8	861.0	862.8	862.6	864.1	869.6	848.5	871.7	872.9	867.5	874.5	658.2	825.4	869.4	877.1
Effective fuel	625.7	642.1	652.0	645.5	642.8	642.0	633.2	630.2	625.0	627.4	625.5	625.4	625.8	623.7	622.4	625.1	625.2
Fraction fuel																	
>850°C	0	0.175	0.113	0.116	0.121	0.121	0.097	0.109	—	0.096	0.100	0.085	0.100	0	0	0.083	0.099
>825°C	0	0.299	0.328	0.300	0.293	0.292	0.250	0.222	0.129	0.205	0.204	0.216	0.197	0	0	0.204	0.187

<sup>a</sup>Each value of the number of pebble passes represents a different situation, the variable within this testing being the number of axial zones; the accuracy of the solution is indicated by *k* which is not given when iterate results were extrapolated.

<sup>b</sup>This is half of the number of data points used to estimate fuel temperature distributions, average and extreme conditions were determined at each of this many sites.

A result such as the fraction of the fuel above a reference temperature has a statistical nature requiring a reasonable number of data points to produce a reasonable result. The extraction of such temperature information is often done in such a way as to be conservative considering that simple sampling would not produce extremes.

As could be expected, the modeling requirements depend on the nature of the problem, and the importance of the specific results desired. Increasing the number of pebble passes tends toward homogenization of the core contents reducing the need for great detail in the axial variation in the nuclide concentrations. Still axial detail is needed to allow detailing the fuel temperature distribution. It may be noted that information such as fuel temperature distributions are somewhat special, being typical of project needs that require an investment in methods development and implementation to satisfy the needs with special results.

### SHUTDOWN REACTIVITY

Shown in Table 13 are reactivity results obtained for the period following shutdown of a high-temperature, gas-cooled, graphite-moderated core using fully enriched uranium fuel with thorium. (These results are for a hot core, excluding the cold shutdown reactivity increase of about 0.035  $\Delta k/k$ .) Making up the  $\Delta k/k$  of 0.060 are the contributions from  $^{135}\text{Xe}$  decay of 0.022 and  $^{149}\text{Sm}$  generation of  $-0.005$ , the remainder of 0.043 being associated with decay of  $^{233}\text{Pa}$  eliminating its neutron absorption (0.008), and the remainder coming from the net of fission and absorption in the fissile decay product  $^{233}\text{U}$ .

Table 13. After-shutdown reactivity history HTR core

Days after shutdown	k	$\Delta k/k$
Reference	0.	1.0
	0.5	0.9438
	1.	0.9689
	2.5	1.0181
	5.	1.0236
	10.	1.0257
	25.	1.0354
	50.	1.0459
	100.	1.0548
	250.	1.0596
	500.	1.0619

## REACTOR HISTORY

A reactor-operating history of 30 years was calculated with the code PREMORÉ<sup>17</sup> applying a simple geometric model and representing regular refueling of one-fourth of the core each time. Since the compacted results of such a calculation contain so much information, they are presented in Table 14 as the calculation of a thermal, gas-cooled, graphite-moderated reactor. The results of calculations are shown for the operating period following start up and after each refueling indicating key nuclear reaction information and an economic analysis for each cycle between fuelings. At the end the operating history is summarized and additional economic information is presented.

These results are hopefully self-explanatory. The use of <sup>232</sup>Th is considered to generate attractive <sup>233</sup>U fuel using highly enriched <sup>235</sup>U feed. To effect reasonable neutron accounting a loss fraction is specified that would be determined with more elaborate core model. It may be noted that nuclide importance results are reported; these are of reactivity importance for the neutronics problem, <sup>232</sup>Th having a large negative value that does not reflect its contribution in time. The calculational procedure allows modeling fixed fuel (critical system at the time of refueling) or moving fuel (critical on the average), and special economic analysis is done at the end in the case of continuous fueling. Note also that the costs are somewhat sensitive to the economical modeling and the interest rate.

Table 14. Reactor history calculation

POINT REACTOR EXPOSURE MODEL CALCULATION (2- GROUP) CODE PREMOR, ORNL VERSION 1, 3/78

BASE DATA FOR NUCLIDES

PEBBLE BED REACTOR DATA, C/HM 250, SIG11,21 .0017684 LATE 77

NUCLIDE	A	DECAY	W/FISS	FAST SIG-A	ALPHA	ETA	THERMAL SIG-A	ALPHA	ETA	*/GM
1	Tl-232	232.1 0.0	3.12000E-11	2.42500	223.51846	0.01043	2.98100	0.0	3.0	0.0400
2	Pa-233	233.1 2.93000E-07	3.13000E-11	20.57001	137.04697	0.01967	58.86000	0.0	3.0	60.0000
3	U-233	233.1 0.0	3.13000E-11	30.23000	0.21552	2.06084	266.89990	0.13240	2.27042	60.0000
4	U-234	234.1 0.0	3.15000E-11	33.12000	137.00000	0.01947	35.18000	0.0	3.0	-10.0000
5	U-235	235.1 0.0	3.17000E-11	19.50999	0.61632	1.51305	256.39990	0.18745	2.34617	50.0000
6	U-236	236.1 0.0	3.18000E-11	16.32001	180.33333	0.01473	2.64800	0.0	3.0	-20.0000
7	U-238	238.1 0.0	3.24000E-11	6.27500	153.16953	0.01761	1.18200	0.0	3.0	0.0
8	Np-239	239.1 3.41000E-06	3.20000E-11	25.72000	97.88460	0.02716	22.89999	0.0	3.0	30.0000
9	Pu-239	239.1 0.0	3.27000E-11	22.12000	0.71847	1.68135	600.00000	0.60428	1.79084	30.0000
10	Pu-240	240.1 0.0	3.29000E-11	9.40400	23.74736	0.12288	698.00000	3672.68433	0.00078	0.0
11	Pu-241	241.1 1.68000E-09	3.30000E-11	35.21001	0.21546	2.41485	750.00000	0.36116	2.15404	30.0000
12	Pu-242	242.1 0.0	3.31000E-11	54.30000	235.08696	0.01296	14.16000	0.0	3.0	0.0
13	Am-243	243.1 0.0	3.32000E-11	16.22000	94.41176	0.03462	126.89999	0.0	3.0	0.0
14	FIXED	12.0 0.0	0.0	0.00009	0.0	0.0	0.00200	0.0	3.0	0.0010
FISSION PRODUCTS										
15	I-135	135.0 2.87000E-05	0.0	0.0	0.0	0.0	0.0	FRACTION YIELD FROM U-233	U-235	0.0639
16	Xe-135	135.0 2.09000E-05	0.0	11.75000	0.0	0.0	108000.00	0.05630	0.06170	0.0027
17	Pm-147	147.0 8.29000E-09	0.0	114.00000	0.0	0.0	100.00000	0.01930	0.02360	0.0210
18	Pm-148	148.0 1.49000E-06	0.0	2760.00000	0.0	0.0	636.00000	0.0	0.0	0.0
19	Pm-148M	148.0 1.98000E-07	0.0	1660.00000	0.0	0.0	11400.0000	0.0	0.0	0.0
20	Pm-149	149.0 3.63000E-06	0.0	0.0	0.0	0.0	0.0	0.00770	0.01130	0.0130
21	Sm-149	149.0 0.0	0.0	49.89999	0.0	0.0	34400.0000	0.0	0.0	0.0
22	Nd-143	143.0 0.0	0.0	3.91600	0.0	0.0	131.10001	0.05990	0.06000	0.0460
23	Fp1	117.0 0.0	0.0	3.98200	0.0	0.0	6.10000	1.02000	1.08000	1.2000
24	Fp2	117.0 0.0	0.0	0.43600	0.0	0.0	0.47100	3.10000	3.30000	3.8000

COST DATA, -- LEAD TIME, LAG TIME, INTEREST, FABRICATION, RECYCLE FAB, PROCESSING, THROWAWAY  
 EXTRA (2), FAB LOSS, PROC LOSS, DISCOUNT FACTOR  
 0.50000 1.00000 0.10000 880.00000 880.000001120.000001050.00000 0.0 0.0 0.30500 0.01000 0.07000

RELATIVE INVENTORY 1.0000 START AND END LOAD FACTORS 0.7500 0.5000

ENRICHMENT DATA 140.00000 88.17999 6.00000 0.00711 0.00200 0.0 0.23070



Table 14. Cont'd

CONTINUING WITH RECYCLE, CYCLE COUNT, MIDCYCLE TIME (FULL POWER YEARS) 3 2.500											
ADJUSTED INITIAL CONCENTRATIONS (SEARCH EIGENVALUE 1.94611 1.08917)											
1.827E-04	0.0	2.572E-06	2.136E-07	1.078E-05	7.842E-07	7.964E-07	0.0	5.171E-09	1.307E-09	7.568E-10	1.876E-10
1.313E-11	4.740E-02	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
DISCHARGE ACTINIDE CONCENTRATIONS, STEPS 2											
1.714E-04	3.712E-07	3.057E-06	8.117E-07	4.882E-07	1.079E-06	3.526E-07	9.505E-11	4.515E-09	1.554E-09	1.417E-09	1.597E-09
3.638E-10	4.740E-02										
REFERENCE CONDITIONS FOR THE EXPOSURE PERIOD (YRS) 1.000 NORMALLY ELECTRICAL POWER BASIS, ITERATIONS 15											
FISSILE LOADING (KGM) 3.0482E-03			FISSILE FEED 1.3016E-06 MAX POWER DENSITY 7.1838E+00								
NUCLIDE	DENSITY	GRAMS	ABSORPTION	CAPTURE	FISSION	PRODUCTION	ETA	IMPORTANCE	DECAY	KGM/MWE-YR	
TH-232	1.7416E-04	6.7124E-02	0.314494	0.313751	0.000730	0.001709	0.005433	-1.5839E+03	0.0	419.80127	
PA-233	3.8230E-07	1.4798E-04	0.009581	0.009559	0.000022	0.000060	0.006264	-2.0717E+04	0.32002	422.75635	
U-233	3.1835E-06	1.2323E-03	0.283918	0.029522	0.254386	0.636790	2.242869	1.2984E+05	0.0	1.08818	
U-234	6.5505E-07	2.5464E-04	0.015100	0.015039	0.000061	0.000164	0.010852	-2.0300E+04	0.0	240.90938	
U-235	2.1807E-06	8.5133E-04	0.178766	0.031904	0.146842	0.356987	1.996950	9.9974E+04	0.0	1.18204	
U-236	1.4673E-06	5.7526E-04	0.010416	0.010365	0.000051	0.000137	0.013138	-6.8177E+03	0.0	197.65567	
U-238	5.4296E-07	2.1468E-04	0.001508	0.001499	0.000009	0.000023	0.015435	-2.6503E+03	0.0	169.23766	
NP-239	1.7029E-10	6.7614E-08	0.000003	0.000003	0.000000	0.000000	0.016303	-1.4723E+04	0.00166	161.22743	
PU-239	9.1978E-09	3.6519E-06	0.001681	0.000636	0.001044	0.003001	1.785694	1.8625E+05	0.0	1.54056	
PU-240	2.8400E-09	1.1323E-06	0.000586	0.000585	0.000001	0.000002	0.002941	-1.5595E+05	0.0	972.75220	
PU-241	2.1775E-09	8.7179E-07	0.000504	0.000131	0.000373	0.001093	2.169442	3.2389E+05	0.00001	1.29281	
PU-242	1.4884E-09	5.9837E-07	0.000038	0.000037	0.000000	0.000000	0.010846	-2.3693E+04	0.0	270.17651	
AM-243	2.8197E-10	1.1383E-07	0.000012	0.000012	0.000000	0.000000	0.005052	-3.3874E+04	0.0	626.83374	
FIXED	4.7400E-02	9.4453E-01	0.029192	0.029192	0.0	0.0	0.0	-4.7359E-01	0.0	0.0	
I-135	2.8221E-10	6.3264E-08	0.0	0.0	0.0	0.0	0.0	0.0	0.02314	0.0	
XE-135	6.6134E-11	1.4826E-08	0.020728	0.020728	0.0	0.0	0.0	-2.3660E+08	0.00395	0.0	
PM-147	6.4844E-08	2.0711E-05	0.006214	0.006214	0.0	0.0	0.0	-6.6130E+04	0.00201	0.0	
PM-148	6.2100E-10	1.5262E-07	0.000779	0.000779	0.0	0.0	0.0	-1.2100E+06	0.00264	0.0	
PM148M	6.6272E-10	1.6779E-07	0.002698	0.002698	0.0	0.0	0.0	-3.1413E+06	0.00039	0.0	
PM-149	7.5309E-10	1.8633E-07	0.0	0.0	0.0	0.0	0.0	0.0	0.00781	0.0	
SM-149	8.1402E-10	2.0141E-07	0.008142	0.008142	0.0	0.0	0.0	-7.5553E+06	0.0	0.0	
NO-143	4.0626E-07	9.6472E-05	0.016074	0.016074	0.0	0.0	0.0	-3.0239E+04	0.0	0.0	
FP1	1.1508E-05	2.2358E-03	0.038147	0.038147	0.0	0.0	0.0	-2.8810E+03	0.0	0.0	
FP2	3.7279E-05	7.2428E-03	0.011400	0.011400	0.0	0.0	0.0	-2.7231E+02	0.0	0.0	
OTHER			0.050000								
SUM		1.0245E+00	0.999981		0.403519	0.999966	2.146568	FISSILE		1.12168	
FLUX, LOSSES, SIGA2, FLUX RATIO (2), SUM IMPORTANCE*N, MULTIPLICATION, RECIPROCAL DOUBLING TIME (YR-1), CONVERSION RATIO (2)											
1.0158E+14	3.5003E+11	2.3391E-03	1.46761	1.33663	0.21642	0.99999	-0.40459	0.63805	0.69114		
FUEL CYCLE ECONOMICS ---- POWER, VOLUME, TIME, LOAD FACTOR, INTEREST, FEED(KGM), DISCHARGE, MWT-D/KGM											
2.00000E+00	1.00000E+00	1.00000E+00	7.46525E-01	1.00000E-01	1.91747E-05	1.69403E-05	7.13857E+01				
	COST	RETURN	DIRECT	INDIRECT	TOTAL	MILL/KW-HR EL. MIDCYCLE REAL YRS 3.338630					
FABRICATION	0.967916	0.0	0.967916	0.307707	1.275623						
PROCESSING	0.0	-1.072070	1.072070	-0.322619	0.749451						
FUEL	3.814868	1.133441	2.681427	1.553862	4.235289						
SUM	4.782784	0.061371	4.721413	1.538949	6.260363	ENERGY (MWE-YR), SUM	2.00000E-06	6.00020E-06			
CYCLE, IT, K, FISS FEED, EXIT, POWER, CR, YRS, COST 3 15 1.0000 1.3016E-06 3.8000E-07 2.0001E+00 0.5381 3.3388 6.2604											
CYCLE, IT, K, FISS FEED, EXIT, POWER, CR, YRS, COST 4 17 1.0000 1.2907E-06 3.6074E-07 1.9998E+00 0.5264 4.6812 6.2562											

Table 14. Cont'd

CONTINUING WITH RECYCLE, CYCLE COUNT, MIDCYCLE TIME (FULL POWER YEARS) 10 9.500												
ADJUSTED INITIAL CONCENTRATIONS (SEARCH EIGENVALUE 1.21969 1.21800)												
1.827E-04	0.0	3.727E-06	1.413E-06	9.677E-06	2.307E-06	1.215E-06	0.0	1.111E-08	3.873E-09	3.514E-09	5.928E-09	
2.123E-09	4.740E-02	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
DISCHARGE ACTINIDE CONCENTRATIONS, STEPS 2												
1.692E-04	3.320E-07	3.419E-06	1.483E-06	7.530E-07	3.011E-06	9.951E-07	2.575E-10	1.478E-08	5.254E-09	4.910E-09	9.035E-09	
3.812E-09	4.740E-02											
REFERENCE CONDITIONS FOR THE EXPOSURE PERIOD (YRS) 1.000 NORMALLY ELECTRICAL POWER BASIS, ITERATIONS 6												
FISSILE LOADING (KGM) 3.3625E-03			FISSILE FEED 1.3066E-06 MAX POWER DENSITY 6.7396E+00									
NUCLIDE	DENSITY	GRAMS	ABSORPTION	CAPTURE	FISSION	PRDUCATION	ETA	IMPORTANCE	DECAY	KGM/MWE-YR		
TH-232	1.7417E-04	6.7127E-02	0.287722	0.287705	0.000704	0.001648	0.005727	-1.5009E+03	0.0	398.21948		
PA-233	3.4799E-07	1.3470E-04	0.007796	0.007776	0.000019	0.000053	0.006758	-1.9453E+04	0.29412	391.83496		
U-233	3.7056E-06	1.4344E-03	0.289012	0.030382	0.258621	0.647397	2.240037	1.0940E+05	0.0	1.08957		
U-234	1.4699E-06	5.7142E-04	0.031125	0.030994	0.000132	0.000355	0.011393	-1.9263E+04	0.0	229.46611		
U-235	2.4092E-06	9.4055E-04	0.171920	0.031065	0.140836	0.342402	1.991639	8.2953E+04	0.0	1.18525		
U-236	3.1041E-06	1.2170E-03	0.021005	0.020901	0.000105	0.000279	0.013293	-6.5513E+03	0.0	195.35979		
U-238	1.0899E-06	4.3092E-04	0.002880	0.002864	0.000017	0.000045	0.015642	-2.5454E+03	0.0	166.99451		
NP-239	3.1363E-10	1.2453E-07	0.000005	0.000005	0.000000	0.000000	0.017034	-1.3994E+04	0.00309	154.31039		
PU-239	1.9354E-08	7.6843E-06	0.003061	0.001160	0.001902	0.005465	1.785108	1.5272E+05	0.0	1.54111		
PU-240	6.3501E-09	2.5318E-06	0.001130	0.001129	0.000001	0.000004	0.003196	-1.4417E+05	0.0	896.40210		
PU-241	5.3248E-09	2.1318E-06	0.001068	0.000277	0.000791	0.002319	2.171171	2.7055E+05	0.00003	1.29179		
PU-242	7.5887E-09	3.0509E-06	0.000181	0.000180	0.000001	0.000002	0.011040	-2.2916E+04	0.0	265.44360		
AM-243	3.4261E-09	1.3831E-06	0.000129	0.000129	0.000000	0.000001	0.005561	-3.1533E+04	0.0	569.38433		
FIXED	4.7400E-02	9.4453E-01	0.025306	0.025306	0.0	0.0	0.0	-4.3884E-01	0.0	0.0		
I-135	2.8231E-10	6.3288E-08	0.0	0.0	0.0	0.0	0.0	0.0	0.00237	0.0		
XE-135	7.4667E-11	1.6739E-08	0.020148	0.020148	0.0	0.0	0.0	-2.1851E+08	0.00450	0.0		
PM-147	9.0731E-08	2.2148E-05	0.006136	0.006136	0.0	0.0	0.0	-6.2881E+04	0.00217	0.0		
PM-148	6.1629E-10	1.5146E-07	0.000734	0.000734	0.0	0.0	0.0	-1.1612E+06	0.00265	0.0		
PM-148M	7.4515E-10	1.8313E-07	0.002585	0.002585	0.0	0.0	0.0	-2.9275E+06	0.00043	0.0		
PM-149	7.3045E-10	1.8073E-07	0.0	0.0	0.0	0.0	0.0	0.0	0.00765	0.0		
SM-149	9.0535E-10	2.2401E-07	0.007798	0.007798	0.0	0.0	0.0	-6.9785E+06	0.0	0.0		
ND-143	4.8002E-07	1.1399E-04	0.016426	0.016426	0.0	0.0	0.0	-2.7989E+04	0.0	0.0		
FP1	1.3703E-05	2.6623E-03	0.041298	0.041298	0.0	0.0	0.0	-2.7239E+03	0.0	0.0		
FP2	4.4661E-05	8.6772E-03	0.012540	0.012540	0.0	0.0	0.0	-2.5841E+02	0.0	0.0		
OTHER			0.050000									
SUM		1.0279E+00	1.000006		0.403127	0.999968	2.145059	FISSILE		1.12326		
FLUX, LOSSES, SIGA2, FLUX RATIO (2), SUM IMPORTANCE*N, MULTIPLICATION, RECIPROCAL DOUBLING TIME (YR-1), CONVERSION RATIO (2)												
8.6613E+13	3.4666E+11	2.6203E-03	1.63928	1.49731	0.17452	0.99999	-0.37545	0.62480	0.67559			
FUEL CYCLE ECONOMICS ---- POWER, VOLUME, TIME, LOAD FACTOR, INTEREST, FEED(KGM), DISCHARGE, MWT-D/KGM												
2.0000E+00	1.0000E+00	1.0000E+00	7.02050E-01	1.0000E-01	1.94895E-05	1.71069E-05	9.36432E+01					
	COST	RETURN	DIRECT	INDIRECT	TOTAL	MILL/KW-HR EL, MIDCYCLE REAL YRS			12.948256			
FABRICATION	0.983811	0.0	0.983811	0.329453	1.313270							
PROCESSING	0.0	-1.082622	1.082622	-0.416679	0.665942							
FUEL	3.654343	1.063251	2.591092	1.632989	4.224081							
SUM	4.638153	-0.019371	4.657524	1.545768	6.203292	ENERGY (MWE-YR), SUM 2.00007E-06 1.99998E-05						
CYCLE, IT, K, FISS FEED, EXIT, POWER, CR, YRS, COST	10	6	1.0000	1.3066E-06	4.3844E-07	2.0001E+00	0.6248	12.9483	6.2033			
CYCLE, IT, K, FISS FEED, EXIT, POWER, CR, YRS, COST	11	9	1.0000	1.2976E-06	4.4448E-07	1.9999E+00	0.5251	14.3840	6.1848			
CYCLE, IT, K, FISS FEED, EXIT, POWER, CR, YRS, COST	12	6	1.0000	1.3104E-06	4.4954E-07	1.9999E+00	0.6241	15.8444	6.1578			
CYCLE, IT, K, FISS FEED, EXIT, POWER, CR, YRS, COST	13	6	1.0000	1.3169E-06	4.5342E-07	2.0001E+00	0.6230	17.3333	6.1933			
CYCLE, IT, K, FISS FEED, EXIT, POWER, CR, YRS, COST	14	6	1.0000	1.3225E-06	4.5475E-07	2.0000E+00	0.6220	18.8555	6.2319			

Table 14. Cont'd

CONTINUING WITH RECYCLE, CYCLE COUNT, MIDCYCLE TIME (FULL POWER YEARS) 20 19.500											
ADJUSTED INITIAL CONCENTRATIONS (SEARCH EIGENVALUE 1.22296 1.226721)											
1.827E-04	0.0	3.841E-06	1.721E-06	9.971E-06	3.947E-06	1.843E-06	0.0	2.169E-08	7.642E-09	7.146E-09	1.380E-08
6.972E-09	4.740E-02	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
DISCHARGE CONCENTRATIONS											
6.980E-04	1.343E-06	1.522E-05	6.845E-06	1.085E-05	1.804E-05	6.703E-06	1.884E-09	1.249E-07	4.169E-08	3.541E-08	5.894E-08
3.419E-08	1.896E-01	1.135E-09	3.169E-10	3.715E-07	2.449E-09	3.093E-09	2.904E-09	3.844E-09	1.975E-06	5.476E-05	1.780E-04
REFERENCE CONDITIONS FOR THE EXPOSURE PERIOD (YRS) 1.000 NORMALLY ELECTRICAL POWER BASIS, ITERATIONS 6											
FISSILE LOADING (KGM) 3.5445E-03				FISSILE FEED 1.3477E-06				MAX POWER DENSITY 6.6481E+00			
NUCLIDE	DENSITY	GRAMS	ABSORPTION	CAPTURE	FISSION	PRODUCTION	ETA	IMPORTANCE	DECAY	KGM/MWE-YR	
TH-232	1.7451E-04	6.7258E-02	0.276766	0.276060	0.000693	0.001622	0.005861	-1.4638E+03	0.0	389.11328	
PA-233	3.3565E-07	1.2992E-04	0.007142	0.007123	0.000018	0.000050	0.006991	-1.8858E+04	0.28325	378.78809	
U-233	3.8054E-06	1.4730E-03	0.278958	0.029480	0.249470	0.624493	2.238659	1.0091E+05	0.0	1.09025	
U-234	1.7113E-06	6.6525E-04	0.034854	0.034703	0.000151	0.000406	0.011638	-1.8798E+04	0.0	224.63762	
U-235	2.7128E-06	1.0591E-03	0.181537	0.033001	0.148517	0.361084	1.989038	7.5901E+04	0.0	1.18683	
U-236	4.5100E-06	1.7682E-03	0.029836	0.029687	0.000149	0.000399	0.013359	-6.4270E+03	0.0	194.39085	
U-238	1.6756E-06	6.6252E-04	0.004326	0.004301	0.000025	0.000068	0.015731	-2.4965E+03	0.0	166.04791	
NP-239	4.7104E-10	1.8702E-07	0.000007	0.000007	0.000000	0.000000	0.017362	-1.3666E+04	0.00463	151.39192	
PU-239	3.1223E-08	1.2397E-05	0.004619	0.001750	0.002869	0.008245	1.784819	1.3885E+05	0.0	1.54138	
PU-240	1.0423E-08	4.1557E-06	0.001731	0.001729	0.000002	0.000006	0.003322	-1.3912E+05	0.0	86.279004	
PU-241	8.8526E-09	3.5443E-06	0.001662	0.000431	0.001231	0.003609	2.172024	2.4842E+05	0.00004	1.29128	
PU-242	1.4736E-08	5.9243E-06	0.000343	0.000341	0.000001	0.000004	0.011123	-2.2463E+04	0.0	263.44653	
AM-243	8.5482E-09	3.4508E-06	0.000304	0.000303	0.000001	0.000002	0.005808	-3.0520E+04	0.0	545.14404	
FIXED	4.7400E-02	9.4453E-01	0.023683	0.023683	0.0	0.0	0.0	-4.2389E-01	0.0	0.0	
I-135	2.8377E-10	6.3616E-08	0.0	0.0	0.0	0.0	0.0	0.0	0.02345	0.0	
XE-135	7.9218E-11	1.7759E-08	0.019937	0.019937	0.0	0.0	0.0	-2.1076E+08	0.00477	0.0	
PM-147	9.2875E-08	2.2671E-05	0.006056	0.006056	0.0	0.0	0.0	-6.1417E+04	0.00222	0.0	
PM-148	6.1223E-10	1.5047E-07	0.000712	0.000712	0.0	0.0	0.0	-1.1386E+06	0.00263	0.0	
PM-148M	7.7315E-10	1.9001E-07	0.002526	0.002526	0.0	0.0	0.0	-2.8348E+06	0.00044	0.0	
PM-149	7.2607E-10	1.7965E-07	0.0	0.0	0.0	0.0	0.0	0.0	0.00759	0.0	
SM-149	9.6105E-10	2.3779E-07	0.007722	0.007722	0.0	0.0	0.0	-6.7314E+06	0.0	0.0	
ND-143	4.9368E-07	1.1723E-04	0.015793	0.015793	0.0	0.0	0.0	-2.7023E+04	0.0	0.0	
FP1	1.3690E-05	2.6598E-03	0.039497	0.039497	0.0	0.0	0.0	-2.6540E+03	0.0	0.0	
FP2	4.4489E-05	8.6436E-03	0.012013	0.012013	0.0	0.0	0.0	-2.5217E+02	0.0	0.0	
OTHER			0.050000								
SUM		1.0290E+00	1.000023		0.403126	0.999987	2.136848	FISSILE		1.12727	
FLUX, LOSSES, SIG2, FLUX RATIO (2), SUM IMPORTANCE*N, MULTIPLICATION, RECIPROCAL DOUBLING TIME (YR-1), CONVERSION RATIO (2)											
8.0908E+13	3.4720E+11	2.7603E-03	1.72373	1.57731	0.15454	0.99998	-0.26934	0.61571	0.66337		
FUEL CYCLE ECONOMICS ---- POWER, VOLUME, TIME, LOAD FACTOR, INTEREST, FEED(KGM), DISCHARGE, MWT-D/KGM											
2.00001E+00	1.00000E+00	1.00000E+00	5.12265E-01	1.00000E-01	1.97864E-05	7.23034E-05	9.22355E+01				
	COST	RETURN	DIRECT	INDIRECT	TOTAL	MILL/KW-HR EL, MIDCYCLE REAL YRS 29.108322					
FABRICATION	0.998826	0.0	0.998826	0.147431	1.146257						
PROCESSING	0.0	-4.575882	4.575882	-1.797485	2.778397						
FUEL	3.575451	6.230789	-2.655338	2.975315	0.319977						
SUM	4.574276	1.654907	2.919369	1.325262	4.244631	ENERGY (MWE-YR), SUM 2.00001E-06 3.99998E-05					
CYCLE THROWAWAY COST ESTIMATE, DIRECT, TOTAL 5.64675 7.13540											
CYCLE, IT, K, FISS FEED, EXIT, POWER, CR, YRS, COST 20 6 1.0000 1.3477E-06 2.6781E-06 2.0000E+00 0.6157 29.1083 4.2446											
SUMMED FERTILE FEED, DISCHARGE, NET USAGE (KGM) 4.07496E-04 3.81025E-04 2.64710E-05											
SUMMED FISSILE FEED, MAKEUP, DISCHARGE, NET PRODUCTION (KGM) 2.78688E-05 1.99747E-05 1.10392E-05 -1.68296E-05											
FISSILE (KGM/MWE-YR), CONVERSION, AND RECIPROCAL DOUBLING TIME (YRS-1) 1.12444 0.62582 -0.11542											

Table 14. Cont'd

SUBZONE FLUX RATIOS	1.51567	1.80896	2.23155	1.33873		
SUBZONE FLUX LEVELS	8.6107E+13	7.8958E+13	7.0522E+13	9.1083E+13		
ORE (U-235 FED) INITIAL, FEED, DISCHARGE, NET (MGM)	6.627678E-07	4.152595E+00	2.546733E-06	4.152592E+00		
MAKE-UP FISSILE ASSOCIATED WITH ORE AND ORE	1.997473E-05	4.608177E-06				
FUEL COST ANALYSIS						
COST LEVELIZED OVER	20 FUEL CYCLES AT DISCOUNT FACTOR	0.0700	REAL YEARS	30.084 ENERGY (MWE-YR)	3.99998E-05	
	COST	RETURN	DIRECT	INDIRECT	TOTAL	MILL/KW-HR ELECTRIC
FABRICATION	1.121621	0.0	1.121621	0.475666	1.597287	
PROCESSING	0.0	-1.258928	1.258928	-0.348844	0.910085	
FUEL	3.896006	1.367197	2.528809	1.775968	4.304776	
SUM	5.017627	0.108269	4.909358	1.902789	6.812147	
TOTAL WITH QUARTERLY ENERGY ACCOUNTING					6.76046	
COST BY DISCOUNTING ONLY AT REFERENCE RATE					0.07000	
FABRICATION	1.121621	0.0	1.121621	0.384090	1.505712	
PROCESSING	0.0	-1.258928	1.258928	-0.153534	1.105394	
FUEL	2.874225	0.363161	2.511064	1.254655	3.765718	
SUM	3.995846	-0.895768	4.891613	1.485211	6.376824	
COST ONLY DISCOUNTING WITH QUARTERLY ENERGY ACCOUNTING					6.32844	AND AT TWICE THE RATE 7.98121
THROWAWAY COST ESTIMATE, DIRECT, TOTAL					6.19787	7.74978 TOTAL ANNUAL AND QUARTERLY ONLY DISCOUNTING, 7.53388 7.47672
THE CHANGE AND TOTAL COST FOR FIFTY PERCENT INCREASE IN UNIT COSTS						
FABRICATION	0.798643	7.610790				
PROCESSING	0.455042	7.267189				
FUEL	2.152388	8.964535				
DISTRIBUTION OF THE COSTS AFTER THE INCREASE BY FIFTY PERCENT						
	COST	RETURN	DIRECT	INDIRECT	TOTAL	MILL/KW-HR ELECTRIC
FABRICATION	1.682431	0.0	1.682431	0.713499	2.395930	
PROCESSING	0.0	-1.888392	1.888392	-0.523265	1.365127	
FUEL	5.844008	2.050796	3.793213	2.663951	6.457164	
SUM	7.526440	0.162403	7.364037	2.854104	10.218221	
ADDITIONAL CONTINUOUS FUELING CHARGES - FABRICATION DIRECT, INDIRECT, FUEL INDIPECT, TOTAL						
ONE CYCLE	0.18627	0.28750	0.32413	0.79791		
HISTORY	0.04657	0.07188	0.08103	0.19948		
COST DEPENDENCE ON INDIRECT CHARGES						
INTEREST RATE	0.0500	0.0750	0.1000	0.1250	0.1500	
TOTAL FUEL COST	5.86075	6.33645	6.81215	7.28784	7.76354	
SUMMARY OF REACTOR HISTORY, ENERGY (MWE-YR) 3.99998E-05						
PERIOD	TIME (YR)	LOAD FACTOR	FISSILE MAKEUP AND FEED AND DISCHARGE	CONVERSION	POWER	COST
1	0.66667	0.75000	2.87285E-06 2.87285E-06 5.19329E-07	0.64917	1.99996E+03	14.80127

Table 14. Cont'd

2	2.00120	0.74866	1.39773E-06	1.39773E-06	4.22856E-07	0.65085	2.00017E+00	6.47273
3	3.33883	0.74653	7.82259E-07	1.30159E-06	3.80001E-07	0.63805	2.00008E+00	6.26036
4	4.68119	0.74339	8.67830E-07	1.29069E-06	3.60736E-07	0.62635	1.99985E+00	6.25520
5	6.03017	0.73923	9.11031E-07	1.29103E-06	4.13049E-07	0.61914	1.99989E+00	6.22552
6	7.38772	0.73403	9.13711E-07	1.27445E-06	4.15151E-07	0.62520	2.00006E+00	5.16455
7	8.75594	0.72775	8.68877E-07	1.28193E-06	4.24199E-07	0.62581	1.99983E+00	6.07584
8	10.13709	0.72036	8.76582E-07	1.29173E-06	4.31822E-07	0.62600	1.99999E+00	6.09874
9	11.53362	0.71181	8.75998E-07	1.30020E-06	4.35300E-07	0.62581	1.99995E+00	6.12450
10	12.94826	0.70205	8.74784E-07	1.30661E-06	4.38442E-07	0.62480	2.00006E+00	6.20329
11	14.38403	0.69101	8.62322E-07	1.29762E-06	4.44479E-07	0.62514	1.99995E+00	6.18477
12	15.84441	0.67861	8.71921E-07	1.31036E-06	4.49536E-07	0.62407	1.99994E+00	6.15779
13	17.33334	0.66476	8.72463E-07	1.31694E-06	4.53423E-07	0.62304	2.00010E+00	6.19333
14	18.85551	0.64932	8.73001E-07	1.32254E-06	4.54745E-07	0.62198	2.00002E+00	6.23190
15	20.41644	0.63217	8.75330E-07	1.32875E-06	4.58386E-07	0.62048	2.00002E+00	6.31813
16	22.02284	0.61312	8.67291E-07	1.32204E-06	4.61610E-07	0.62022	1.99997E+00	6.33708
17	23.68300	0.59194	8.74711E-07	1.33310E-06	4.64330E-07	0.61921	2.00000E+00	6.35783
18	25.40739	0.56835	8.76691E-07	1.33830E-06	4.66688E-07	0.61816	2.00004E+00	6.02789
19	27.20970	0.54196	8.78346E-07	1.34268E-06	4.67004E-07	0.61710	2.00003E+00	5.66935
20	29.10832	0.51226	8.81045E-07	1.34773E-06	2.67809E-06	0.61571	2.00001E+00	4.24463
OVERALL	30.08437	0.67337	1.99747E-05	2.78688E-05	1.10392E-05	0.62581	1.99999E+00	7.75441
COST ESTIMATE DISCOUNTING ENERGY ON THE BASIS OF ONE- QUARTER YEARS								7.09558
COST ESTIMATE DISCOUNTING ENERGY FROM MID-CYCLE EXPOSURE POINTS (NOT A BETTER ESTIMATE)								7.09581
A DIRECT ACCOUNTING OF THE TIME OCCURANCE OF COSTS YIELDS A FUEL COST OF (SEE SUMMARY ABOVE)								6.81215
CASE END NORMAL, U-235 FEED, SUBZONES 4 4 YR FIXED FUEL HTR MODEL, RECYCLE , PROCESSOR (SEC)								9.43

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