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PROCEEDINGS OF THE JOINT NEACRP/CSNI SPECIALISTS' MEETING ON NEW DEVELOPMENTS IN THREE-DIMENSIONAL NEUTRON KINETICS AND REVIEW OF KINETICS BENCHMARK CALCULATIONS

Garching, 22nd - 24th January 1975

The Specialists' Meeting was organized by the OECD Nuclear Energy Agency Committee on Reactor Physics (NEACRP), the Committee on the Safety of Nuclear Installations (CSNI) and the Laboratorium für Reaktorregelung und Anlagensicherung der Technischen Universität München (LRA)
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LABORATORIUM FÜR REAKTORREGELUNG UND ANLAGENSICHERUNG
D-8046 Garching
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ABSTRACT

The papers presented at the meeting discuss problems related to three-dimensional kinetics calculations of nuclear reactors with the inclusion of feedback effects.

Solutions of benchmark problems posed by NEACRP/CSNI and submitted by various contributors are compared and discussed.
INTRODUCTION

The main topics of the papers are the following:

1. Recent developments of computational methods for the analysis of 3-d neutron kinetics:
   - Numerical methods general.
   - Coarse mesh methods.
   - Analysis and evaluation of 3-d neutron kinetics calculations.

2. Comparison and discussion of benchmark problems posed by NEACRP/CSNI:
   - Four 1-d benchmark problems for a gas-cooled thermal reactor (9 submitted solutions)
   - 2-d benchmark problem for a LWR (5 submitted solutions)
   - 3-d benchmark problem for a LWR (2 submitted solutions)
   - Four 2-d benchmark problems for a fast reactor (4 submitted solutions)

The meeting was attended by 41 officially accepted participants from 15 countries and international organisations. 14 papers have been presented from 8 different countries and organisations.

W. Werner
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Session I

NUMERICAL METHODS GENERAL

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APPROXIMATIONS THAT MAKE SPACE-DEPENDENT KINETICS COMPUTATIONS MORE EFFICIENT

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APPROXIMATIONS THAT MAKE SPACE-DEPENDENT KINETICS COMPUTATIONS MORE EFFICIENT

MIT, Cambridge, Massachusetts, USA
Approximations That Make Space Dependent Kinetics Computations More Efficient

A. F. Henry    M.I.T.

Introduction

The predicted behavior of power reactors during transient operation strongly influences certain design features of the system. The overall core size, the coolant-to-fuel volume ratio and the safety detection system are examples. There is thus a significant economic incentive for developing accurate methods for predicting how a reactor will behave under transient conditions.

To predict transient behavior requires that both thermal-hydraulic and neutron behavior be modeled and that the resultant equations be solved simultaneously. Fortunately, this non-linear problem in both the thermal-hydraulic and neutron flux parameters can be solved during each of a sequence of small time intervals by a thermal-hydraulic computation, for which the local power distribution is predicted from the local fluxes at the beginning of the interval, followed by a neutron flux computation based on local temperatures and densities obtained from the just-completed thermal-hydraulics calculation. If this tandem procedure is used the numerical models for thermal-hydraulic behavior and neutron behavior both become linear. Driving terms and coefficients in the thermal-hydraulics model involve time-dependent neutron fluxes, and coefficients (D's and Σ's) in the neutron equations are functions of the local thermal-hydraulic parameters.

In this paper we shall be concerned with approximate methods for solving equations belonging to the neutron part of this dual set. Moreover, we shall concentrate on schemes applicable to situations where there is no disassembly of the core. Thus we shall be concerned with methods used to analyse transients associated with normal maneuvering or with accidents that the core is designed to withstand rather than with catastrophies that lead to its destruction.

1) The Basic Neutron Model

Comparisons with experiments and with sophisticated analytical techniques provide strong support for the belief that energy group diffusion theory is capable of predicting criticality and detailed static power distributions for large reactors. For this model to be valid it is first necessary to find equivalent group-diffusion theory parameters that account properly for the transport effects associated with control rods or lumps of burnable poison, and that permit a pin cell of fuel, clad and associated moderator to be represented by homogenized group parameters that are averaged over energy ranges containing a number of resonances. But when this is done and homogenized fuel regions, control rods, flux suppressors, etc. are represented as geometrically distinct regions, the evidence is that diffusion theory, with 20 to 30 groups for a fast reactor or 2 to 4 groups for a thermal reactor, is an acceptably accurate model.
The assumption that the same group diffusion models are applicable to time dependent cases has been made primarily on the grounds that the time derivative terms \( \frac{\partial \phi_q(z,t)}{\partial t} \) for group \( q \) are usually very small compared to other terms in the group equations. Thus, in times longer than those required for neutrons to travel across a few pin cells or to slow down through a few energy groups, static equivalent group diffusion theory parameters are expected to be valid for transient situations. There is one qualification that must be imposed on this statement. It appears necessary to use effective delayed neutron fractions rather than physical ones in the time dependent equations\[1\]. With that qualification, we shall assume that time dependent group diffusion theory provides an accurate prediction of reactor behavior. Thus the basic set of equations for which we shall discuss approximate solution methods are:

\[
\nabla \cdot D_g(r,t)\nabla \phi_g(r) - \Sigma_g(r,t)\phi_g(r,t) + \sum_{q'=1}^{G} \Sigma_{g'q'}(r,t)\phi_{g'}(r,t) + \sum_{q'=1}^{G} \beta^{q'q} \psi_{g'}(r,t) = \frac{d}{dt}(\phi_g(r,t))
\]

The notation in these group diffusion equations is fairly standard. Subscripts \( q \) refer to group; superscripts \( j \) to different fissionable isotopes; subscripts \( i \) to different precursor groups; \( \Sigma_{g'q'}(r,t) \) is the transfer cross section from \( g' \) to \( q \).

2) Synthesis Methods

The geometrical complexity of most large power reactors is so great that it is impractical to solve Eqs. (1) by standard finite difference procedures. For example, in thermal reactors, if control rods or fingers, different zones of enrichment, lumps of burnable poison, etc. are all represented as explicit regions, several million mesh points may be needed just to describe the geometry. For such a case, even with only two groups, the solution of Eqs. (1) for more than a few time steps would be unacceptably expensive. In my opinion, if such geometrical complexity is to be represented explicitly, the flux synthesis technique \[2,3\] remains the most efficient procedure for providing detailed flux information during a transient.

The basic idea of flux synthesis methods is to approximate the group fluxes \( \phi_g(r,t) \) as

\[
\phi_g(r,t) = \sum_{k=1}^{K} \psi_g^k(x,y) z_g^k(z)
\]
where the $\psi_k^g(x,y)$ are predetermined expansion functions and the $Z_g^K(z)$ are mixing functions generally found by variational procedures. Usually different sets of expansion functions are used at different elevations [4].

For the analysis of transients involving possible tilting of the flux in the XY-plane (caused, for example, by the withdrawal of an asymmetrically positioned control rod) expansion functions capable of representing that tilt must be included. Several alternative methods that account for flux tilts without requiring that extra two-dimensional calculations be run have been suggested. These may all be described by a slight generalization of Eq. (2) so that it becomes

$$\phi_g(r,t) = \sum_{k=1}^{K} [F_g(x,y) \psi_k^g(x,y)] Z_k^g(z)$$

(3)

where the $F_g(x,y)$ are modulating functions having a single mathematical form that does not reflect any geometrical fine structure. In the multichannel synthesis method [5] the $F_g(x,y)$ $(=F(x,y))$ are the same for all groups $g$, have a unit value over certain zones in the XY-plane and are zero elsewhere. For example four $F(x,y)$'s may be chosen, each equal to unity in one quadrant of the XY-plane and zero elsewhere. Four different expansion functions $[F(x,y) \psi_k(x,y)]K$, all with the same detailed $\psi_k(x,y)$ but non-zero in different quadrants, result. The discontinuities in the radial planes resulting from use of this approximation are conceptually unsatisfying and apparently lead to numerical difficulties. I am unaware of any three-dimensional computer programs implementing the idea. Selecting the $F(x,y)$ to be overlapping tent-functions [6] avoids any radial discontinuities. This idea is being implemented for three-dimensional static problems.

Another choice of modulating functions has been explored at MIT [7]. For this scheme the $\psi_k(x,y)$ are not computed for the full XY-planes. Instead zero-current boundary conditions are used to compute $\psi_k(x,y)$ appropriate to various subregions of the XY plane (fuel subassemblies or clusters of fuel subassemblies). The $F_g^K(x,y) Z_g^K(z)$ are then modulating functions of the finite element type. The $F_g^K(x,y)$ as well as the $Z_g^K(z)$ contain unknown parameters (such as the magnitude of the flux at nodal corner points. The notation in Eq. (3) is rather clumsy for representing this particular "cell stitching" approximation. It may help to clarify matters to point out that, in this method, if the $\psi_k^K(x,y)$ are taken to be spatially flat, the scheme provides a three-dimensional finite element approximation for the $\phi_g(r)$.

The cell stitching scheme has been tested successfully for one-dimensional static cases [7]. The testing for a two-dimensional extension is now in progress.

Synthesis methods have not been widely accepted by the reactor analysis community for several reasons. The primary one is that there is no systematic error criterion through which their accuracy can be tested. (Halving the spatial mesh intervals of a finite difference solution for Eqs. (1) is guaranteed to improve accuracy; doubling the number of expansion functions in Eq. (2) is not.) Thus
it is necessary to validate synthesis methods empirically. A corollary of this situation is the fact that it is necessary to build experience before synthesis methods can be used in an optimum fashion. The various modulating schemes now being tested for static cases are basically attempts to ease this problem. Finally, synthesis methods, although relatively fast running, are very difficult to program.

Despite these limitations they remain the only practical, tested method for obtaining detailed solutions for Equations (1) for geometrically complicated situations.

3) Response Matrix Techniques

The geometry of some reactors permits a partitioning into rather large "nodes" (subvolumes) in such a way that the spatial, angular and energy behavior of the directional flux density \( \psi(x,\Omega,E) \) is a smooth function of \( x,\Omega,E \) over the nodal surfaces, even though it may be a very complicated function of these arguments in interior parts of the node. A two-dimensional example of this situation is provided by a D_2O moderated reactor in which the fuel is present as clusters of cylindrical fuel rods contained in widely spaced pressure tubes. If two-dimensional nodes are formed from the cross section of the pressure tube and its associated moderator (as in the figure)

\[
\psi(x,y,\Omega,E) \text{ along (ab) will be a simple function of its arguments, whereas inside the pressure tube (containing seven fuel rods - possibly all different) it will be a complicated function of these arguments.}
\]

For a situation of this kind the response matrix method is a very appealing scheme for determining the criticality of the reactor as well as the power level within any desired fuel rod. The basic idea of the scheme is to take as unknowns partial inward and outward group currents on the nodal surfaces such as (ab). If \( n \) is assumed to be an outward directed normal to (ab), these currents are

\[
\begin{align*}
J_{\text{in}}^g(x,y_0) &\equiv - \int dE \int d\Omega \frac{n \cdot \Omega}{n \cdot \Omega < 0} \psi(x,y_0,\Omega,E) \\
J_{\text{out}}^g(x,y_0) &\equiv \int dE \int d\Omega \frac{n \cdot \Omega}{n \cdot \Omega > 0} \psi(x,y_0,\Omega,E)
\end{align*}
\]

(4)
If, further, one assumes that the X-dependence of these partial currents has some simple mathematical form, the unknowns become the parameters that specify this form. Thus, if it is assumed that $J_{g1}^{\text{in}}(x,y_0)$ and $J_{g}^{\text{out}}(x,y_0)$ are linear functions of $x$, the unknowns of the problem become $J_{g}^{\text{in}}(x_1^+,y_0)$, $J_{g}^{\text{out}}(x_2^-,y_0)$, $J_{g}^{\text{in}}(x_3,y_0)$ and $J_{g}^{\text{out}}(x_4,y_0)$ where superscripts (+ and -) mean, for example, that $J_{g}^{\text{in}}(x^+,y_0)$ is the inward, group-$g$ partial current across $(ab)$ just to the right of point $(a,y_0)$. ($J_{g}^{\text{in}}(x_1,y_0)$ belongs to the node to the left of the one in the figure and need not necessarily equal $J_{g}^{\text{in}}(x_2^+,y_0)$.)

For each different kind of node making up the overall reactor the output currents from all faces and for all energy groups due to a given, group, unit input current along $(ab)$ can be determined by solving auxiliary problems for the node isolated in a vacuum. Methods ranging in sophistication from Monte Carlo to few group diffusion theory may be used for these auxiliary computations as the complexity of the problem demands. Assumptions about the angular and energy shape of the incoming neutrons (as well as the spatial shape mentioned above) must be made in performing these calculations, and the resultant output currents must be fit to these assured shapes. It is for this reason that $\psi(x,\Omega)$ must be a smooth function of its arguments over the nodal surfaces. (Or, if not simple, it must be known fairly accurately.) Otherwise one must decompose the incoming and corresponding outgoing currents into more component space, angular or energy shapes and do many more auxiliary problems in order to determine all output components for each input component.

When the auxiliary computations are done, it is possible to express a given outgoing partial current across a surface such as $(ab)$ as a linear combination of all input partial currents to the node for which $(ab)$ is a surface. Since the output partial current across $(ab)$ is the input partial current for the adjacent node, a matrix relationship involving only input partial currents can be constructed. Thus, if $[J^{\text{in}}]$ is a column vector of all nodal-incoming partial currents for all energy groups, we may construct an equation

$$\gamma[J^{\text{in}}] = [R][J^{\text{in}}]$$

where $[R]$ is the response matrix for the reactor, its elements being computed by performing the auxiliary computations just described. The scalar quantity $\gamma$ is an eigenvalue that will be unity if the reactor is critical.

The same auxiliary calculations used to determine the elements of $[R]$ can be made to generate extra response matrices that allow various reaction rates within a node to be computed once $[J^{\text{in}}]$ is known. Thus the method can yield both criticality and power distributions that are as detailed as desired.

For static problems sophisticated methods for determining response matrices have been used for thermal heavy water reactors [8] and for fast reactors [9]. Results have been very encouraging. At MIT we have been looking at applications to light water moderated thermal reactors [10] but with the response matrices (for heterogeneous nodes containing cross shaped control rods or water holes)
computed only by diffusion theory. Again results are very encouraging.

The extension of the response matrix technique to transient situations [11] is in principle straightforward. One merely defines a time dependent response matrix \([R(t,\tau)]\) giving the incoming currents at time \(t\), \([J_{\text{in}}(t)]\) in terms of the incoming currents at time \(\tau\):

\[
[J_{\text{in}}(t)] = \int_{-\infty}^{t} [R(t,\tau)] [J_{\text{in}}(\tau)] d\tau
\]  

(6)

In practice the determination of \([R(t,\tau)]\) and the solution of Eq.(6) is very complicated, particularly if delayed neutron and feedback effects are considered. The strategy that is being explored to overcome these difficulties at the Savannah River Laboratory [12] and at MIT is to separate prompt and delayed neutron effects by treating the population of delayed precursors within a node as an independent variable. Matrices specifying the creation rates of delayed precursors within a node due to unit incoming currents at time \(\tau\):

\[
[R_{\text{p}}(t,\tau)]
\]

are computed. In addition, matrices specifying outgoing neutron currents due to decay of an average precursor are thus computed. These matrices are assumed to depend on the instantaneous physical characteristics of the node. Thus Eq.(6) will be approximated by

\[
[J_{\text{in}}(t)] = \int_{-\infty}^{t} [R_{\text{p}}(t,\tau)] [J_{\text{in}}(\tau)] d\tau + \int_{-\infty}^{t} [E(t,\tau)] \Xi \lambda_i [C_i(\tau)] d\tau
\]  

(7)

where \([R_{\text{p}}(t,\tau)]\) is a response matrix analogous to \([R(t,\tau)]\) but with all neutrons emitted by the precursors that have been created by neutrons belonging to \([J_{\text{in}}(\tau)]\) omitted; \([C_i(\tau)]\) is a column vector of the total number of group-\(i\) precursors present in the various nodes of the reactor at time \(\tau\), and \([E(t,\tau)]\) is a matrix giving the incoming partial currents at time \(t\) through the faces of all the nodes of the reactor due to emissions of delayed neutrons at time \(\tau\) in the various nodes. Again, if the delayed neutrons emitted by the \([C_i]\) themselves create delayed precursors, any neutrons emitted from these secondary precursors and subsequently crossing a nodal face are not accounted for by \([E(t,\tau)]\). Thus, for a fixed \(t\), the dependency of the elements of both \([R_{\text{p}}(t,\tau)]\) and \([E(t,\tau)]\) on \(\tau\) is a very fast decaying function of \((\tau-t)\). As a result it is a good approximation to use the values of these matrices appropriate to time \(t\). Moreover, since the matrix elements of \([R_{\text{p}}(t-\tau)]\) and \([E(t,\tau)]\) are very small except for \(\tau\) close to \(t\), it may be permissible for relatively slow transients to approximate \([J_{\text{in}}(\tau)]\) and the \([C_i(\tau)]\) in Eq.(7) by \([J_{\text{in}}(t)]\) and the \([C_i(t)]\). Then Eq.(7) becomes

\[
[J_{\text{in}}(t)] = [R^\text{ST}_\text{p}(t)][J_{\text{in}}(t)] + [E^\text{ST}(t)] \Xi \lambda_i [C_i(t)]
\]  

(8)

where \([R^\text{ST}_\text{p}(t)]\) and \([E^\text{ST}(t)]\) are the static matrices appropriate to the reactor at time \(t\) and related to the corresponding time dependent matrices by
The response matrix technique shows promise of being able to deal practically with time dependent problems of considerable geometrical complexity. Moreover, it is not restricted to a diffusion theory model. Its continued study therefore seems very worthwhile.

4) The Determination of Homogenized Group Diffusion Parameters

Synthesis and response matrix methods make it possible to predict the criticality and power distribution of geometrically complex reactors for which detailed finite difference solutions of Eqs. (1) are impractical to obtain. There is another, much more common class of methods for dealing with such problems, the common feature of the class being that the behavior of heterogeneous nodes, containing possibly several zones of enrichment, lumps of burnable poison, control rods or water holes, is represented by equivalent homogenized group diffusion theory parameters, spatially constant over the entire node. A very common method for determining such parameters is to compute detailed group flux shapes $\phi_g(c)(r)$ throughout the node using zero current boundary conditions on the nodal surfaces and representing all material compositions in the node explicitly. An equivalent parameter such as $\Sigma_fg$, the homogenized fission cross section for group-$g$ is then defined as

$$\Sigma_fg = \frac{\int_{\text{node}} \tilde{\Sigma}_{fg} (r) \phi_g(c)(r) dv}{\int_{\text{node}} \phi_g(c)(r) dv}$$

where $\tilde{\Sigma}_{fg}(r)$ is the spatially dependent fission cross section for group-$g$ corresponding to the true enrichments and loading pattern within the node.

This is an appealing procedure since, if the difference between $\phi_g(c)(r)$ and the "true" detailed flux $\phi_g(r)$ throughout the node (i.e., the one corresponding to a full core solution and thus to non-zero-current boundary conditions) is disregarded, the ratio of group reaction rates determined when the homogenized parameters are used (along with the flux $\phi_g(r)$ resulting from such use) will be correct. Thus, if $\Sigma_{ag}$ is the homogenized, group-$g$ absorption cross section, we have

$$\frac{\int_{\text{node}} \Sigma_{ag} \tilde{\phi}_g(r) dv}{\int_{\text{node}} \Sigma_{fg} \phi_g(r) dv} = \frac{\int_{\text{node}} \Sigma_{ag} \phi_g(c)(r) dv}{\int_{\text{node}} \Sigma_{fg} \phi_g(c)(r) dv}$$

$$= \frac{\int_{\text{node}} \Sigma_{ag}(r) \phi_g(r) dv}{\int_{\text{node}} \Sigma_{fg}(r) \phi_g(r) dv}$$ (11)
Unfortunately there is no guarantee that an individual reaction rate such as \( \int_{\text{node}} \hat{f}_g(r) \Phi(r) \, dv \) will equal \( \int_{\text{node}} \hat{f}_g(r) \phi_g(r) \, dv \). Equality can be forced for one node by normalization of \( \phi_g(r) \). However the normalization of the flux will then be fixed for other groups and other nodes, and the desired equality may be lost.

A recent thesis [10] by John Kollas at MIT indicates that there may be reason for concern about the use of Eq. (10) for obtaining equivalent homogenized parameters. It is shown that, for one-dimensional (and only one-dimensional) slab geometry it is possible to determine equivalent homogenized parameters that are "exact" in the sense that their use leads to nodal absorption, fission and leakage rates (and hence critical eigenvalues) that agree identically with detailed solutions in which the geometrical heterogeneities within nodes are represented explicitly. For a symmetric slab subassembly consisting of a 0.5 cm thick absorbing sheet (one group parameters \( D=1.0 \, \text{cm}, \Sigma_a=1.0 \, \text{cm}^{-1}, \nu \Sigma_f=0 \)) surrounded by 3.75 cm thick homogeneous fuel regions (\( D=0.8 \, \text{cm}, \Sigma_a=0.015 \, \text{cm}^{-1}, \nu \Sigma_f=0.060 \, \text{cm}^{-1} \)) the "exact" homogenized parameters and the corresponding flux-weighted values obtained from Eq. (10) were

<table>
<thead>
<tr>
<th>Homogenized Parameter</th>
<th>&quot;Exact&quot; Value</th>
<th>Flux Weighted Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D )</td>
<td>0.553</td>
<td>0.807</td>
</tr>
<tr>
<td>( \Sigma_a )</td>
<td>0.0502</td>
<td>0.0587</td>
</tr>
<tr>
<td>( \nu \Sigma_f )</td>
<td>0.0491</td>
<td>0.0573</td>
</tr>
</tbody>
</table>

While this example is extreme, it does suggest that some improvement over the conventional flux weighting procedure is called for. The flux weighting scheme has been validated many times for more realistic situations by comparison with detailed, full core solutions. Generally, however, testing has been for symmetric, two-dimensional situations. For transients involving significant tilting of the flux the conventional flux weighting procedure may be inadequate.

At MIT we are examining an alternate scheme for determining homogenized group diffusion parameters. The basic idea is to compute response matrices for the heterogeneous node to be homogenized and then to find homogeneous group parameters that reproduce these response matrices. This approach has the virtue of yielding the "exact" parameters for the one-dimensional case. In two and three dimensions there are strong arguments suggesting that "exact" homogenized parameters do not exist. Thus we expect to determine only an approximate set for such cases. The hope is that, since they do become exact for the one-dimensional case, they will be superior to flux-weighted values in two and three dimensions.

The whole question of the adequacy of equivalent homogenized diffusion theory parameters becomes even more complex for transient analysis. Kollas [10] has shown that, here, even in slab geometry, parameters that are "exact" for static situations yield incorrect predictions of transient behavior. The hope is that they are inadequate only for very fast transients. But a thorough study of the matter has not as yet been carried out.
5) Methods For Predicting Flux Behavior in Reactor Composed of Large Homogeneous (or Homogenized) Nodes

If the methods just discussed for finding equivalent homogenized parameters are successful, or if it turns out that flux weighted parameters are adequate for cases of practical interest, the solution of Eqs.(1) becomes much more simple since many fewer mesh points are needed to describe geometrical details of the reactor. Under these circumstances, a spatial finite difference solution of Eqs.(1), while quite possible, may be unnecessarily expensive. A number of alternative procedures are currently being investigated. These fall roughly into two categories: higher order difference equation methods and nodal coupling schemes.

To the first category belong the finite element methods [13], the scheme of Robinson and Eckard [14] and the method of Antonopoulos described in Reference [15] (although the latter two might be viewed as nodal coupling schemes). To date only the first of these methods has been extended to treat transient situations. For a given degree of accuracy it appears to be faster than a standard finite difference solution [16]. But, although there are many fewer unknowns in a given problem the equations determining them have a higher degree of coupling. Thus the gain in running time is as yet not so great as had been hoped originally.

One attractive feature of finite element schemes should be noted. They are not restricted to completely homogeneous nodal compositions [17]. Mild heterogeneities, such as different zones of enrichment or non-uniform fuel loading due to depletion effects can be accommodated.

The other two higher order difference equations mentioned have fewer unknowns. Moreover the difference equations which result have the same form as the standard finite difference equations except that the coefficients in the flux equations depend on the flux values at previous time steps. Thus they should be much faster. However their time dependent extensions have not yet been tested. Moreover, the Robinson and Eckard scheme is restricted to one-energy group, and, although an extension of the Antonopoulos scheme to two groups has been worked out theoretically, it has not yet been tested even for static cases.

The notion of nodal coupling schemes is essentially to deal with nodal averaged or center point group-fluxes as unknowns and to express the group currents across nodal interfaces in terms of these fluxes. They are discussed in a general way in Reference [15], and References [18-22] deal with specific examples as applied to static situations. The recent extension of the method of Birkhoff and Werner to time-dependent situations [23] appears to be a particularly attractive approach. Like the finite element method, it appears to be able to accommodate mild heterogeneities in the material compositions of the nodes. It is not restricted to one-group problems. However, it involves difference equations that have the same non-linear form as those encountered by Robinson and Eckard. Thus it shows real promise of being both accurate and fast-running.
6) The Use of Boundary Conditions to Replace Reflectors

Explicitly representing the reflector when solving the group diffusion equations for a reactor adds considerably to the cost of the calculation. This is particularly true if the reflector is light water and there is no core baffle, for then, rather small mesh spacings must be used in the reflector or else returning neutron currents will not be correctly described with the result that criticality and the relative power level at the center of the reactor may be poorly estimated.

The one-group nodal code FLARE [18] and the code embodying the Robinson and Eckard scheme circumvent this difficulty by using albedo type boundary conditions relating flux to current over the surface of the reactor. The required flux-to-current ratios are specified as input and determined empirically by comparison with experiment or with more detailed, few group calculations. Generally the flux-to-current ratio is taken to be some constant average value over the entire interface between the core and the reflector.

At MIT we have been examining more systematic ways for deriving such boundary conditions. Specifically we are trying to find appropriate two-group boundary conditions for light water reflector power reactors. We want to generate them internally, and we want them to apply to transient situations when the reflector properties may be changing. The detailed study is being carried out by Panos Kalambokas for two-dimensional radial slices of reactors having the usual staircase-like interfaces between core and reflector. Such interfaces are typical of PWR's and BWR's composed of sub-assemblies having a square cross section. In the reflector of such a reactor, which for simplicity we shall assume to be homogeneous and infinitely thick, the two-group counterparts of Eqs. (1) are

\[
\begin{align*}
D_1 \left( \frac{\partial^2 \phi_1(x,y,t)}{\partial x^2} + \frac{\partial^2 \phi_1(x,y,t)}{\partial y^2} \right) - \Sigma_1 \phi_1(x,y,t) &= \frac{1}{v_1} \frac{\partial \phi_1(x,y,t)}{\partial t} \\
D_2 \left( \frac{\partial^2 \phi_2(x,y,t)}{\partial x^2} + \frac{\partial^2 \phi_2(x,y,t)}{\partial y^2} \right) - \Sigma_2 \phi_2(x,y,t) + \Sigma_{21} \phi_1(x,y,t) &= \frac{1}{v_2} \frac{\partial \phi_2(x,y,t)}{\partial t} \\
\end{align*}
\] (12)

Let us suppose that \((x,y)\) is a point on a segment of the surface of the core perpendicular to the \(x\)-direction so that the reflector extends in the \(x\)-direction from \((x_1,y_1)\) to \((x_2,y_1)\) where we shall take \(x_2 \gg x_1\). Then, at \(t=t_1\), we arbitrarily define parameters \(B^2_{g_1}(x,y_1,t_1)\) and \(\omega_g(x,y_1,t_1)\) such that

\[
\begin{align*}
B^2_{g_1}(x,y_1,t_1) &= -\frac{1}{\phi_1(x,y_1,t_1)} \left. \frac{\partial^2 \phi_1(x,y,t)}{\partial y^2} \right|_{y=y_1} \\
\omega_g(x,y_1,t_1) &= \frac{1}{v_g} \phi_g(x,y_1,t_1) \left. \frac{\partial \phi_g(x,y,t)}{\partial t} \right|_{t=t_1} \\
\end{align*}
\] (13)

\(g=1,2\)
As a result, Eq. (12) at \((y_1, t_1)\) becomes

\[
D_1 \frac{\partial^2 \phi_1(x, y_1, t_1)}{\partial x^2} - [D_1 B_{2y}^2(x, y_1, t_1) + \Sigma_1 + \frac{\omega_1(x, y_1, t_1)}{v_1}] \phi_1(x, y_1, t_1) = 0
\]

\[
D_2 \frac{\partial^2 \phi_2(x, y_1, t_1)}{\partial x^2} - [D_2 B_{2y}^2(x, y_1, t_1) + \Sigma_2 + \frac{\omega_2(x, y_1, t_1)}{v_2}] \phi_2(x, y_1, t_1) +
\]

\[
\Sigma_2 \phi_1(x, y_1, t_1) = 0
\]

(14)

If now the fundamental assumption is made that the \(B_{qy}\) and the \(\omega_g\) may be approximated by their values at \(x_1\) for the whole range \(x_1\) to \(x_2\), a solution of Eq. (14) in terms of the fluxes and currents at \((x_1, y_1, t_1)\) is easily obtained, and it is simple to show that

\[
\begin{bmatrix}
-D_1 \frac{\partial \phi_1(x_1, y_1, t_1)}{\partial x} \\
-D_2 \frac{\partial \phi_2(x_1, y_1, t_1)}{\partial x}
\end{bmatrix} =
\begin{bmatrix}
\alpha_{11} & 0 \\
\alpha_{21} & \alpha_{22}
\end{bmatrix}
\begin{bmatrix}
\phi_1(x_1, y_1, t_1) \\
\phi_2(x_1, y_1, t_1)
\end{bmatrix}
\]

(15)

\[
\alpha_{11} \equiv D_1 \kappa_1; \quad \alpha_{22} \equiv D_2 \kappa_2; \quad \alpha_{21} \equiv -\frac{\Sigma_2 \kappa_1}{\kappa_2 \kappa_1 + \kappa_2}
\]

(16)

Then, since fluxes and the normal components of currents are continuous across interfaces, Eq. (15) becomes a homogeneous boundary condition applicable to any segment of the core surface that is perpendicular to the \(x\)-direction. A completely analogous treatment for segments of core surface perpendicular to the \(y\)-direction (along with definition of parameters \(B_{qy}^2(x_1, y, t_1)\) and \(\omega_g(x_1, y, t_1)\) analogous to (13) ) then yields homogeneous boundary conditions over the entire core surface. We may then solve Equations (1) within the core using these boundary conditions and omitting any explicit treatment of the reflector. Since, in the course of solving the equations in the core, the flux as a function of time and position over the core surface is obtained, the transverse bucklings \(B_{qy}^2\) and \(B_{qy}^2\), and the instantaneous periods \(\omega_q^2\) may be obtained from the solution itself as the problem proceeds. If the properties of the reflector materials change uniformly, the
effect can be accounted for by changing the \( D_q \), \( \Sigma_q \) and \( \Sigma_2 \) in the formulas (16). If the changes are not uniform, the reflector can be partitioned into regions and Eq. (16) generalized so that the \( \alpha \)'s are found for a multislab reflector. The generalization is straightforward although it does lead to complicated algebraic formulas for the \( \alpha \)'s.

The accuracy of this procedure for replacing explicit consideration of a reflector by boundary conditions at the core surface depends on the magnitudes of the \( D_q B_{qx} \), \( D_q B_{qy} \) and \( \omega_q / v_q \) compared to the \( \Sigma_q \) and, if they are not small, on the validity of replacing values of these parameters throughout the reflector by values on the surface of the core. For light water reflectors (or steel-water mixtures) the \( \omega_q / v_q \) will be negligible for all but the most extreme transients. Moreover, since the linear segments making up the perimeter of a radial slice of a light water power reactor are about 20 cm in length, we expect the \( B_{qx} \) and \( B_{qy} \) to be small except near corners where two segments join (forming a 90° angle facing either the reflector or the core material).

Numerical testing of the method to date has been sufficiently encouraging that we are incorporating the boundary conditions (15) (along with the capability for treating jagged outer boundaries) into a three-dimensional, transient code being developed for the electric utility industry.
References


DISCUSSION

J.J. Dorning

My question concerns the response matrix method studies which you described. Have you or the group at SRL studied the effect of varying the order of the spatial expansion (flat, linear, etc.) of the partial currents on the volume element surfaces?

A.F. Henry

As far as I know the studies at Savannah River have involved only spatially constant partial currents over the faces of the hexagons. At MIT we have the capability of looking at both flat and linearly varying distributions. I cannot recall any actual studies using the flat distributions. For light water moderated systems I would not expect the flat approximation to be adequate.

J.J. Dorning

In connection with the nodal methods, have you tried renormalizing via the ratio of homogenized $\nu\xi_f$ to the exact $\nu\xi_f$ which you mentioned, followed by adjusting the diffusion coefficient to preserve neutron balance?

A.F. Henry

No, we haven't. Our basic idea is to try to find homogenized constants that reproduce the same response matrices as those found when the true heterogeneous nature of the
region being homogenized is explicitly accounted for. We have so far stuck closely to the one criterion.

J.J. Dorning

How are you "matching" your coarse representation and fine representation response matrices?

A.F. Henry

We average absorption, fission and removal constants over the detailed fluxes found when the heterogeneous problems are run to obtain the "exact" response matrices. Then we adjust the (two group) homogenized diffusion constants until the matrices are produced when these homogenized parameters are used to determine response matrices.

H. Küsters

From the various methods you have outlined as possibilities to achieve better efficiency in 3d calculations, what would be the favourable one in your opinion?

A.F. Henry

In my opinion, syntheses methods provide the most accurate, feasible procedures for determining detailed flux behaviour when geometrical structure is represented explicitly. They are fast-running and I believe, with further development, they can be made accurate. Their main drawback is of course the fact that they can provide no accurate measure of their own error, but I believe that, with experience, we could live with that drawback.
J. Devooght / E. Mund

A - STABLE ALGORITHMS FOR NEUTRON KINETICS

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ABSTRACT

Benchmark problems are interesting not only as a common meeting ground of different numerical algorithms but as a mean to check their soundness or conformity to the underlying theory, if any. Although some numerical algorithms devised to integrate the space dependent kinetics are well founded, others are on a more shaky ground and therefore not completely trustworthy. On the other hand, numerical schemes with a theoretical small truncation error may not always fare as well as they are supposed to. The first part of this paper deals with some general features of a space dependent kinetics code, stressing the properties of A-stability and spectral matching. The second part summarizes the main characteristics of a new A-stable algorithm that is flexible enough and encompasses many existing schemes. Some extrapolation procedures are discussed. A Newton series interpolation with a permanence property is introduced. The third part, finally, describes two numerical applications of the \( W_{11}(u_1|u_1,u_2) \) time-integration scheme and their related conclusions.
1. General Features of a Reactor Dynamics Code

1.1. Introduction

Point kinetics is a very simple problem, computationally speaking, compared to space dependent kinetics, especially 2D and 3D. It is hardly necessary to improve methods, as far as point kinetics alone is concerned, considering the very small computing time. However some methods used can be extended readily to space dependent kinetics (most of them not) and therefore it is useful to improve the computing efficiency: lengthening of time steps, memory and core storage etc... Moreover some methods like the quasistatic method rely on the frequent solution of a point kinetics problem and the infrequent solution - which means with large time steps - of a space dependent problem. It is sometime argued that it is unnecessary to extend the time step because in some reactor dynamics problems the time needed for the computation of the thermohydraulic feedback is the commanding factor. First, it should be kept in mind that as long as neutronics is not a negligible part of the problem, the lengthening of the time step is not unwarranted. Second, any technique that allows a lengthening of the time step can likely be applied also to the thermohydraulic variables.

1.2. Limits to time step lengthening

There are three main obstacles to the step lengthening in the integration of the initial value problem \( \frac{dY(t)}{dt} = A(t) Y(t) \) : (1.1)

a. the global accuracy limitation

b. the non-constancy of the operator \( A(t) \) which yields usually a local truncation error \( O(h^3) \)

c. the non-commutation of the operators when they are splitted, like the ADI methods for 2D and 3D.

Some methods have all limitations, some only the first two. As far as we are aware there is yet no complete analysis for neutron kinetics of the three problems. It has been recognized for a long time that owing to the stiff nature of the equations (i.e. large spread
in the eigenvalues of \(A\), the time step should be small for short times and presumably long in the asymptotic range, if any. The need for an adaptive method that yields the optimal time step compatible with a given global accuracy is as great as ever since only rules of thumb are available. Error monitoring should take into account all three types of error. Up to now, authors have been satisfied by errors of type 2 of order no less than errors of type 1, for which there is usually a qualitative knowledge, i.e. the absolute truncation error is bounded by \(Ch^n\). The order \(n\) is known but \(C\) is generally unknown. The ambiguity resulting thereof will be shown in a later paragraph.

1.3. One step method and rational approximations

We are interested in point kinetics problems to the extent that methods are transposable to space dependent problems. Aside from the problem of computing time, the most pressing problem is memory storage which can be troublesome even for 2D-multigroup problems. Therefore multistep methods are almost automatically excluded, except maybe two-step methods. The restriction is severe for integral formulation of the kinetics problems which need more than two points for the quadrature. Since any interpolatory quadrature method is based on an assumption for the integrand behaviour, usually the flux, the accuracy can be improved by a judicious choice of the assumed time dependence, like for instance exponential behaviour. However the accuracy is mostly dependent upon the number of points for a given time step and the simplest scheme is given by:

\[
N(t) = N(0) f_1(t) + N(h) f_2(t)
\]

with

\[
f_1(o) = \delta_{i1}, \quad f_1(h) = \delta_{i2}
\]

Introducing (1.2) into \(N(h) - N(0) = \int_0^h A(s) N(s) ds\) yields essentially a scheme of the Crank-Nicolson (or Padé 11) family. Higher order schemes based on more than two points quadrature yield similarly higher order Padé approximations or generalizations thereof. Confluent points yield Hermite interpolation. Moreover it is known that methods like collocation, Galerkin and interpolatory quadrature...
are all equivalent [1]. Similarly WRIGHT [2] has shown the equivalence between collocation and a subclass of implicit Runge-Kutta methods. BUTCHER, EHLE, CHIPMAN, AXELSSON have shown that various well known quadrature schemes like Gauss-Legendre, Radau, Lobatto, led to Pade approximants of order \((n,n)\), \((n,n-1)\) and \((n,n-2)\) [3,4,5,6]. Reciprocally GEAR has shown that any rational approximation \(P(A)/Q(A)\) where the \(n\) poles are distinct and the degree of \(P\) \(\leq\) degree of \(Q\) \((\leq n)\) is equivalent to an implicit Runge-Kutta scheme [7]. Two point Hermite interpolations have also been used to generate rational approximations.

It can therefore be asserted that in spite of appearances all methods of integration that do not split operators based either on rational approximations or on the treatment of integral (or integro-differential) forms of the kinetics equations, by collocation or Galerkin weighting, are all basically alike. It is then sufficient to investigate rational approximations to \(e^{HA}\) where \(A\) is suitably defined. Some investigations have started directly from that point of view. Granting that any integration scheme of the kinetics equation is essentially a rational function \(P(A)/Q(A)\) of \(A\), we immediately encounter the difficulty of evaluating powers of \(A\) which is out of question for space dependent problems. Factoring \(P(A)/Q(A)\) gives almost always complex numbers. Although TURNAGE extending a scheme of DA NOBREGA and HENRY [8] has shown how to deal with such problem in the case of a multipoint reactor, his method cannot be extended to full space dependent problems because of the need of explicitly inverting matrices [8]. Therefore, we are left either with first degree rational approximations (like \(P_1\)) or approximations which have real coefficients and may be factorized like all those resulting from extrapolation.

1.4. Equivalent constant operators

In the case of time dependent operators we are left yet with the problem of defining a suitable average operator. Although this can be done rigorously by means of

\[
N(h) = \exp\left\{\int_0^h A(s) \, ds + \frac{1}{2} \int_0^h d\sigma \int_0^\sigma d\xi \left[A(\xi), A(\sigma)\right] + \ldots\right\} N(0) \quad (1.3)
\]

in practice \(A(t)\) will be known only at discrete times, and an approximate quadrature should be used. As a rule the first operator in
brackets is approximated by \( \frac{h}{2} \left[ A(0) + A(h) \right] \) which gives an error \( O(h^2) \) and the second is neglected.

1.5. Spectral matching

Many methods make assumptions, one way or another, about the flux behaviour. The flux is expressed as a linear combination of functions of time. A popular choice of the basis is either a polynomial, or an exponential times a polynomial. The first choice is dictated by the vast literature on spline functions. We believe however that polynomials are unsuitable for the description of transients with large steps and that a more natural choice is a basis of exponentials \( \left\{ e^{\lambda_1 t} \right\} \) were the \( \lambda_1 \) are close to the eigenvalues. With such a choice we know at least then—when the operator A is constant— that the solution is exact when the initial vector belongs to the subspace spanned by the eigenvectors associated with the eigenvalues \( \lambda_1 \). This property of spectral matching is a very essential requirement for any method devised to cope with large time steps. On the contrary, polynomials basis and the ensuing Padé approximations are founded implicitly on the false assumption that all eigenvalues are zero.

1.6. A-stability

The stability of the integrating scheme is a necessary requirement for any proposed method. Lax equivalence theorem provides the necessary link between stability, convergence and consistence (cfr [9], p. 13). Although some schemes have been proved to be stable, some are not or at best uncertain. For stiff systems like the neutronics equations an even stronger condition is necessary, namely the A-stability of Dahlquist, which is defined as follows [10]:

**Definition 1**: a one step method \( \gamma_{i+1} = w(\lambda h) \gamma_i \) applied to the equation \( \frac{d \gamma}{dt} = \lambda \gamma \) is A-stable iff \( |w(\lambda h)| \leq 1 \) for \( Re \lambda \leq 0 \).

It is obvious that if the condition is valid only in a finite portion of \( Re < 0 \) errors would grow exponentially for the eigenvectors associated for instance with large values of \( |\lambda h| \). Some approximations like the Crank-Nicolson \( \frac{1+\lambda h}{2} \) are such that \( \lim_{h \to 0} |w(\lambda h)| = 1 \). This is
an important defect for stiff systems or (and) large time steps. Accordingly, we have:

Definition 2: a one step method is strongly A-stable if $|w(\lambda h)| \to 0$ when $|\lambda h| \to \infty$ for $\Re \lambda < 0$.

In the words of GEAR [11] a method is strongly (or stiffly) A-stable if for the equation $\frac{d\vec{y}}{dt} = \lambda \vec{y}$, the rapidly decaying components also decay rapidly in the numerical approximations, so that it would not be necessary to use small steps even when the components were still present. Any method supposed to deal efficiently with step lengthening in stiff systems is bound to be A-stable. The nature of the space or energy discretization is not essential for the discussion, as long as the discretization of $A$ is dissipative.

1.7. Summary

To summarize, a suitable method for space dependent reactor dynamics must fulfill the following conditions:

1. The algorithm must be consistent and convergent which by Lax theorem ensures stability.

2. The systems studied being "stiff", the algorithm should be not only stable, but A-stable (or A($\alpha$)-stable [11]), in order to handle correctly large time constants with medium to large time steps.

3. The approximate solution should possibly contain some essential characteristics of the exact solution, which can be done best by spectral matching.

4. The global error should be controlled in order to obtain at a given time a stated accuracy with the minimum number of time steps. The local error should be decreased preferably without discarding previous results, a requirement which points towards iterative methods with a permanence property (see §2.1).

5. In order to minimize memory requirements, the algorithm must be one-step, either of first degree or factorizable in first degree rational operator-valued functions. Extrapolation is a possible method for both 4 and 5: it has also the distinct advantage to use factorized approximations and therefore need only to invert linear systems one at a time without squaring matrices. This is the case for instance for:
Although, as will be seen in §2.3, this approximation is not A-stable.

We close this paragraph with two general remarks:

1. We do not refer to any explicit form of neutron kinetics equations which are only supposed to be linear or linearized. However the quasistatic method which gives probably the most general and versatile algorithm yields two systems of equations: "point kinetics" and "space kinetics" with a translated spectrum. [29] [30]

2. A complete theory of the spectrum of the matrix A is lacking. However some results, on particular cases obtained by Henry [24], Foulke and Gyftopoulos [25], and Porshing [26] suggest that the eigenvalues occur in I+G clusters (I precursors, G groups) associated with eigenvectors of similar shape. Insofar as the stiffness of the matrix is involved in the algorithm described below, only order of magnitudes of the eigenvalues (except for the dominant one) are needed (see §3.3) and the cluster assumption will be made.
2. A FIRST ORDER A-STABLE ALGORITHM WITH SPECTRAL MATCHING

2.1. Introduction

We shall, in this introductory paragraph, recall some theoretical preliminaries which form the basis of the present work. For the sake of conciseness, only the statements of the theorems will be given. For further details, the readers are referred to [12, 13].

We are interested, generally speaking, by the construction of rational approximations $W(u)$ of the complex function $e^u$ having the interpolation property at arbitrarily given points $\{u_i\}$, $i=1,\ldots,n$ and whose moduli $|W|$, for stability reasons, satisfy the inequality $|W| \leq M < 1$ in the open left half plane. Some fifty years ago, an analog problem was formulated and solved by NEVANLINNA and SCHUR.

More precisely, given a real positive constant $M$ and two sets of $n$ complex values $\{z_i\}$, $\{W_i^{(1)}\}$, $i=1,\ldots,n$ the first of which is entirely located in the unit disc $|z| \leq 1$, the following question was raised: would it be possible to find an analytic function $W(z)$ -unique, if any- having its modulus less or equal to $M$ in the unit disc and taking at $\{z_i\}$ the corresponding values $\{W_i^{(1)}\}$? The complete answer to that question as well as Schur-Nevanlinna's (SN) algorithm which gives the solution of the problem may be summarized in a few theorems stated below [13].

First, we want to define a sequence of functions:

$$W_k(z) = \frac{M^2}{f_k(z)} \cdot \frac{W_{k-1}(z) - W_k^{(k-1)}}{M^2 - W_k^{(k-1)}W_{k-1}(z)} \quad k=1,\ldots,n \quad (2.1)$$

with

$$f_k(z) = \frac{z - z_k}{1 - \bar{z}_k \bar{z}}$$

$$W_0(z) = W(z)$$

$$W_k^{(v)} = W_v(z_k) \quad k = v+1, v+2,\ldots,n \quad (2.2)$$

$W_0(z)$ is the, yet hypothetical, solution of the problem. Functions like $f_k(z)$ or products thereof play an essential role in this theory. Called Blaschke products, they are bounded analytic functions inside
the unit disc with a modulus equal to 1 on \(|z|=1\). Using the sequence (2.1) and (2.2), a triangular scheme is built without difficulty, running downwards line by line and from the left to the right:

\[
\begin{align*}
W_1^{(0)} &
W_2^{(0)} \rightarrow W_2^{(1)} \\
W_3^{(0)} &\rightarrow W_3^{(1)} \\
& \vdots \\
W_n^{(0)} &\rightarrow W_n^{(1)} \\
& \vdots \\
& \vdots \\
W_n^{(n-1)} &
\end{align*}
\]

(2.5)

We have then, the first and main theorem:

**Theorem 2.1.1:** The SN problem admits at least one solution iff one of the two situations occurs:

1. \(|W_k^{(k-1)}| < M\) \(k=1,2,\ldots,n\)

\[
|W_{\mu+1}^{(\mu)}| = M \\
W_{\mu+1}^{(\mu)} = W_{\mu+2}^{(\mu)} = \ldots = W_n^{(n)}
\]

2. \(|W_k^{(k-1)}| \leq M\) \(k=1,2,\ldots,n\)

In the first case (i.e. when it happens that all elements along a vertical line in (2.5) are equal, their modulus being equal to \(M\)), the solution is **unique** and given by the sequence (2.1) running backwards with the initial function \(W_n(z) = W_n^{(n)}\).

In the other case, the solution is **not unique** : any analytical function having its modulus \(\leq M\) along \(|z|=1\), serving as initial function \(W_n(z)\) in the sequence (2.1) taken in reverse order, will give a correct answer to the problem.
One may easily verify that, given the analytical structure of (2.1), \( W(z) \) will be a rational function iff the initial function introduced in SN's algorithm is rational. We have also:

**Theorem 2.1.2**: Given \( \{ z_i \} \) and \( \{ W_i^{(0)} \} \) \( i=1,2,\ldots,n \), there is a minimum value of \( \mu \) to which corresponds a unique solution of SN's problem. The algebraic equation for the determination of the smallest \( \mu \) is

\[
|W^{(n-1)}_n| = |W_{n-1}(z_n)| = \mu
\]

The smallest real positive value of \( \mu \) is taken.

**Theorem 2.1.3**: A sufficient condition that there exists a function \( W(z) \) of modulus \( \leq N \) along \( |z| = 1 \) which takes on the values \( W_k^{(0)} \) at \( z_k \) is that \( W_k^{(0)} \) are the values taken at \( z_k \) by a bounded analytic function \( \sigma(z) \) (with \( |\sigma(z)| \leq N \) along \( |z|=1 \)) and \( N \geq \sigma^{(n-1)}(z) \).

Let us now introduce the conformal mapping of the complex left-half plane \( \text{Re} \, u \leq 0 \) on the closed unit disc \( |z| \leq 1 \), defined by:

\[
z = \frac{u-a}{u+a} \quad a, \text{ real } < 0 \quad (2.4)
\]

Our original problem may be stated in the equivalent form: find \( \phi(u) \) whose image in the closed unit disc is such that \( |W| \leq \mu \leq 1 \) along \( |z|=1 \) and interpolates \( \tau(z) = \exp(-a \frac{z+1}{z-1}) \) at a finite number of arbitrarily given points \( \{ z_i \} \) \( i=1,\ldots,n \). The function \( \tau(z) \) is a bounded analytic function in \( |z| < 1 \), but has an essential singularity at \( z=1 \), the image point of \( u=\infty \). Moreover \( |\tau(e^{i\theta})| = 1 \) almost everywhere. It may be shown that this is not a restriction to the validity conditions of theorem 2.1.3 which guarantees the existence of at least one solution, provided \( N \geq |\tau^{(n-1)}| \).

We further introduce a class of functions \( W(z) \) which are said to satisfy property-M if for all \( |z| \leq 1 \):

\[
W(z) = \frac{M^2}{W(\frac{1}{z})} \quad (2.5)
\]

Analytic functions in the closed unit disc satisfy property-M iff they have a constant modulus \( M \) on \( |z|=1 \). It is easily verified that \( \sigma(z) \),
although not analytic in the closed unit disc, has property-$M$ ($M=1$) everywhere except at its essential singularity. It has been shown [13] that when SN's algorithm is applied to elements of the class (2.5), $n$ additional interpolation properties may be stated outside the unit circle. More precisely, we have:

Theorem 2.1.4.: Let $W(z)$ be a rational function with $|W(e^{i\theta})| \leq M$ which interpolates at $n$ arbitrarily given points $\{z_i\}_{i=1}^n$ inside the unit circle a function $\sigma(z)$ satisfying property-$N$. Then $W(z) - \sigma(z)$ has also $n$ zeros $\{\gamma_k\}_{k=1}^n$ outside the unit circle and there exists a positive constant $L$ such that:

$$|z_k - \frac{1}{\gamma_k}| < L|M-N|$$

(2.6)

Returning once more to the exponential function and putting $N=1$, we find that each interpolation point $u_k$ in the left half plane $\Re u < 0$ has an associated interpolation point $v_k$ in $\Re u > 0$ with the remarkable relationship:

$$u_k = -v_k, \quad k=1, \ldots, n$$

(2.7)

which will be used extensively in the next paragraph.

Up to now, no particular assumption was made for the "arbitrary" starting function $W_n(z)$ of SN's algorithm, when $|\sigma^{(n-1)}_n| < M$, save its rational nature. One might try, for instance, to take opportunity of the algorithm's flexibility to implement additional interpolation conditions. This possibility, indeed, has been shown by DEVOOGHT [13]. More precisely

Theorem 2.1.5.: If the rational function $W_0(z)$ satisfies the condition of theorem 2.1.3., it can be made to interpolate $\sigma(z)$ at the additional point $z_{n+1}$ provided $W_n(z_{n+1}) = \sigma^{(n)}_{n+1}$, with $|W_n(z_{n+1})| = M_{n+1} < M$. If the equality applies, $W_n(z)$ is constant and $W_0(z)$ is the unique function of least maximum modulus in $\Re u \leq 0$ as established in case I of theorem 2.1.1.

It should be noted, however, that this additional matching point has no counterpart outside the unit circle, giving a total of $2n+1$ interpolation points for the most general $(n,n)$ rational approximation.
This is by no means a surprise, since such expressions contain precisely \((3n+1)\) independent coefficients.

We may now proceed to the explicit construction of the first-order rational approximation of maximum modulus \(M\) in \(\text{Re} \, u < 0\), \(W_{11}(u)\) interpolating \(e^u\) at a real abscissa \(u_1 < 0\). Using (2.3), one obtains:

\[
W_0(u) = M^2 \frac{e^{u_1}(u+u_1) + W_1(u)(u-u_1)}{N^2(u+u_1) + W_1(u)(u-u_1)} e^{u_1} \tag{2.8}
\]

According to (2.7), this expression matches also \(e^u\) at \(u=-u_1\). Requiring further \(W_0(u)\) to interpolate \(e^u\) at \(u_2\) gives -provided \(M \geq M_{\min}\) - the unique solution:

\[
W_0(u) = W_{11}(u|u_1,u_2;M^2) = M^2 \frac{\frac{e^{u_1+W_1}}{u(M^2+W_1e^{u_1})} + \frac{e^{u_1-W_1}}{u_1(M^2-W_1e^{u_1})}} {u(M^2+W_1e^{u_1}) + u_1(M^2-W_1e^{u_1})} \tag{2.9}
\]

with

\[
W_1 = M^2 \frac{u_2+u_1}{u_2-u_1} \frac{e^{u_1-u_2}}{e^{u_1+u_2}-M^2} \tag{2.10}
\]

The minimum value \(M_{\min}\) is obtained by solving the quadratic equation associated to the condition \(|W_1| = M_{\min}\). One obtains easily, for given \(u_1\) and \(u_2\):

\[
M_{\min} = e^{-\frac{u_1+u_2}{2}} \left[ B(u_1,u_2) + \sqrt{1 + B^2(u_1,u_2)} \right]
\]

\[
B(u_1,u_2) = \frac{u_2+u_1}{u_2-u_1} \sinh \frac{u_1-u_2}{2} \tag{2.11}
\]

2.2. Some properties of \(W_{11}(u|u_1,u_2;M^2)\)

Let us go further into details to examine what happens when some particular choices are made for the interpolation points. First of all, we shall try to release somewhat the symmetry property of two among the three interpolation points of \(W_{11}(u|u_1,u_2;1)\), without
losing A-stability for the result.

Indeed, we have trivially \( e^u = e^a \cdot e^{u-a} \). Replacing the exponential function in the right member of the equality, by its \( \tilde{W}_{11} \) approximation adequately shifted, gives a new rational scheme \( \tilde{W}_{11} \):

\[
\tilde{W}_{11}(u|u_1,u_2,u_3) = e^a W_{11}((u-a)|(u_1-a),(u_2-a);1)
\]  

(2.12)

interpolating \( e^u \) at \( u_1, u_2 \) and \( u_3=2a-u_1 \). A-stability will be preserved provided the domain \( \mathcal{D} \) of the complex plane with \( |\tilde{W}_{11}| > 1 \), be entirely located in \( \text{Re} \, u \geq 0 \). Since \( \tilde{W}_{11} \) has the rational form:

\[
\tilde{W}_{11} = \frac{A_0 + A_1 u}{B_0 + B_1 u}
\]  

(2.13)

\( \mathcal{D} \) is a circle of radius \( R_c \) whose center lies at \( u_c \) on the real axis:

\[
u_c = \frac{B_0 B_1 - A_0 A_1}{A_1^2 - B_1^2}
\]  

(2.14)

\[
R_c = \frac{A_0 B_1 - A_1 B_0}{A_1^2 - B_1^2}
\]

When \( a=0, W_{11}(0) < 1 \) and \( \mathcal{D} \), entirely in \( \text{Re} \, u > 0 \), encompasses \( u=-u_1 \). The A-stability requirement limits the "shift" \( a \) in the negative direction to an extreme value such that \( u_c = R_c \) or equivalently, from (2.14), \( A_0 = B_0 \). Using (2.9), (2.10) and (2.12), after some elementary algebra, this is found to be equal to \( \frac{u_1}{2} \), which brings the third interpolation point \( u_3 \) at the origin. We must keep in mind that the variable \( u \) in all this subject-matter refers to the product \( \lambda h \) of a characteristic time-decay constant by the integration step, interpolation meaning "spectral-matching". For small integration steps, the error \( \varepsilon(\lambda h) = \exp(\lambda h) - \tilde{W}_{11}(\lambda h) \) is approximately given by:

\[
\varepsilon(\lambda h) = C (\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3) h^3 (1 + O(h))
\]  

(2.15)

i.e. vanishes identically, whatever the value of \( h \), for \( \lambda \) equal either to \( \lambda_1, \lambda_2 \) or \( \lambda_3 \). \( C \) is a constant factor, easily found by particularizing the \( \lambda \)'s.
2.2.1. Let us first put \( u_1 = u_2 = u_3 = 0 \) (or equivalently \( \lambda_1 = \lambda_2 = \lambda_3 = 0 \)) into (2.12). One easily finds:

\[
W_{11}(u|0,0,0) = \frac{1 + \frac{u}{12}}{1 - \frac{u}{12}}
\]  

(2.16)

which is the Padé \((1,1)\) \((P_{11})\) approximation of the exponential function also known, when expressed in the variable \( \lambda h \), as the Crank-Nicolson integration scheme or the trapezoidal rule \([14]\). Its local truncation error is equal to:

\[
e^{\lambda h} - P_{11}(\lambda h) = -\frac{1}{12} \lambda^3 h^3
\]  

(2.17)

which gives immediately the value of \( C \) in (2.15): \( C = -\frac{1}{12} \). The Crank-Nicolson approximation has, at small time steps, the highest order of a \((1,1)\) type approximation. At large values of \( |u| \), on the contrary, it is badly behaved since \( \lim_{|u| \to \infty} P_{11}(u) = -1 \) whereas the exponential function tends to zero.

2.2.2. To cope with "stiff" problems one may, for instance, interpolate at infinity. Putting \( u_1 = u_2 = 0 \) and \( u_3 = -\infty \) in (2.12) gives:

\[
W_{11}(u|0,-\infty,0) = \frac{1}{1-u}
\]  

(2.18)

which is the Padé \((0,1)\) \((P_{01})\) approximation of \( e^u \), known as the backward Euler formula. This is a strongly A-stable one-step integration scheme according to Definition 2 of §1.6. A satisfactory behaviour at large time steps (i.e. \( O(\frac{1}{h}) \)) is obtained at the expense of one order in the local truncation error near the origin. Indeed, a series expansion gives:

\[
e^{\lambda h} - P_{01}(\lambda h) = -\frac{1}{2} \lambda^2 h^2
\]  

(2.19)

\( W_{11} \) is not strongly A-stable since \( \lim_{|u| \to \infty} W_{11} \neq 0 \) in general. But, nevertheless, it is interesting to examine more closely its behaviour at large values of \( u \). This is important both for step-lengthening and for a correct description of those eigenvalues of large absolute value.
which cannot be matched with 2 or 3 degrees of freedom at most. Suppose the interpolated eigenvalues satisfy the inequality \( \lambda_2 < \lambda_1 < 0 \); introducing \( \lambda \) in (2.9) and (2.10) (with \( N = 1 \)), gives:

\[
W_{11}(\lambda h, \lambda_1 h, \lambda_2 h; 1) = \frac{\lambda_1 h}{\lambda + \lambda_1} \frac{(\lambda_2 - \lambda_1)(e^{\lambda_2 h} - 1)}{(\lambda_2 + \lambda_1)(e^{\lambda_1 h} - 1)} + \frac{\lambda_1 h}{\lambda + \lambda_1} \frac{(\lambda_2 - \lambda_1)(e^{\lambda_1 h} - 1)}{(\lambda_2 + \lambda_1)(e^{\lambda_2 h} - 1)}.
\]

Since both \( \exp(\lambda_1 h) \) and \( \exp(\lambda_2 - \lambda_1)h \) tend to zero for increasing values of \( h \), one finds immediately:

\[
\lim_{h \to \infty} W_{11}(\lambda h, \lambda_1 h, \lambda_2 h; 1) \leq e^{-(\lambda_1 h)} \frac{1 + (\lambda_2 + \lambda_1)}{(\lambda + \lambda_1)(\lambda_2 - \lambda_1)}.
\]

The error, for given \( \lambda_1 \) and \( \lambda_2 \), vanishes exponentially with increasing time steps as fairly well illustrated by the numerical example shown on Fig. 1. We have evaluated the approximation errors \( \delta(\lambda) \) as a function of \( h \), for a series of values of \( \lambda \), with interpolation at \( \lambda_1 = -1.5 \) and \( \lambda_2 = -5.0 \). Also shown on the figure are the \( P_0 \) and \( P_1 \) approximations for \( \lambda = -1.0 \). The superiority of the \( W_{11} \) scheme appears quite clearly: time-step lengthening should be much more feasible in the latter case than with both former ones.

2.2.3. Let us pursue our investigation concerning the choice of the interpolation points. It might appear that in many instances, the use of \( \lambda_2 = -\infty \) is unnecessary to cope with rapidly decaying components. An exact treatment of the eigenvalue with greatest absolute value is quite sufficient, indeed. Letting \( \lambda_1 \) and \( \lambda_2 \) successively tend to zero, one obtains through (2.12):

\[
W_{11}(\lambda h, \lambda_1 h, \lambda_2 h; 0) = \frac{1 + e^{\lambda h}}{1 - (1 - \lambda)\lambda h}
\]

with

\[
\lambda = \frac{\lambda_2 h}{e^{\lambda_2 h} - 1} = \frac{1}{\lambda_2 h}.
\]
This is the approximation suggested by LINIGER and WILLOUGHBY in
[\textit{15}], \(\textit{LW}\), whose local truncation error is given by (2.15):
\[
\exp(\lambda h) = \tilde{w}_{11}(\lambda h, \lambda_2 h, 0) \leq -\frac{1}{12} (\lambda - \lambda_2) \lambda^2 h^2
\]
(2.23)

For large time-steps \(\textit{LW}\), unfortunately, has the same characteristics
as \(\textit{P}_{11}\) which prevents it from being an interesting tool for time-step
lengthening.

2.2.4. A more valuable suggestion consists of the interpolation
at infinity and at two adequately chosen eigenvalues of the problem.
Provided \(\lambda_2 > 0\), this integration scheme guarantees A-stability
and even strong A-stability. Let \(\lambda_2\) tend to \(-\infty\); one obtains:
\[
\tilde{w}_{11}(\lambda h, \lambda_1 h, \infty, \lambda_2 h) = \frac{(\lambda_2 - \lambda_1) h}{(\lambda_2 h - \lambda_1 h) + \lambda h(e^{\lambda h} - 1)}
\]
(2.24)

This result, known as the G01 approximation, has been given previously
by DEVOGHT, JAUCOT and MACHGEELS from a quite different point of view
and has proved to be quite useful \([16]\). Once again, strong A-stability
is obtained at the price of one order in the truncation error
near the origin:
\[
\exp(\lambda h) - G_{01}(\lambda h) \leq -\frac{1}{2} (\lambda - \lambda_1)(\lambda - \lambda_2) h^2
\]
(2.25)

2.2.5 We wanted to show in this paragraph, how the \(W_{11}\) algorithm
unifies most of the existing first-order integration schemes. There
is but one important of them which does not fit into our framework:
the Chebyshev-type approximation suggested by VARGA \([17,18]\) \(\text{Ch}_{11}(\lambda h)\),
which among all rational functions of type \((1,1)\) minimizes the maximum
approximation error, over the entire spectrum:
\[
\text{Ch}_{11}(\lambda h) = \min_{a_{i, b_i}} (\max_{\lambda h \geq 0} |\exp(\lambda h) - \frac{a_{o+1} \lambda h}{1 + b_i \lambda h}|)
\]
(2.26)
The result, unfortunately, is not A-stable but this may be compensated by using a "shift" analogous to the one suggested at the beginning of this paragraph \([18]\). The coefficients which define \( C_{11}(\lambda h) \) as well as those corresponding to higher-order rational approximations are given in \([19]\).

The main results of this paragraph are synthesized in Table 1: the \( W_{11} \) algorithm provides an integration scheme with spectral matching at three eigenvalues at most. Its A-stability is ensured provided one interpolation point be located in \( \Re(\lambda h) > 0 \). If, moreover, \( \lambda_2 \) is set equal to \(-\infty\), the algorithm is strongly A-stable in the sense of GEAR.

2.3. The extrapolation technique

Extrapolation is a well known and widely used technique allowing the acceleration of convergence in the numerical process which leads to the determination of an unknown quantity \([20]\). We shall briefly recall its principle.

If the current numerical process \( T \) used to evaluate the quantity \( a_o \) has a power series expansion in terms of a parameter \( h \):

\[
T(h) - a_o = \sum_{k=1}^{\infty} a_k h^k
\]

\( y_k \) being positive and \( y_1 < y_2 < y_3 \ldots \), one might try to combine in some way, evaluations of \( T \) at different values of \( h \), to get a resulting process \( \hat{T} \) whose power expansion (2.27) does not contain anymore some of the lowest powers of \( h \). The interest of the method lies in the fact that for a given total number of arithmetic operations, one might obtain a better global accuracy using the extrapolation process \( \hat{T} \) instead of \( T \) with the corresponding refined mesh. There are various ways leading to that objective: polynomial extrapolation or rational extrapolation. The technique which is used here belongs to the first family: it is called Romberg's iterative linear extrapolation.

Let \( h_i = h/2^i \) (\( i=0,1,\ldots \)) and \( T_i^o \), the corresponding value \( T(h_i) \). A triangular scheme is built column by column, starting from the
The diagonal elements are the successive extrapolation schemes. An explicit determination of the first two terms gives:

$$T_0^0 = \frac{(4T_0^1 - T_0^0)}{3}$$  \hspace{1cm} (2.30)

$$T_0^2 = \frac{(64T_0^2 - 20T_0^1 + T_0^0)}{45}$$

These expressions are known, respectively, as Simpson's rule and Boole's rule when applied to the trapezoidal quadrature formula. Romberg's extrapolation algorithm eliminates one term of (2.27) at each stage. It happens that when applied to the trapezoidal approximation of $e^{\lambda h}$, the Simpson's rule $(\frac{4}{3}, - \frac{1}{3})$ increases the convergence of two orders of magnitude, i.e.:

$$e^{\lambda h} - (\frac{4}{3} P_{11}^{2}(\frac{\lambda h}{2}) - \frac{1}{3} P_{11}^{1}(\lambda h)) \approx \frac{1}{720} (\lambda h)^5$$  \hspace{1cm} (2.51)

which is comparable to the truncation error of a second-order diagonal Padé approximation. Each stage of the computation involves 3 arithmetic operations instead of 1: the extrapolated formula is expected to give better accuracy than $P_{11}^{2}(\frac{\lambda h}{2})$, as will be shown in the next section. Moreover it has the computational advantage of being factorized as mentioned in the first section. When integrating the system (1.1) in the interval $(0,t)$ with time step $h(t=nh)$, two possibilities occur:
\[ e^{\lambda h} = \left( \frac{4}{3} P_{11}^{h2} \left( \frac{\lambda h}{2} \right) - \frac{1}{3} P_{11}(\lambda h) \right)^N \]

\[ \frac{4}{3} P_{11}^{2N} \left( \frac{\lambda h}{2} \right) - \frac{1}{3} P_{11}(\lambda h) \]

A series expansion shows that both cases give rise to the same error at time \( t \). However these two schemes are not equivalent on computational grounds, the first one necessitating twice the storage of the operator.

Since \( W_{11}(\lambda h) \) has exactly the same type of error expansion than \( P_{11}(\lambda h) \) except for the coefficient \((\lambda - \lambda_1)(\lambda + \lambda_1)(\lambda - \lambda_2)\) which may be factorized, one has to expect similar results. This is indeed the case when the interpolation points are not too widely spaced. For "stiff" systems such that \(|\lambda h| \gg 1\), \( W_{11}(\lambda h) \not\gg P_{01}(\lambda h) \) and in the latter case the Simpson's rule is no more valid. Pursuing Romberg's idea, a straightforward calculation gives:

\[ e^{\frac{\lambda h}{2}} - (2 P_{01}^{h2} \left( \frac{\lambda h}{2} \right) - P_{01}(\lambda h)) = \frac{1}{6} \lambda^2 h^3 \]

The Simpson's rule applied to \( W_{11}(\lambda h) \) is not unconditionally A-stable as shown by:

\[ \lim_{|\lambda h| \to \infty} \left[ \frac{4}{3} P_{11}^{h2} \left( \frac{\lambda h}{2} \right) - \frac{1}{3} P_{11}(\lambda h) \right] = \frac{5}{3} \]

To keep A-stability, the quantities \( \lambda_1 h \) and \( \lambda_2 h \) are restricted to a domain of values shown on Fig. 2, whose frontier may be determined using the Newton-Raphson method and has a lower bound given by

\[ |\lambda_1 h|_{\min} = \ln \frac{5}{3} \approx 0.511 \]

This does not happen for the extrapolated \( P_{01}(\lambda h) \) and related schemes.

\[ \text{Figure 2.} \]
having one interpolation point at infinity which are always A-stable provided the restrictions given in 2.3 are fulfilled.

2.4. \textbf{The Newton Series}

2.4.1. Among interpolation methods, the Newton series has a definite advantage of being \textbf{permanent} \cite{21} : the addition of a new interpolation point, i.e. of a supplementary term of the series, does not modify the previous terms \textbf{(1)}. This feature makes it worthwhile for iterative type calculations or when the accuracy must be improved. Let $W(z)$ be one of the rational approximations defined in section 2.1. Therefore:

\begin{equation}
\frac{u}{e} = e^{-a} \frac{z+1}{z-1} = e^{-\frac{z(W)+1}{z(W)-1}} = F(W)
\end{equation}

where we have selected one of the branches of the inverse function $z(W)$ which is rational only if $W$ is of degree 1. A natural variable to expand $e^u$ in Newton series is $W$. Since the only singularity of $e^u$ in the unit disc is the essential singularity at $z=1$, $F(W)$ will be analytic inside the disc of radius $|W(1)| \leq 1$. We have:

\begin{equation}
F(W) = F(W_1) + \sum_{k=2}^{\infty} \left[ F_1, \ldots, F_k \right] \left( W(z_i) - W(z_{i-1}) \right)
\end{equation}

where

\begin{align*}
F_1 &= F(W_1) \\
W_1 &= W(z_1) \\
\left\{ z_i \right\} &= \text{the set of interpolation points } |z_i| < 1
\end{align*}

and the divided difference of $F(W)$ is:

\begin{equation}
\left[ F_1, F_2, \ldots, F_k \right] = \begin{vmatrix}
1 & \ldots & 1 \\
W_1 & \ldots & W_k \\
W_{k-1} & \ldots & W_k \\
F_1 & \ldots & F_k
\end{vmatrix}
\end{equation}

\textbf{(1)} This feature has been exploited in \cite{16,22} by reproducing kernel techniques.
Assume that \( W(z) = W_n(z) \). It therefore follows that \( W(z) \) interpolates \( F(W) \) at \( n \) points \( z_1, z_2, \ldots, z_n \) and \( F_k = W_k \) for \( k = 1, \ldots, n \). If \( 2 \leq k \leq n \), two lines of the numerator's determinant in (2.38) will be equal and 
\[
[F_1, F_2, \ldots, F_k] = 0.
\]
On the other hand:
\[
F_1 + [F_1, F_2] (W(z) - W(z_1)) = W_1 + \frac{W_2 - W_1}{W_2 - W_1} (W(z) - W_1) = W(z) \tag{2.39}
\]
and
\[
F(W) = W(z) + \left[ \sum_{i=1}^{n} (W(z) - W(z_i)) \prod_{k=n+1}^{i-1} [F_1, F_2, \ldots, F_k] \prod_{j=n+1}^{k} (W(z) - W(z_j)) \right] \tag{2.40}
\]
Let \( F_N(z) \) be the truncated series, whose last term is
\[
[F_1, F_2, \ldots, F_N] \prod_{i=1}^{N-1} (W(z) - W(z_i)) \tag{2.41}
\]
The remainder \( F(W) - F_N(W) \) may be cast in the following form:
\[
F(W) - F_N(W) = \left[ F(W), F_1, F_2, \ldots, F_N \right] \prod_{i=1}^{N} (W(z) - W(z_i)) \tag{2.42}
\]
It is known \([21]\) that:
\[
\left| [F(W), F_1, \ldots, F_N] \right| \leq \frac{1}{(N+1)!} \max_{z \in D} \left| F(N+1)(z) \right| \tag{2.43}
\]
where \( D \) is the smallest convex set which contains all \( z_i \). Introducing (2.36) into (2.42), we have:
\[
\left| F(W) - F_N(W) \right| \leq \frac{1}{(N+1)!} \max_{z(u) \in D} \left| e^u \right| \prod_{i=1}^{N} \left| (W(z) - W(z_i)) \right| \leq \frac{e^{\omega h}}{(N+1)!} \prod_{i=1}^{N} \left| (W(z) - W(z_i)) \right| \tag{2.44}
\]
where
\[
\max_{z(u) \in D} \left| e^u \right| \leq \max_{\text{Re } u < \omega h} \left| e^u \right|
\]
When \( N > n \), a more convenient expression for the error is:

\[
F(W) - F_N(W) = \frac{1}{i \pi} \sum_{j=1}^{N} \frac{F(\frac{j}{j - W})}{j - W} \prod_{i=1}^{j} (\frac{W - \frac{1}{j}}{\frac{j}{j - W}}) \, d_j^2
\]  

(2.45)

Let \( W \) be interior to the lemniscate \( \xi_j = \prod_{i=1}^{N} (W - W_i)^{1/2} \). We have \( \xi_j < \xi_j' \) for \( j > j' \). For a given set \( \{ W_i \} \), there is a maximum value of \( j' \) such that \( \xi_j < \xi_j' \). Therefore:

\[
|F(W) - F_N(W)| \leq \left( \frac{1}{i \pi} \right)^{N/2} \prod_{j=1}^{N} \frac{|F(\frac{j}{j - W})|}{|j - W|} \prod_{j=1}^{N} \frac{|d_j|}{2\pi} = \left( \frac{1}{i \pi} \right)^{N/2} \prod_{j=1}^{N} \frac{|d_j|}{2\pi} \frac{d_j}{2\pi j - W_i} = \left( \frac{1}{i \pi} \right)^{N/2} \prod_{j=1}^{N} \frac{|d_j|}{2\pi j - W_i} = \left( \frac{1}{i \pi} \right)^{N/2} \prod_{j=1}^{N} \frac{|d_j|}{2\pi j - W_i}
\]  

(2.46)

for \( W < \xi_j < \xi_j' \) since \( F(\frac{j}{j - W}) \) on the unit circle boundary is the modulus of \( e^u \) on the imaginary axis of \( u \). The optimal set \( \{ W_i \} \) necessary in order that \( \xi_j' \) fills the unit circle "as well as possible" is an open problem.

Translating the results for matrix-valued functions, one has:

\[
F_n(hA) = W(hA) + \left[ e^{\lambda_1}, \ldots, e^{\lambda_n} \right] \prod_{i=1}^{N} (W(hA) - W(h\lambda_i))
\]  

(2.47)

where, for short, we write \( W(hA) \) instead of \( W(z(hA)) \). We remind that, in fact, \( W(hA) \) is a function of \( h \) and \( A \) and not only of the product. Moreover:

\[
\|F_N(W(hA)) - e^{hA} - 1\|_{(N+1)!} \leq \frac{1}{(N+1)!} e \prod_{j=1}^{N} (W(hA) - W(h\lambda_j))
\]  

(2.48)

2.4.2. We shall now look for a development valid for the intermediate time \( 0 \leq t \leq h \). We approximate

\[tA \underset{\text{approx}}{=} e^{hA} = e^{\frac{t}{h}A} \]

by the full development:

\[
F_N(W) = F_1 + \sum_{k=2}^{N} \frac{F_1, \ldots, F_k}{k!} \prod_{i=1}^{k-1} (W(hA) - W(h\lambda_i))
\]  

(2.49)
But \( F_j - F(W) = \frac{t}{h} u_j = e^{\frac{t}{h}} j \), and therefore we obtain the interpolation formula for \( e^{t/\lambda} \):

\[
F_N(t, W) = e^{\frac{t}{\lambda}} + \sum_{j=1}^{N} e^{\frac{t}{\lambda}} ... e^{\frac{t}{\lambda} + \left(\frac{h}{\lambda} \right) j} (W(h) - W(h)) \quad (2.50)
\]

where the divided difference is given by (2.38). Eventually, when \( W(u) \) interpolates \( e^u \) at \( u_j = \lambda_j h \), \( j=1, \ldots, n \) we can replace \( W(\lambda_j h) \) by \( e^{\lambda_j h} \). For \( t=0 \), \( F_N(0, W) = 1 \) and for \( t=h \), \( F_N(h, W) = W(h) \) defined by (2.49).

Explicitly, when \( W(h) = W_{\lambda_1}(h) \), interpolating for \( \lambda_1, \lambda_2, \lambda_3 \):

\[
F_1(t, W) = e^{\frac{t}{\lambda_1}} I \\
F_2(t, W) = e^{\frac{t}{\lambda_2}} I + e^{\frac{t}{\lambda_1}} \left( \frac{W(h) - e^{\lambda_1}}{W(h) - e^{\lambda_1}} \right) \quad (2.51)
\]

\[
F_3(t, W) = e^{\frac{t}{\lambda_3}} I + e^{\frac{t}{\lambda_1}} \left( \frac{W(h) - e^{\lambda_1}}{W(h) - e^{\lambda_1}} \right) + e^{\frac{t}{\lambda_2}} \left( \frac{W(h) - e^{\lambda_2}}{W(h) - e^{\lambda_2}} \right) \quad (2.52)
\]

\[
F_4(t, W) = e^{\frac{t}{\lambda_4}} I + e^{\frac{t}{\lambda_1}} \left( \frac{W(h) - e^{\lambda_1}}{W(h) - e^{\lambda_1}} \right) + e^{\frac{t}{\lambda_2}} \left( \frac{W(h) - e^{\lambda_2}}{W(h) - e^{\lambda_2}} \right) \quad (2.53)
\]

and

\[
F_1(h, W) = e^{\frac{t}{\lambda_1}} I \\
F_2(h, W) = F_3(h, W) = W(h)
\]

Characteristically, \( F_3(h, W) = F_2(h, W) \) although \( F_3(t, W) \neq F_2(t, W) \) for \( 0 \leq t < h \). Let us see why. We have:
Developing the first bracket in powers of $h$ and introducing (3.15) into the second one gives:

$$F_2(t,w) - e^{tA} = (t_{1}-A)(t_{2}-A) \frac{t(h-t)}{2}$$

$$+ \frac{h^3}{12} (t_{1}-A)(t_{2}-A)(A+\lambda_1) \frac{t \lambda_2 - t \lambda_1}{\lambda_2 - \lambda_1} + O(h^4) \quad (2.56)$$

Therefore, the error is $O(h^3)$ at the end-point only, and only $O(h^2)$ for $t < h$. Moreover as it should, the error is zero for vectors that belong to the subspace spanned by the eigenvectors associated with the eigenvalues $\lambda_1, \lambda_2$ for all $t$. If we enlarge that subspace to $\lambda_3$ by a suitable shift, the result is only exact for the end-point. We see that the last term of $F_2(t,w)$ brings the missing term containing $e^{t_3t}$ giving an exact result for the subspace associated with $(\lambda_1, \lambda_2, \lambda_3)$ for all $t$, without modifying $F_2(hw)$ at the end-point, which is already exact.

### 2.4.3. The evaluation of the solution of $\frac{d\psi}{dt} = A\psi(t) + Q(t)$, i.e.

$$\psi(t) = e^{tA} \psi(0) + \int_0^t e^{(t-\tau)A} Q(\tau) \, d\tau \quad (2.57)$$

can be made approximately by:

$$\psi_N(t) \approx F_N(t,w) \psi(0) + \int_0^t F_N(t-\tau,w) Q(\tau) \, d\tau \quad (2.58)$$
\[
\psi_N(t) = \sum_{k=1}^{N} \left[ e^{t\lambda_1}, \ldots, e^{t\lambda_k} \right] \int_{\mathcal{O}} (W(hA)-W(hA)) \psi_0(t)
\]

\[
+ \sum_{k=1}^{N} \left[ e^{t(t-\tau)\lambda_1}, \ldots, e^{t(t-\tau)\lambda_k} \right] \int_{\mathcal{O}} q(\tau) d\tau
\]

(2.59)

By (2.38) \[e^{t\lambda_1}, \ldots, e^{t\lambda_k} = \sum_{j=1}^{k} \alpha_j e^{t\lambda_j} \psi_k(t)\] where the \(\alpha_j\) are constants.

Let:

\[
Z_k = \sum_{i=1}^{k-1} \left[ W(hA)-W(hA) \right] \psi_0(t)
\]

(2.60)

\[
V_k(t) = \sum_{i=1}^{k-1} \left[ W(hA)-W(hA) \right] Q(t)
\]

(2.61)

The solution is built sequentially, using the following set of equations:

\[
\psi_N(t) = \psi_{N-1}(t) + f_N(t) Z_N + Q_N(t)
\]

\[
Z_N = (W(hA)-W(hA)) Z_{N-1}
\]

\[
Q_N(t) = Q_{N-1}(t) + \int_{0}^{t} f_N(t-\tau) V_N(\tau) d\tau
\]

(2.62)

\[
Z_1 = e^{t\lambda_1} \psi_0(t)
\]

\[
V_N(t) = (W(hA)-W(hA)) V_{N-1}(t)
\]

\[
V_1(t) = Q(t)
\]
2.4.4. As final remarks, let us point the following:

1. \( F_N(t,W) \) is not in general A-stable, even if \( W \) is A-stable. However the standard Schur test can be applied to the power series of \( W \), in order to find the set of interpolation points compatible with A-stability.

2. \( F_1(t,W) \) is connected with the metastatic method of GALATI [23], provided that an additional normalization factor be introduced.

3. Each step \( Z_{N-1} \rightarrow Z_N \), or in general the evaluation of \( W(hA) \) needs the inversion of a matrix \( I - EA \) where \( E \) is a constant. Whenever the multinode model is used DA NOBREGA-TURNAGE-HENRY scheme [8,26] can be used, therefore combining the advantages of spectral matching, A-stability and fast inversion.

4. The scheme proposed by DA NOBREGA and HENRY starts from the identity

\[
e^{hA} = W(hA) + \sum_{i=1}^{K} \left( e^{h\lambda_i} - W(h\lambda_i) \right) P_i
\]

where \( P_i \) is the projector on the \( i \)th eigensubspace of \( A \) and \( K \) the total number of eigenvalues (supposed distinct). The sum is truncated and the projector evaluated by diagonalization which can be done explicitly for small matrices. If we use instead the equivalent operator

\[
P_i = \prod_{k \neq i}^{K} \left( \frac{A - \lambda_k}{\lambda_i - \lambda_k} \right) \quad \text{or what amount to the same}
\]

\[
P_i = \prod_{k \neq i}^{K} \frac{W(hA) - W(h\lambda_k)}{W(h\lambda_i) - W(h\lambda_k)},
\]

we end up with a Lagrange interpolation series for \( e^{hA} \).

Therefore our scheme is different in the following respects:

(a) \( W(hA) \) is a general A-stable approximation interpolating at arbitrary points, instead of a Padé approximation with osculating interpolation at the origin;

(b) a Newton series is used instead of a Lagrange series, adding a permanence property;

(c) the annihilation of the error of the \( i \)th eigenmode is done
sequentially by solving a linear system instead of computing explicitly the eigenvectors. Both problems boil down to solving a static "prompt neutron" problem.

2.5. The equivalent integral formulation

2.5.1. Let \( \frac{dy}{dt} = A(t) y(t) + S(t) \). Multiplying both members to the left by the operator \( V(t) \) and integrating by parts over \( t \in [0,h] \) gives:

\[
V(h)y(h) - V(0)y(0) = \int_0^h \left( \frac{dV}{dt} + V(t)A(t) \right)y(t)dt + \int_0^h V(t)S(t)dt \tag{2.63}
\]

Let \( V^{-1}(h)V(t) = T(h,t) \) with \( V(0) = I \). We have then:

\[
y(h) = T(h)y(0) + \int_0^h T(h,t)S(t)dt + \int_0^h \left[ \frac{dT}{dt} + T(h,t)A(t) \right] y(t)dt \tag{2.64}
\]

This is an identity, so far as \( T(h,t) \) is defined. If we choose

\( T(h,t) = F_2(h-t,W) \), and \( A \) some "average" value of \( A(t) \), it is easily shown by substitution of (2.52) into (2.64) that:

\[
y(h) = W(h,A)y(0) + \int_0^h F_2(h-t,W)S(t)dt + \\
\left\{ \begin{array}{c}
\frac{(A-\lambda_2)(W(h,A)-e)}{h\lambda_2 - e\lambda_1} \int_0^h e^{(h-t)\lambda_2} y(t)dt \\
- \frac{(A-\lambda_1)(W(h,A)-e)}{e^{h\lambda_2} - h\lambda_1} \int_0^h e^{(h-t)\lambda_1} y(t)dt \\
+ \int_0^h F_2(h-t,W)(A(t)-A)y(t)dt
\end{array} \right. \tag{2.65}
\]
The third term incurred by the use of the approximate semi-group $F_2$ is of order $O(h^2)$. The last term is also of order $O(h^2)$ if we define, for instance, $A$ as $A(h/2)$. If we assume now, for simplicity, $A(t)$ constant over the interval $[0,h]$ and decompose $A=M+N$, we have the more general identity:

$$y(h) = T(h)y(0) + \int_0^h T(h-t)S(t)dt + \int_0^h \left[ \frac{dT(h-t)}{dt} + T(h-t)N \right] y(t) dt$$

If we substitute in the right-hand side integrals, two-point interpolation formulas for $y(t)$ involving $y(h)$ and $y(0)$, we obtain a general canvass for (probably) all known integration schemes of neutron kinetics, provided that:

a/ the interpolation is not necessarily identical for each integral

b/ the calculation is cyclic, each step being in fact one-half step.

Table 2 contains a few examples of known algorithms, for both split- ted and unsplit operators. A glance at the table shows that only a fraction of the possible choices for $T(h)$, $N$, $N$, $y_1(t)$ and $y_2(t)$ has been used.

2.5.2. As a final remark, we note that the operator-splitting may be handled in a much more natural way. For instance:

$$S(h,A,B) = e^{\frac{hA}{2}} e^{\frac{hB}{2}} e^{\frac{h(A+B)}{2}} = e^{hA} + O(h^2)$$

or

$$T(h,A,B) = \frac{hA}{6} e^{\frac{2hA}{3}} e^{\frac{2hB}{3}} e^{\frac{1hB}{3}} - \frac{1}{6} e^{hA} e^{hB} + O(h^4)$$

Both expressions are optimal for their respective order of accuracy as far as the number of operations is concerned. If each exponential $e^{hA}$ and $e^{hB}$ is replaced by $W(hA)$, correct to $O(h^2)$, we have
which is $A$-stable with respect to $A+B$, but does not reproduce correctly, in general, the spectrum unless $A$ and $B$ commute.

On the other hand, $O(h^4)$ accuracy is retained in (2.68) only if $W(hA)$ and $W(hB)$ are correct to $O(h^4)$ which involves higher order formulas like $W_{22}$. However, the extrapolation $\frac{4}{3} S^2(h, A, B) - \frac{1}{3} S(h, A, B)$ gives $O(h^4)$ with 8 matrix inversions, and is $A$-stable if the maximum modulus of $W(hA)$ and $W(hB)$ is about 0.9.
3. NUMERICAL TEST PROBLEMS.

Two model problems will be analysed to illustrate the content of the preceding section.

3.1. A one-dimensional diffusion problem.

Let $T(x,t)$ be the temperature distribution at time $t$, in a finite one-dimensional medium devoid of any heat source (or heat sink):

$$\frac{\partial T(x,t)}{\partial t} = \frac{\partial^2 T(x,t)}{\partial x^2} \quad 0 < x < 1 \quad (3.1)$$

with the boundary conditions

$$T(0,t) = T(1,t) = 0 \quad \forall t \in (0, \infty) \quad (3.2)$$

Given any initial temperature distribution $T(x,0)$, (3.1)-(3.2) is known to admit a unique solution which is easily obtained using Fourier series. If, for instance, $T(x,0) = \sin \frac{2\pi}{x}$, one finds:

$$T(x,t) = -\frac{8}{\pi} \sum_{k=0}^{\infty} \frac{\sin \left(\frac{(2k+1)\pi}{x}\right)}{(2k-1)(2k+1)(2k+3)} e^{-\left(2k+1\right)^2 \pi^2 t} \quad (3.3)$$

We, first, discretise spatially the problem by introducing an equidistant grid $G$ on $[0,1]$ with $N$ subintervals of length $h=1/N$:

$$G = \left\{ x_{\nu} = \frac{\nu}{N}, \ \nu=0(1)N \right\} \quad (3.4)$$

If $T(x_1,t) = T_1(t)$, and the usual finite difference representation is used for the spatial derivatives, the "continuous problem" (3.1)-(3.2) with initial condition $T(x,0)$ is transformed into:

$$\frac{dT}{dt} = A \vec{T}(t) \quad (3.5)$$

with

$$\vec{T}(t) = (T_1(t), T_2(t), \ldots, T_{N-1}(t))^T \quad (3.6)$$
and $A$ a $(N-1) \times (N-1)$ matrix with the familiar tridiagonal form:

$$
A = \begin{pmatrix}
-\frac{2}{h^2} & \frac{1}{h^2} & 0 \\
\frac{1}{h^2} & -\frac{2}{h^2} & \frac{1}{h^2} \\
0 & \frac{1}{h^2} & -\frac{2}{h^2}
\end{pmatrix}
$$

(3.7)

The eigenvalues of $A$, $\lambda_k (k=1, \ldots, N-1)$ are approximations of the $(N-1)$ first eigenvalues of the continuous operator defined by (3.1) and (3.2). The latter, $\mu_k$, are in infinite number along the negative real axis, the system being dissipative:

$$
\lambda_k = -k^2 \pi^2 \\
\lambda_k \approx \mu_k \\
\mu_k = -k^2 \\
k=1, \ldots, N-1
$$

(3.8)

When $N=20$, the extreme eigenvalues of $A$ are respectively equal to $-9.849$ and $-1.590 \times 10^3$; we are faced to solve a stiff system of equations as defined in Section 1. It happens, however, that for realistic initial conditions such as those leading to (3.3), the various eigenmodes of the equation are not excited in the same way: in that case the initial amplitudes are proportional to $1/k^3$. The problem (3.5), therefore, is not truly stiff, the eigenvalues with large absolute magnitude having almost no influence on the final result.

The exact solution of (3.5) is easily obtained using, for instance, a fast diagonalisation routine: we call it $\bar{T}$ _ex_. We have made a series of calculations with the various approximate schemes mentioned in Section 2 at $t=0.1$ s with $N=20$ and the initial condition:

$$
T_i(0) = \sin^2 \pi \frac{i}{N} \quad i=0, \ldots, N
$$

(3.9)

The table 3 gives a sample of our results with the corresponding
curves on Fig. 3. The numerals between parentheses indicate the interpolated eigenvalues. The results are given in terms of a discrete $L^2$-norm:

$$n = - \log_{10} \frac{\| T_{\text{ex}} - T_{\text{app}} \|_{L^2}}{\| T_{\text{ex}} \|_{L^2}}$$

(3.10)

with

$$\| T_{\text{ex}} - T_{\text{app}} \|_{L^2} = \left( \sum_{i=1}^{N-1} (T_{\text{ex},i} - T_{\text{app},i})^2 \right)^{1/2}$$

(3.11)

n is almost equal to the number of exact digits in the approximation. The best results are those with $\omega_{11}$ or $G_{01}$ interpolating $\lambda_1$ and $\lambda_2$. This is no surprise since (cfr. (3.3)) even-order eigenmodes are not excited with the given initial condition. A few refinements of the time integration step are quite enough to attain the maximum accuracy allowed by round-off errors. Fig. 3 displays, in fact, two families of curves, according to their slopes: those which, like $P_{01}$, have an $O(h)$ time-integrated behaviour and those, like $P_{11}$, with an $O(h^2)$ global error. We remark that whenever a judicious interpolation is made, the accuracy may be considerably enhanced. This is the case, for instance, for $LW(1)$ and $W(1,2)$ whose curves are above and parallel to $P_{11}$. $LW(2)$ and $LW(19)$, on the contrary are located well below $P_{11}$ which is not surprising given the distribution (5.8) of the eigenvalues. In the latter case, for $h=10^{-1}$, $\lambda_{19}h = -1.60 \times 10^2$, and this is almost equivalent to an interpolation at $-\infty$ as evidenced by the numerical results: $LW(19) \approx P_{01}$ for time steps $h > 5.10^{-3}$. $G_{01}(1,2)$ gives an excellent result when the calculation is made in one or a few steps. Its convergence order being equal to that of $P_{01}$, successive step refinements are not as effective as one should expect.

Potential consequences of the lack of A-stability are clearly shown by the results obtained with $Ch_{11}(\lambda h)$ which for $|\lambda h| < 3.63 \times 10^{-2}$ is such that $|Ch_{11}(\lambda h)| > 1$. The minimum step associated is given by

$$h_m = 3.63 \times 10^{-2}/\pi^2 \approx 3.68 \times 10^{-5}$$

which corresponds approximately to our transition point of steadily growing errors.

The Fig. 4. displays the results obtained when applying the first and second order extrapolation rules (2.30 a) and (2.30 b) to $W_{11}(1,2)$. The global errors are equal, respectively, to $O(h^4)$ and $O(h^6)$ which is quite in agreement with theoretical predictions [20]. Also drawn
on the figure are $W_{11}(\frac{\delta}{3})$ and $W_{11}(\frac{\delta}{7})$ which for a given value of $h$ correspond to the same amount of matrix inversions as Simpson's or Boole's rule respectively. It appears quite clearly that for relatively low error levels the use of extrapolation rules is systematically to be preferred to step refinements especially if computation economy is a major requirement.

3.2. The point kinetics equations.

Point kinetics is a much more valuable testing problem for time-integration algorithms since, as we shall see below, this is a truly stiff system of differential equations. The problem was solved in its simplest form [27] without any external neutron sources or thermohydraulic coupling:

\[
\frac{dn}{dt} = \frac{f(t) - \beta}{\Lambda} n(t) + \sum_{i=1}^{I} \lambda_i c_i(t) \tag{3.12}
\]

\[
\frac{dc_i}{dt} = -\lambda_i c_i(t) + \frac{\beta_i}{\Lambda} n(t) \quad i=1, \ldots, I
\]

in standard notations. Various step-insertions of reactivity for fast as well as thermal reactors have been studied, one of which is analysed in details here. Numerical values for the delayed neutron groups and $\Lambda$ were taken from DA NOBREGA [28].

The case selected is a step of 0.5 $\$ reactivity in the fast reactor described in Table 4. The ratio of the extreme eigenvalues $|\frac{\omega_1}{\omega_{11}}| < 1.4 \times 10^5$ is fairly large. The exact number of digits

\[
p = -\log_{10} \frac{|n_{ex} - n_{app}|}{|n_{ex}|} \tag{3.13}
\]

is plotted as a function of $h$ or of the number of time steps. We have in this case essentially three different behaviours: a slope $-2$, a slope $-1$ and a step behaviour. Since the truncation error is $O(h^3)$.
for \( \tilde{w}_{11} \), the global error may be expected to be \( N \cdot O(h^3) = O(h^2) \) giving a slope -2 as exemplified by \( \tilde{w}_{11}(1,2,6) \) on Fig. 6. However this is not true of all \( \tilde{w}_{11} \) approximations, and even less of the \( P_{11} \) approximation which has the step behaviour on Fig. 5. This is a reminder that the order of the truncation error is not a good predictor of the global accuracy especially in stiff systems. Let:

\[
\begin{align*}
    n_{\text{app}}(t) &= \sum_{i=1}^{7} \alpha_i \varphi_i P_{11}^{N}(\omega h) \\
    n_{\text{ex}}(t) &= \sum_{i=1}^{7} \alpha_i \varphi_i e^{\omega h}
\end{align*}
\]

with:

\[
\begin{align*}
    \alpha_i &= \langle \overline{\phi}(0), \overline{v}_i \rangle \\
    \varphi_i &= \langle \overline{u}_i, \overline{e}_i \rangle
\end{align*}
\]

\( \overline{\phi}(0) \) is the initial vector \( (n(0), c_1(0), ..., c_7(0))^T, \overline{v}_i^T \) and \( \overline{u}_i \) respectively the left and right-hand eigenvectors of the kinetics matrix and \( \overline{e}_i \) the unit vector \( (1, 0, ..., 0)^T \). We have therefore:

\[
\mathcal{E}(t) = \sum_{i=1}^{7} \alpha_i \varphi_i \left[ e^{\omega_i t} - \frac{1}{1 - \frac{\omega_i t}{2N}} \right]^{N}
\]

the error for a fixed time \( t \) and a variable number of time steps \( N \). There are two extreme cases:

\[1^o/|\omega_i t| \gg 1 \text{, } N \ll |\omega_i t| \text{ and } \left| \frac{N + \frac{1}{2} \omega_i t}{N - \frac{1}{2} \omega_i t} \right| \geq 1 \]  \hspace{1cm} (3.17)

\[2^o/ N \to \infty \text{ and } \lim_{N \to \infty} \left( \frac{1 + \frac{1}{2} \frac{\omega_i t}{N}}{1 - \frac{1}{2} \frac{\omega_i t}{N}} \right) = e^{\omega_i t} \]  \hspace{1cm} (3.18)

When \( |\omega_i t| \gg 1 \), \( i=2, ..., 7 \), \( e^{\omega_i t} \approx 0 \); for \( N \ll |\omega_i t| \), the contribution
The error is approximately $-\varphi_i\psi_i$, although for $N\not\sim |\omega_1t|\gg 1$, the contribution to the error is virtually nil and we have therefore a step increase of $p$ reflecting the step behaviour of

$$
\left(\frac{N + \frac{1}{2} \omega_1 t}{N - \frac{1}{2} \omega_1 t}\right)^N.
$$

The greater $|\omega_1t|$, the sharper is the transition. Once $N \gg \omega_1t$, the error becomes almost independent of $N$. Similarly, because of (3.17), as long as $N \gg |\omega_1t|$, the error stays constant. We might now expect that the transition appears somewhere near the seven values of $N\not\sim |\omega_1t|$. There are, in fact, roughly two clusters of eigenvalues, one of which around 0 and the other near $-2.10^4$, since even $|\omega_2| = 7.10^5$. One step behaviour appears therefore near $N\not\sim |\omega_1t|$. The value of $N$ corresponding to the transition is determined by the initial conditions, i.e. by the relative amplitude of the eigenmodes. When $N$ is large enough:

$$
\varepsilon(t) = \sum_{i=1}^{7} \kappa_i \varphi_i \left[ e^{\omega_1 t} - \left( e^{\omega_1 h} + \sum_j \omega_j h^{j} \right)^N \right]
$$

$$
= - \sum_{i=1}^{7} \kappa_i \varphi_i \omega_1 h(N-1) = - \left( \sum_{i=1}^{7} \kappa_i \varphi_i \omega_1 h \right) h^{N-1}.
$$

This is the case for $P_{11}$ in Fig. 5 where $k=3$. On the other hand in Fig. 5, the error is drastically reduced to the level of round off ($p=8$) before the asymptotic behaviour in $h^2$ is observed. The conclusions are essentially the same for $W_{11}(1,2)$ and $W_{11}(1,6)$ because, for $t=0.1\ s$, $|\omega_6t| \not\approx 0.1$ and the interpolation points are virtually at the origin. Similarly $W_{11}(1,7) \not\approx P_{01}$ and even for $h$ down to $10^{-3}$, there is no noticeable difference between the results. However below $h=10^{-3}\ s$, the $\omega_7$ eigenvalue comes into play.

Let us turn now to the comparison of the $W_{11}$ approximations. It is essential to choose $\omega_4$ as an interpolation point in order to have a correct asymptotic behaviour. A second interpolation point should be taken near the origin: $\omega_2$ for instance. Letting the third interpolation point take successively the values $\omega_2, \ldots, \omega_6$ once again gives the 3 types of behaviour:
a/ the step behaviour for $\omega_3$, $\omega_4$, $\omega_5$

b/ the $O(h^2)$ truncation error for $\omega_6$

c/ the $O(h)$ truncation error for $\omega_7$

The step behaviour for (a) results from the fact that $\tilde{W}_{11}(\omega_1, \omega_2, \omega_3)$, $i=3,4,5$ is essentially $P_{11}$. On the other hand, $\omega_7$ is relatively far away ($\omega_7 h = 22$ even down to $h=10^{-3}$) and $\tilde{W}_{11}(\omega_1, \omega_2, \omega_7)$ is essentially equal to $P_{01}$ which explains (c). In case (b), $|\omega_6 t| \leq 30$, a very low value which means that most of the plot is left of the transition which is moreover well rounded. Therefore, we are truly in the asymptotic range. We see also that $\tilde{W}_{11}(\omega_1, \omega_2, \omega_5)$ is much better than $\tilde{W}_{11}(\omega_1, \omega_2, \omega_4) \approx P_{11}$ by displacing the interpolation point from $\omega_4$ to $\omega_5$ the overall agreement is improved.

Fig. 7, finally, gives some results concerning the application of the Newton series and the extrapolation rules. From the point of view of the computation expenses, the first order extrapolation rule is equivalent to the interpolation of four eigenvalues, both implying three matrix inversions. One has, however, to take care of the fact that when $|\omega_7 h| \gg 1$, $\tilde{W}_{11} \approx P_{01}$ which implies that (2.33) should be used instead of Simpson's extrapolation rule. This is fairly well illustrated numerically since the overall accuracy increases until $h=5 \times 10^{-2}$ after which it is maintained at a constant level. An application of the $(\frac{1}{3}, -\frac{1}{3})$ rule results in a convergence curve with the same slope as the non-extrapolated one, except for a slight displacement towards the right. The use of the Newton series with four interpolation points gives an $O(h^2)$ convergence (instead of $O(h^3)$). This is due to the interpolation at $\omega_7$ almost at infinity. The results, however, seem to be less favourable than those given by the extrapolation rule, especially with a few integration steps. This can be explained by the fact that the extrapolation rule improves the approximation accuracy, "on the average", whereas the Newton series acts pointwise. Also shown on the figure is a curve corresponding to the use of the Newton series with four interpolation points endowed with a 50% error on the exact eigenvalues in the same sense at each point. The result, clearly is not very sensitive to such uncertainties which might occur in the estimation of higher-order eigenvalues for space dependent problems. More precisely, in this case, the increase of the relative error does not exceed a factor 4, which is quite reasonable given the relatively important amount of error allowed.
CONCLUSIONS

We have shown how to develop a general $A$-stable algorithm for the integration of the neutron kinetics equations. The algorithm can be used itself as an element of a Newton series or of an extrapolation process. The implementation calls for the solution of static problems with modified absorption and sources.

The sensitivity of the results to the choice of the interpolating points, and therefore to a knowledge of the kinetics matrix eigenvalues is not important, and except for the asymptotic eigenvalue, orders of magnitude are sufficient. Most known algorithms enter into the framework of this integration scheme.

Sample problems indicate that improvements of accuracy ranging from one to two order of magnitude can be obtained either by one $W_{\text{eff}}$ method or by combination of spectral matching and extrapolation. The optimal choice of the interpolating points must probably change as the transient develops and further study on the subject is needed. Evidence has been given over the influence of the stiffness of the kinetics matrix on the effective local truncation error which may be quite different from the theoretical one.

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Figure 1.

Absolute error $\delta(h) = W_{11}(\lambda h | \lambda_1 h, \lambda_2 h; 1) - e^{\lambda h}$

- $\lambda_1 = -1.5$
- $\lambda_2 = 0.0$

$W_{ij}(\lambda h) = e^{\lambda h}$

$\lambda = 0.0$

$\lambda = 1.0$

$\lambda = 0.5$
Normalised Heat Equation

\[ \frac{\partial T}{\partial t} = \frac{1}{\alpha} \frac{\partial^2 T}{\partial x^2} \]

\[ T(x,0) = \sin^2 \pi x \]
\[ T(0,t) = T(1,t) = 0 \quad \forall t \in [0,\infty) \]

Study of convergence for various one step, first order approximations at \( t=0.1 \epsilon \)

\[ n = -\log( \frac{\| u_{\text{ex}} - u_{\text{app}} \|_{L^2}}{\| u_{\text{ex}} \|_{L^2}} ) \]
Normalized Heat Equation

Study of convergence for the \( W_{11} \) approximation with interpolation at two eigenvalues of the discretized operator \( t = 0.1s \)

Application of the first and second-order Romberg extrapolation rules to \( W_{11} \)

\[
S^{(W_{11})} = (\frac{4}{9} W_{11}^{(h)} - W_{11}^{(2h)})/2
\]

\[
B^{(W_{11})} = (\frac{5}{12} W_{11}^{(h)} - 2 W_{11}^{(2h)} + \frac{1}{3} W_{11}^{(3h)})/45
\]

\[
W_{11}^{(h)}
\]

\[
W_{11}^{(2h)}
\]

\[
W_{11}^{(3h)}
\]

\[
S^{(W_{11})}
\]

\[
B^{(W_{11})}
\]

\[
10^{-3}
\]

\[
10^{-2}
\]

\[
10^{-1}
\]

Figure 2.
Study of convergence for various one-step, first-order approximations at $t = 0.1s$

$$p = - \log \left( \frac{|\phi_{ex} - \phi_{ap}|}{\phi_{ex}} \right)$$

$N = \text{number of steps}$

Figure 5.
Point Kinetics/Fast-Reactor step reactivity insertion $\rho = 0.5$ \\

Study of convergence for various $\bar{U}_{11}$ approximations at $t=10s$

$$p = - \log_{10}(\frac{|\varphi_{ex} - \varphi_{ap}|}{\varphi_{ex}})$$

$N = \text{number of steps}$

Figure 6.
Point Kinetics/Fast-Reactor step reactivity insertion $\gamma = +0.5$ 

Application of the Newton series and extrapolation rules to the $W_{11}$ scheme at $t=0.1s$. 

---

Figure 7.
<table>
<thead>
<tr>
<th>Name</th>
<th>Type of interpolation</th>
<th>Truncation error for small h</th>
<th>Truncation error for large h</th>
<th>A-stability</th>
<th>Strong A-stability</th>
</tr>
</thead>
<tbody>
<tr>
<td>P11</td>
<td>$\tilde{w}_{11}(0,0,0)$</td>
<td>$\frac{1}{12} \lambda^3 h^3$</td>
<td>$O(1)$</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>LW</td>
<td>$\tilde{w}_{11}(0,0,1)$</td>
<td>$\frac{1}{12}(\lambda-\lambda_2) \lambda^2 h^3$</td>
<td>$O(1)$</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>P01</td>
<td>$\tilde{w}_{11}(0,-\infty,0)$</td>
<td>$\frac{1}{2} \lambda^2 h^2$</td>
<td>$O(1)$</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>$W_{11}(\lambda_1,\lambda_2)$ (M=1)</td>
<td>$\tilde{w}_{11}(\lambda_1,\lambda_2,-\lambda_1)$</td>
<td>$\frac{1}{12}(\lambda-\lambda_1)(\lambda+\lambda_1)(\lambda-\lambda_2)h^3$</td>
<td>$\frac{1}{h}\left[1 - \frac{(\lambda-\lambda_1)(\lambda_2+\lambda_1)}{(\lambda+\lambda_1)(\lambda_2-\lambda_1)}\right]$</td>
<td>Yes</td>
<td>Yes (3)</td>
</tr>
<tr>
<td>$W_{11}(\lambda_1,\lambda_2,\lambda_3)$ (M=1)</td>
<td>$\tilde{w}_{11}(\lambda_1,\lambda_2,\lambda_3)$</td>
<td>$\frac{1}{12}(\lambda-\lambda_1)(\lambda-\lambda_2)(\lambda-\lambda_3)h^3$</td>
<td>$\frac{1}{h}\left[1 - \frac{(\lambda-\lambda_1)(\lambda_2+\lambda_1+2a)}{(\lambda_3-\lambda_1)(\lambda+\lambda_1+2a)}\right]$</td>
<td>Yes</td>
<td>Yes (3)</td>
</tr>
<tr>
<td>G01(\lambda_1,\lambda_3) (1)</td>
<td>$\tilde{w}_{11}(\lambda_1,-\infty,\lambda_3)$</td>
<td>$\frac{1}{2}(\lambda-\lambda_1)(\lambda-\lambda_3)h^2$</td>
<td>$\frac{1}{h}\left[1 - \frac{(\lambda-\lambda_1)(\lambda_3+\lambda_1)}{(\lambda_3-\lambda_1)(\lambda+\lambda_1)}\right]$</td>
<td>Yes</td>
<td>Yes (3)</td>
</tr>
<tr>
<td>Ch_{11} (2)</td>
<td>Interpolation replaced by best Chebychev approximation</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>

(1) Ref : [16]
(2) Ref : [19]
(3) See discussion in the text

Table 1.
\[
y(h) = T(h)y(o) + \int_0^h \frac{dT(h-t)}{dt} + T(h-t)N_1 y_1(t) \, dt + \int_0^h (1-\alpha) \frac{dT(h-t)}{dt} + T(h-t)N_2 y_2(t) \, dt
\]

<table>
<thead>
<tr>
<th>Name</th>
<th>(T(h))</th>
<th>(\alpha)</th>
<th>(M)</th>
<th>(N)</th>
<th>(y_1(t))</th>
<th>(y_2(t))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gakkin</td>
<td>(e^{\Gamma h})</td>
<td>(\alpha)</td>
<td>(L+U+\xi \Gamma)</td>
<td>(D+(1-\alpha)^\Gamma)</td>
<td>(y(h))</td>
<td>(e^{\omega(h-t)})</td>
</tr>
<tr>
<td>Du.-Hansen (ADL) (1)(2)</td>
<td>(e^{\omega h})</td>
<td>1</td>
<td>(E_2 + \Lambda_2)</td>
<td>(\Lambda_1 + E_4)</td>
<td>(y_1(t) = e^{\omega h} \phi(h))</td>
<td>(y(o))</td>
</tr>
<tr>
<td>(\omega)-method (1)</td>
<td>1</td>
<td>-</td>
<td>(1-hA(e^{hA} - 1))^{-1}</td>
<td>(A-M)</td>
<td>(y(h))</td>
<td>(y(o))</td>
</tr>
<tr>
<td>(\omega)-method (simplified)(1)</td>
<td>1</td>
<td>-</td>
<td>(\omega A)</td>
<td>((1-\omega)A)</td>
<td>(y(h))</td>
<td>(y(o))</td>
</tr>
<tr>
<td>Time-integrated (1)</td>
<td>1</td>
<td>1</td>
<td>(A)</td>
<td>(C)</td>
<td>(y(o)(1 - \frac{t}{h}) + y(h)\frac{t}{h})</td>
<td>(-\frac{t}{h})</td>
</tr>
<tr>
<td>this paper</td>
<td>(W(h,A))</td>
<td>1</td>
<td>(A)</td>
<td>(C)</td>
<td>(p_1(t)y(o) + p_2(t)y(h)) (3)</td>
<td>(-\frac{t}{h})</td>
</tr>
</tbody>
</table>

(1) See for instance ref. [30]
(2) For one half-step only
(3) \(p_1(C) = \zeta_1^i\), \(p_1(h) = \zeta_2^i\)

Table 2.
Problème de la chaleur

\[ \frac{\partial T(x,t)}{\partial t} = \frac{\partial^2 T(x,t)}{\partial x^2} \quad 0 < x < 1 \]

\[ T(0,t) = T(1,t) = 0 \]

\[ T(x,0) = \sin^2 \pi x \]

Etude de la convergence de différentes solutions approchées vers la solution exacte en \( \tau = 10^{-1}s \).

| \( n \)   | \( n_{p01} \) | \( n_{p11} \) | \( n_{\text{cheb11}} \) | \( n_{\text{LW}(\kappa^s)} \) | \( n_{\text{LW}[1]} \) | \( n_{\text{LW}[2]} \) | \( n_{\text{LW}[19]} \) | \( n_{w_{11}[1,2]} \) | \( n_{w_{11}[1,3]} \) | \( n_{w_{11}[1,19]} \) | \( n_{G_{01}[1,3]} \) |
|----------|-------------|-------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| \( 10^{-1} \) | 0.4519 | 0.4506 | 1.2576 | 0.5792 | 0.6201 | 0.7225 | 0.4546 | 1.1646 | 2.2344 | 1.3618 | 5.3592 |
| \( 5 \times 10^{-2} \) | 0.6926 | 1.0551 | 0.6268 | 0.8152 | 1.2461 | 1.2514 | 0.7036 | 1.8615 | 2.6850 | 1.8186 | 5.8153 |
| \( 2 \times 10^{-2} \) | 1.0469 | 2.2564 | 0.6334 | 1.1682 | 2.4924 | 2.0266 | 1.0748 | 2.9427 | 3.6845 | 2.5788 | 6.8909 |
| \( 10^{-2} \) | 1.3316 | 3.0871 | 1.3486 | 1.4528 | 3.8726 | 2.6269 | 1.3397 | 4.2810 | 5.0700 | 3.1765 | 7.9653 |
| \( 5 \times 10^{-3} \) | 1.6424 | 3.7002 | 1.4472 | 1.7454 | 4.9853 | 3.2729 | 1.7494 | 5.1905 | 8.8492 | 3.7434 | 8.8767 |
| \( 2 \times 10^{-3} \) | 2.0167 | 4.4961 | -1.0215 | 2.1382 | 5.7682 | 4.0234 | 2.3565 | 5.9795 | 9.0131 | 4.4961 | 9.0120 |
| \( 5 \times 10^{-4} \) | 2.6161 | 5.7004 | -5.2704 | 2.7376 | 6.9703 | 5.2274 | 3.5003 | 7.1827 | 9.0145 | 5.6878 | 9.0128 |

\[ n = - \log_{10} \left( \frac{\| \overline{\bar{T}}_{\text{ex}} - \overline{\bar{T}}_{\text{app}} \|_{L^2}}{\| \overline{\bar{T}}_{\text{ex}} \|_{L^2}} \right) \]

Table 3.
Point kinetics / Fast-Reactor study

Step reactivity \( \xi = +0.5 \) $ - Numerical Data

<table>
<thead>
<tr>
<th>( i )</th>
<th>( \lambda_i )</th>
<th>( \beta_i )</th>
<th>( \omega_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0129</td>
<td>1.672 ( 10^{-4} )</td>
<td>( 1.536 ) ( 10^{-1} )</td>
</tr>
<tr>
<td>2</td>
<td>0.0311</td>
<td>1.232 ( 10^{-3} )</td>
<td>( -1.358 ) ( 10^{-2} )</td>
</tr>
<tr>
<td>3</td>
<td>0.154</td>
<td>9.504 ( 10^{-4} )</td>
<td>( -5.379 ) ( 10^{-2} )</td>
</tr>
<tr>
<td>4</td>
<td>0.331</td>
<td>1.443 ( 10^{-3} )</td>
<td>( -2.003 ) ( 10^{-1} )</td>
</tr>
<tr>
<td>5</td>
<td>1.26</td>
<td>4.534 ( 10^{-4} )</td>
<td>( -1.056 )</td>
</tr>
<tr>
<td>6</td>
<td>3.21</td>
<td>1.540 ( 10^{-4} )</td>
<td>( -3.030 )</td>
</tr>
<tr>
<td>7</td>
<td>-</td>
<td>-</td>
<td>( -2.2 ) ( 10^4 )</td>
</tr>
</tbody>
</table>

\[ \Lambda = 10^{-7} \text{ s} \]

Table 4
DISCUSSION

A.F. Henry

Could you comment on extension to space dependent problems and also to situations in which the A matrix changes in time?

J. Devooght

A two-dimensional 1-group code, with triangular cell, cubic finite elements is now in the process of debugging. The code incorporates the features mentioned in the paper. In general, one matrix inversion is needed per time step; the case of splitted operators is dealt with on p. 50.

When the matrix is time dependent, it is necessary to deal with proper averages, i.e. consistently keep the error to the same order \( o(h^3) \) as the one used in the \( W_{11} \) approximation.
A.A. Harms, W.J. Garland, W.A. Pearce, M.F. Harding, O.A. Trojan, J. Vlachopoulos

MULTIPLE TEMPORAL-MODE ANALYSIS FOR THREE-DIMENSIONAL REACTOR DYNAMICS

McMaster University, Hamilton, Ontario, Canada
MULTIPLE TEMPORAL-MODE ANALYSIS FOR THREE-DIMENSIONAL REACTOR DYNAMICS

A.A. Harms, W.J. Garland, W.A. Pearce,
M.F. Harding, O.A. Trojan, and J. Vlachopoulos

Faculty of Engineering
McMaster University
Hamilton, Ontario, Canada

Abstract

A multiple temporal-mode transformation combined with spatial differencing is developed and applied in a two-group, three-dimensional reactor dynamics analysis using the diffusion approximation. It is found that this solution formalism leads to an apparently efficient and effective method for the study of fast transients for time intervals before a global flux trend has been established. Calculational results for a simplified cylindrical reactor under conditions of a fast transient and some general properties of the formalism are discussed.
Introduction

The development of efficient and effective analytical and calculational models which describe a wide range of dynamic characteristics of a nuclear reactor in three dimensions has long represented a desirable goal. Experience with low-dimensional calculations involving suitably chosen analytical descriptions and numerical strategies suggests that this goal may be attainable.

The three-dimensional, multi-group, time-dependent analysis of a nuclear reactor generally provides a basis for considerable scope in exploring various strategies. Factors such as available computational resources, detail of system description, temporal domain of interest, and others combine to provide various though restricted options.

Here we describe a three-dimensional, two-group, time-dependent neutron diffusion analysis based on the use of a multiple temporal-mode transformation combined with finite differencing in space. As will become clear, the chosen analytical formalism seems particularly applicable for fast transients; in this context, this defines the dynamics of a nuclear reactor before a dominant global flux trend has been established. In the following we will describe the solution formalism and relate it to a dynamic discretization. Finally, some preliminary calculational results will be presented and some general features of the solution formalism will be identified.

Multiple-Mode Solution Representation

The three-dimensional, multi-group, time-dependent neutron diffusion description of a nuclear reactor with or without delayed neutron can be represented in symbolic form by

\[ \frac{\partial}{\partial t} \psi(r,t) = A\psi(r,t), \]  

(1)

where \( A \) is a systems matrix and \( \psi(r,t) \) is the vector containing the neutron group fluxes and the neutron precursor groups. We choose to base our analysis on a functional prescription used effectively by Hansen and associates (1-3) and restrict our solution to the form

\[ \psi(t_{i+1}) = \psi'(t_i)\exp[\alpha \Delta t_i], \]  

(2)

for a time step \( \Delta t_i = t_{i+1} - t_i \). Here, \( \alpha \) is a suitable parameter valid during \( \Delta t \).

To be specific, we consider the two-group, time-dependent equation in three-dimensions written in its common form
for \( g = 1,2 \) and where the symbols possess the usual meaning. Note that herein we do not include delayed neutron precursors although the solution formalism to be described here can be readily extended to include this effect as well as more than two groups. We interject to note that the exclusion of delayed neutron precursors will clearly effect the characteristic temporal evolution of the neutron flux in a calculational context. The above equations, Eq. (3), are coupled implying that a solution which retains this coupling explicitly is desirable. Thus we choose to use an Ansatz given by

\[
\phi_g(r,t) = \phi_g(r,t) \sum_{\lambda=1}^{2} \beta_{g\lambda}(r) \exp[\alpha_{g\lambda}(r)t],
\]

for \( t \geq t_i \). Here \( \phi_g(r,t) \) may be called a transformed flux while \( \beta_{g\lambda}(r) \) and \( \alpha_{g\lambda}(r) \) may be termed moments and frequencies respectively. We emphasize two important properties of this Ansatz. First, the flux-coupling property specifies here that the \( g' \)th flux, \( \phi_{g'}(r,t) \), is given in terms of the moments and frequencies associated with all other neutron group terms. Second, the proposed solution, Eq. (4), reduces to the standard point-kinetics solution if no spatial dependence is assumed to exist.

To place the multi-mode Ansatz, Eq. (4), in historical perspective we point out that it does possess some relation to the Ansatz previously used by Reed et al. (1) and Wight et al. (2)

\[
\phi_g(r,t) = \psi_g(r,t) \exp[\alpha_g(r)t],
\]

and that used by Ferguson and Hansen (3)

\[
\phi_g(r,t) = \psi_g(r,t) \exp[\alpha(r)t].
\]

The distinction in these three solution models rests primarily in the extent to which the time variations of the various neutron groups are explicitly listed as contributors in effecting a change in any given group flux.

**Analytical Development**

In the analysis to be pursued here, we restrict ourselves to an arbitrary time step, \( \Delta t_i = t_{i+1} - t_i \), for which the system parameters, \( D_g(r) \) and \( \Sigma g_g'(r) \), are assumed to be given as a function of position only. Thus, our describing equation for the \( g' \)th neutron energy group is now given by

\[
\frac{1}{\nu_g} \frac{\partial}{\partial t} \phi_g(r,t) = \nu \cdot D_g(r) \phi_g(r,t) + \sum_{g' \neq 1} \Sigma g_g'(r) \phi_g'(r,t),
\]
where again $g = 1, 2$ and $t \in \Delta t$. Substituting Eq. (4) into Eq. (7) yields, after some algebraic rearrangement, the describing equations in terms of $\phi_g(\tau, t)$, $\beta_g(\tau)$, and $\alpha_g(\tau)$:

$$
\sum_{g=1}^{N} \alpha_g(\tau) \phi_g(\tau, t) = -\sum_{g=1}^{N} \beta_g(\tau) \alpha_g(\tau) \phi_g(\tau, t)
$$

$$
+ \sum_{g=1}^{N} \beta_g(\tau) \phi_g(\tau, t) \left\{ v \cdot g(\tau) \phi_g(\tau, t) \right\} + \sum_{g=1}^{N} \beta_g(\tau) \phi_g(\tau, t) \left\{ v \cdot g(\tau) \phi_g(\tau, t) \right\}
$$

$$
+ \sum_{g=1}^{N} \beta_g(\tau) \phi_g(\tau, t) \left\{ v \cdot g(\tau) \phi_g(\tau, t) \right\}
$$

(8)

Writing the transformed describing equations in this form identifies the common multiplier containing the $\xi$th order frequency, $\exp[\alpha_\xi(\tau)t]$, in each but the third term of the right hand side of this equation; the "del" operator prevents a convenient extraction of this exponential term. Although an argument could be attempted that the contribution of this term might be small and hence could be neglected, we propose to set this term equal to zero on the grounds that the resultant equation will be used only to evaluate the moments, $\beta_g(\tau)$, and the frequencies, $\alpha_g(\tau)$, at $t_i = 0$. This latter imposition possesses the feature that it renders the terms upon which $v$ operates a constant and hence defines the entire $3^{rd}$ term equal to zero. We will comment on this point again in a subsequent section. Thus, viewing the leading term, $\exp[\alpha_\xi(\tau)t]$, as a common coefficient requires that the $\xi$th term in each summation be equated as follows:

$$
\frac{\beta_g(\tau)}{v_g} \left\{ \alpha_g(\tau) \phi_g(\tau, t) \right\} = -\frac{\beta_g(\tau)}{v_g} \alpha_g(\tau) \phi_g(\tau, t)
$$

$$
+ \sum_{g'=1}^{N} \beta_g'(\tau) \phi_g'(\tau, t) + \sum_{g'=1}^{N} \sum_{g''=1}^{N} g'(\tau) g''(\tau) \phi_g'(\tau) \phi_g''(\tau, t)
$$

(9)

for $g = 1, 2$ and $t \in \Delta t_i$. This equation will now be examined to permit the evaluation of $\phi_g(\tau, t)$, $\beta_g(\tau)$, and $\alpha_g(\tau)$ at all discrete values of $\tau$ and for $\xi = 1, 2$.

**Finite Analysis**

We consider arbitrary time steps $\Delta t_i = t_{i+1} - t_i$ and, for convenience, choose to use $t_i = 0$ for all iterative time intervals. Either from the time when the simulation is initiated or from the beginning of an arbitrary iteration in time, we set $t = t_i = 0$ and use Eq. (4) to write
\begin{align}
\Phi_g(r,0) &= \Phi_g(r,0) \sum_{\lambda=1}^{2} \beta g_\lambda(r). \\
\text{We choose to use a normalization on the moments } \beta g_\lambda(r) \text{ defined by}
\sum_{\lambda=1}^{2} \beta g_\lambda(r) &= 1, \tag{11}
\text{and thus have}
\Phi_g(r,0) &= \Phi_g(r,0) \tag{12}
\text{at the beginning of each timestep.}
\end{align}

To find the moments and frequencies, we use the value, \(\Phi_g(r,0)\), associated with the beginning of each interval and assume that the temporal evolution of the neutron flux during the interval \(\Delta t_i\) is predominantly exponential. That is, in Eq. (9) we impose the following condition on the transformed flux \(\Phi_g(r,t)\)

\[\frac{3}{\Delta t} \Phi_g(r,t) \bigg|_{t = \Delta t_i} = 0, \tag{13}\]

and obtain an equation in terms of \(\beta g_\lambda(r), \alpha_\lambda(r)\) and the initial conditions, \(\Phi_g(r,0)\):

\[\begin{align*}
-\beta g_\lambda(r) \alpha_\lambda(r) + \beta g_\lambda(r) \nu_g \frac{v \cdot D_g(r) \nu \Phi_g(r,0)}{\Phi_g(r,0)} \\
+ \frac{2}{g} g_\lambda'(r) \beta g_{\lambda'}(r) \nu_g \frac{\Phi_g(r,0)}{\Phi_g(r,0)} = 0
\end{align*} \tag{14}\]

This equation can be written as an eigenvalue equation for the frequencies \(\alpha_1(r)\) and \(\alpha_2(r)\) corresponding to the values of \(D_g(r)\) and \(\beta g_\lambda(r)\) at \(r\) and \(\Phi_g(r,0)\) about \(r\):

\[
\begin{bmatrix}
\Sigma_{11}(r) v_1 + \frac{v_1 v \cdot D_1(r) v \Phi_1(r,0)}{\Phi_1(r,0)} \\
\Sigma_{21}(r) v_2 + \frac{v_2 v \cdot D_2(r) v \Phi_2(r,0)}{\Phi_2(r,0)}
\end{bmatrix}
\begin{bmatrix}
\Phi_1(r,0) \\
\Phi_2(r,0)
\end{bmatrix}
= \begin{bmatrix}
\alpha_1(r) \\
\alpha_2(r)
\end{bmatrix}
\tag{15}
\]

or, symbolically,

\[\Phi_\lambda = \alpha_\lambda \beta_\lambda. \tag{16}\]
Since all elements of \( \zeta \) are assumed known at the coordinate of interest, \( r \), the eigenvalues \( \alpha \) can be found by the solution to

\[
|\zeta - \alpha \Gamma| = 0 , \tag{17}
\]

In this two-group representation, \( \alpha_1(r) \) and \( \alpha_2(r) \), are the two solutions of a quadratic equation.

The components of the eigenvector \( \beta \), Eq. (17), are given by any non-zero column of the adjoint of \([C-\alpha \Gamma]\), \( ADJ[C-\alpha \Gamma] \), to within an arbitrary constant. Supposing that these vector components are identified by \( \beta'_\alpha(r) \). Then, according to the normalization condition, Eq. (12), we find a constant \( h_\alpha \), \( \alpha = 1,2, \) such that

\[
h_\alpha[\beta'_\alpha(r) + \beta'_\alpha(r)] = 1 . \tag{18}
\]

Hence, the moments \( \beta'_\alpha(r) \), \( \alpha = 1,2, \lambda = 1,2 \), are determined. With the functions \( \phi_\alpha(r,0) \), \( \alpha_\lambda(r) \) and \( \beta_\lambda(r) \) all known at \( t_i = 0 \), we insert these values into Eq. (8) and, by finite numerical methods solve for \( \phi_\alpha(r,t_{i+1}) \). With the use of Eq. (4), this resultant expression yields the flux \( \phi_\alpha(r,t_{i+1}) \) at the end of the time step.

**Numerical Modeling and Calculational Results**

For the purpose of an initial exploratory three-dimensional examination of our formalism, it is advantageous to adopt a simple and direct numerical model and to concentrate on relatively large scale effects. Our simplified three-dimensional reactor is therefore chosen to be a homogeneous, bare cylinder penetrated by a control rod perpendicular to the axial direction.

We choose to restrict ourselves to a coarse spatial mesh describing the whole reactor with 1320 mesh points. Errors may arise from three sources: 1) numerical round-off, 2) finite difference expressions, and 3) boundary condition approximations.

Round-off errors will not be a severe problem in our calculation both because of the precision of the long (60 bit) capacity of the CDC-6400 computer used in our calculation and because our equations involve only tridiagonal (three-stripe) matrices. Computer memory size limits the number of values of the flux which can be conveniently stored; in particular, we cannot keep the value of the flux at many past times and thus are forced to compute the flux at time \( t \) based on values of the flux and system parameters at time \( t - \Delta t \) and accept the attendant truncation error in the time step. If the boundaries of the reactor do not lie on our chosen grid points then we must take an approximation to the actual boundary values; we can avoid this error, however, by describing our reactor in cylindrical co-ordinates \((r, \theta, z)\).
We have chosen to describe the spatial domain by two diametrically opposite 90° wedges of the core. Use of the physical bi-lateral symmetry of our reactor model allows us to construct all values not explicitly lying within our grid thus reducing our computer storage requirements. The control rod has been made to appear more regular by weighting the parameters accordingly within the control rod region. A grid with 12 points in the r-direction, 10 points in the $\theta$-direction and 11 points in the z-direction yielding 1320 grid points has been chosen.

Starting with some initial array of values for the flux $\phi_g(r_i) = \phi_g(r_i, \theta_i, z_i), g = 1, 2$, we solve Eq. (17) - which here represents a quadratic equation - for the spatial frequencies $a_k(r_i)$ and for the spatial moments $B_{kg}(r_i)$ according to Eq. (11) and Eq. (18). The diffusion term in Eq. (18) is represented at the point $r_i = (r_i, \theta_i, z_i)$ in finite different form. Equation (8) may subsequently be written as a tri-diagonal system which is implicit in one of the three spatial directions and explicit in the remaining two. In solving this system we have chosen to use the alternating two-direction implicit method (2).

The data used in the sample calculation here are listed in Table I and correspond approximately to those appropriate for a heavy water reactor. Figure 1 shows the fast and thermal flux rise associated with two sudden withdrawals of the control rod described by the following. At steady state we consider the axial flux traverse adjacent to the cylindrical axis with the control rod inserted 55% of the full cylindrical diameter. At $t = 0$ the control rod is suddenly withdrawn so that only 27.5% of the diametrical distance of the core contains the control rod. After a time interval of 320 $\mu$s the control rod is withdrawn entirely. The flux rise is followed for another 320 $\mu$s up to $t = 640 \mu$s, Fig. 1.

We note that during this very fast transient, the induced reactivity disturbance effects both the fast and thermal flux only in the region close to the control rod position. We also observe a contrast in the flux perturbation and response between the fast and thermal flux.

The computer time requirements for this three-dimension, two-group, 1320 mesh-point calculation was found to be 0.84 s/step on the CDC-6400 computer used here. This is almost identical to the computer time requirements reported by Reed (5) for an efficient two-dimensional calculation using a faster computer (CDC-6600).

Discussion of Solution Formalism

The describing equation, Eq. (1), used here can be easily extended to G energy groups and include I delayed neutron precursor groups. For this case we write the vector $\psi(r,t)$ and the matrix $\hat{A}$ in Eq. (1) as
\[ \psi(t, \tau) = [\psi_1, \psi_2, \ldots, \psi_G, C_1, \ldots, C_I]^T, \] (19)

and

\[ A = \begin{bmatrix}
D_1 + T_{11} & T_{1G} & \cdots & F_{11} & \cdots & F_{1I} \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
T_{G1} & D_G + T_{GG} & \cdots & F_{G1} & \cdots & F_{GI} \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
P_{11} & \cdots & P_{1G} & -A_1 & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
P_{11} & \cdots & P_{1G} & 0 & \cdots & A_1
\end{bmatrix} \] (20)

Here, the notation conforms to that used by Ferguson and Hansen (3). The matrix \( A \) is real, irreducible, square and "essentially positive"; these properties are independent of the number of energy groups or delayed neutron precursor groups.

The transformation used in our work herein may be represented by

\[ \psi = \mathcal{Q}^\Phi, \] (21)

where the matrix operator \( \mathcal{Q} \) is defined by

\[ \mathcal{Q} = \begin{bmatrix}
G & \sum_{\xi=1}^G \beta_{1\xi}(r)\exp[\alpha_{1\xi}(r)t] & 0 \\
0 & \cdots & G \\
0 & \sum_{\xi=1}^G \beta_{G\xi}(r)\exp[\alpha_{G\xi}(r)t]
\end{bmatrix} \] (22)

which, upon substitution in Eq. (1) yields,

\[ \frac{\partial}{\partial t} \Phi = \mathcal{Q}^{-1}(\mathcal{A} - \mathcal{Q}^{-1})\mathcal{Q}\Phi. \] (23)

The moments \( \beta_{G\xi}(r) \), and the frequencies \( \alpha_{G\xi}(r) \), are found from the condition

\[ \frac{\partial}{\partial t} \Phi = \mathcal{Q}^{-1}(\mathcal{A} - \mathcal{Q}^{-1})\mathcal{Q}\Phi = 0. \] (24)

This relationship suggests the following condition
for the determination of the moments and frequencies; here \( \hat{A}' \) is simply \( \hat{A} \) in which \( \nabla \cdot D(\mathbf{r}) \nabla \) is evaluated using the flux at \( t = 0 \). This eigenvalue equation, Eq. (25) is, of course, the same equation as Eq. (17) obtained by a different algebraic method.

It is important to note that the difference matrix \((\hat{A} - \hat{A}')\), appearing by subtraction involving Eq. (1)

\[
\frac{\partial}{\partial t} \phi = \hat{\omega}^{-1}(\hat{A} - \hat{A}')\phi ,
\]

(26)
is composed only of terms containing the Laplacian \( \nabla^2 \) along the main diagonal (4). Thus, the equations are separable in the neutron group flux and can be solved by sequential elimination. This is a most useful consequence since it eliminates the need for group scanning (3).

Some additional points of observation seem pertinent to this solution formalism. As indicated, the moments and frequencies, \( \beta g(\mathbf{r}) \) and \( \alpha g(\mathbf{r}) \), are calculated from \( \hat{A}' \), that is, the matrix \( \hat{A} \) appropriate to the beginning of the time step. An improved value for \( \hat{A}' \) might be obtained using a predictor-corrector scheme although it appears that the benefits from such a scheme would be highly dependent upon the reactor system of interest.

Further, we approximated the fourth term in Eq. (8)

\[
T_4 = \nabla \cdot D(\mathbf{r}) S_4(\mathbf{r},t) \int \sum_{\xi=1}^{G} \exp[\alpha_{\xi}(\mathbf{r})t] g_{\xi}(\mathbf{r}) ,
\]

(27)
at \( t = 0 \) while permitting the rest of the equation to be a function of time. This equation could be expanded to yield

\[
T_4 = \sum_{\xi=1}^{G} \exp[\alpha_{\xi}(\mathbf{r})t] g_{\xi}(\mathbf{r}) r(\mathbf{r},t) ,
\]

(28)
where \( r(\mathbf{r},t) \) is obtained by performing the spatial operations suggested in Eq. (27). Equation (9) could be expanded to include this additional term and therefore provide for an improved estimate for the moments and frequencies in Eq. (17).

Although the calculational experience with this new formalism is limited, it does appear to possess considerable merit particularly in the descriptions of fast reactor transients.
Fig. 1: Fast and thermal neutron flux rise. At $t = 0$ the control rod is suddenly raised from 55% of full diametrical insertion in core to 27.5%; at $t = 320 \mu s$ the rod is withdrawn entirely. During the 640 $\mu s$ time interval, the flux perturbations are found to be contained close to the region of the radial direction of control rod location.
Table I: Data used in sample calculation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reactor Core</th>
<th>Control Rod</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_{11}$ ($\text{cm}^{-1}$)</td>
<td>$-0.97 \times 10^{-3}$</td>
<td>$-0.97 \times 10^{-3}$</td>
</tr>
<tr>
<td>$\Sigma_{22}$ ($\text{cm}^{-1}$)</td>
<td>$-0.41 \times 10^{-2}$</td>
<td>$-0.10 \times 10^{0}$</td>
</tr>
<tr>
<td>$\Sigma_{21}$ ($\text{cm}^{-1}$)</td>
<td>$0.86 \times 10^{-2}$</td>
<td>$0.86 \times 10^{-2}$</td>
</tr>
<tr>
<td>$\Sigma_{12}$ ($\text{cm}^{-1}$)</td>
<td>$0.48 \times 10^{-2}$</td>
<td>$0.48 \times 10^{-2}$</td>
</tr>
<tr>
<td>$D_1$ (cm)</td>
<td>1.40</td>
<td>1.30</td>
</tr>
<tr>
<td>$D_2$ (cm)</td>
<td>0.92</td>
<td>0.86</td>
</tr>
</tbody>
</table>

$v_1 = 2.0 \times 10^6 \text{ cm/s}$ ; $v_2 = 2.0 \times 10^5 \text{ cm/s}$

$R = 3.50 \text{ m}$ $H = 5.94 \text{ m}$

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DISCUSSION

A. Siebertz

Your method could be called a quasi-static method with specialized exponential form amplitude function.

Could you comment on the relative merits of both methods (accuracy, computing time ...)?

A.A. Harms

First, for very rapid changes with highly localized effects, this method seems more accurate and at least as fast. Second, the one additional important merit point is associated with the group-coupling solution representation which describes an arbitrary group flux in terms of all other groups; thus, increases in one group and concurrent decreases in another group can be both described.

A.F. Henry

The improvement caused by these methods when applied to alternating directions schemes is much greater than when they are applied to fully implicit schemes.

D.A. Meneley

1) The quasi-static method is best suited to fast reactor problems.

2) Hansen's and Harm's methods have pointwise or/and groupwise exponential transformations with extrapolated coef-
ficients. The quasi-static method has a single amplitude function obtained by solution of the point kinetic equation. Quasi-static methods are presently limited to linear variation of shape functions with time; on the other hand, the Hansen-Harm's methods are limited in maximum time step length because of the extrapolation, constant properties over the time step, and by alternating-direction solution method. The question can only be answered by running a series of benchmark problems with all methods.
Session II

COARSE MESH METHODS

Chairman: F.J. Fayers, United Kingdom

W. Werner

MATHEMATICAL PROBLEMS IN THREE-DIMENSIONAL REACTOR CALCULATIONS
Laboratorium für Reaktorregelung und Anlagen- sicherung, Technische Universität München, Germany

T.J. Burns / J.J. Dorning

THE PARTIAL CURRENT BALANCE METHOD: A NEW COMPUTATIONAL METHOD FOR THE SOLUTION OF MULTIDIMENSIONAL NEUTRON DIFFUSION PROBLEMS
Oak Ridge National Laboratory, Oak Ridge, Tennessee / University of Illinois, Urbana, Illinois, USA

H. Finnemann

A CONSISTENT NODAL METHOD FOR THE ANALYSIS OF SPACE-TIME EFFECTS IN LARGE LWR
Kraftwerk Union AG, Erlangen, Germany
S. Langenbuch, W. Maurer, W. Werner

SIMULATION OF TRANSIENTS WITH SPACE-DEPENDENT FEEDBACK BY COARSE MESH FLUX EXPANSION METHOD

Laboratorium für Reaktorregelung und Anlagen sicherung, Technische Universität München, Germany

O. Norinder

THE BITNOD METHOD OF REACTOR COARSE MESH CALCULATIONS

AB Atomenergi, Studsvik, Sweden
W. Werner

MATHEMATICAL PROBLEMS IN THREE-DIMENSIONAL REACTOR CALCULATIONS

Laboratorium für Reaktorregelung und Anlagensicherung, Technische Universität München, Germany
1. Introduction

The necessity of genuine 3d-calculations for the analysis of the time dependent behaviour of modern LWR's is generally recognized by now.

Basis of these calculations is the multigroup-neutron diffusion equation

\[
\left( \nabla \cdot \frac{\partial}{\partial t} - \mathbf{L} \right) \phi - \nabla \cdot \mathbf{C} = \sigma, \quad \left( \frac{\partial}{\partial t} + \Lambda \right) \mathbf{C} - \mathbf{B} \phi = \sigma
\]

where

\[
\phi(x,t) = (\phi_1(x,t), \ldots, \phi_m(x,t))^T, \quad \mathbf{C}(x,t) = (C_1(x,t), \ldots, C_m(x,t))^T
\]

\[
\mathbf{L} = \nabla \mathbf{D} \nabla - \mathbf{A}, \quad \mathbf{D} = \text{diag}(D_i),
\]

\[
(A)_{ik} = \delta_{ik} \rho_i^{\text{rem}} - \chi_i \nu(1-\beta) \Sigma^f_{ik} - \Sigma^s_{ik}, \quad \Sigma^s_{ik} = \sigma \text{ for } i \leq k, \quad i, k = 1, 2, \ldots, m.
\]

The cross-sections \(D, \Sigma^f, \Sigma^{\text{rem}}, \text{ and } \Sigma^s\) are piecewise continuous functions of \(x\), and continuous functions of \(t\) and \(\mathbf{y} = (\phi, \mathbf{C})^T\). The dependence on \(t\) and \(\mathbf{y}\) is described by a set of "feedback" equations.
Furthermore, \[
\begin{align*}
(\mathbf{r})_{i\kappa} &= \chi_{i\kappa} \lambda_{\kappa}, \\
\Lambda &= \text{diag}(\lambda_{\kappa}), \\
(\mathbf{B})_{i\kappa} &= \gamma \beta_k \sum_{\kappa}^{g} \mathbf{f}_k, \\
&\quad i = 1, \ldots, m, \quad \kappa = 1, \ldots, g,
\end{align*}
\]
\(\lambda_{\kappa}\) and \(\beta_k\) are given constants.

Together with suitable initial conditions and boundary conditions of the reactor, and continuity conditions cross interfaces, the solution of eq. (1.1) poses a nonlinear parabolic problem (I). Obviously, it is impossible to find explicit solutions of problem I for any reasonably realistic reactor model. Therefore, approximation \(\Psi\) to the true solution \(\psi\) must be sought.

It is commonly agreed, that for thermal reactors, 2-4 groups of prompt neutrons and 6 groups of delayed precursors are needed for realistic problems.

For fast reactors at least 6, but often more than 15 groups of prompt neutrons are needed, and also 6 groups of delayed precursors.

All practicable approximation methods are based on the use of discrete variables (Finite Difference Methods (FD), Nodal Methods (NM), Expansion Methods (EM) and Finite Element Methods (FEM)).
2. Direct and Indirect Methods

Very coarsely, these approximation methods can be classified into direct and indirect methods.

In direct methods, the space \( \mathbb{R}^{n+1} = \mathbb{R}^n \times \mathbb{R}^1 \) of independent variables \( x_1, \ldots, x_n, t \) is subdivided into discrete regions \( G_i, i = 1, \ldots, N, \cup G_i = G, \)

\( \Delta t_j = t_j - t_{j-1}, j = 1, \ldots, M. \) On \( G_i \), resp. \( \Delta t_j \), suitable "Basisfunctions" \( P_i(k), i = 1, \ldots, N, \) resp. \( Q_j(t) \) are defined.

Upon substitution of \( P_i \) and \( Q_j \) into 1.1, and replacement of differential operators by difference operators, eq. 1.1 is converted into a matrix equation, which permits to compute basisfunction \( P_i^{j+1}(x) \), \( i = 1, \ldots, N \), at time \( t_{j+1} \) from the knowledge of basisfunctions \( P_i^j(x), \ldots, P_i^{j-\ell}(x), i = 1, \ldots, N, \) at times \( t_j, \ldots, t_{j-\ell}. \)

The propagation of the approximate solutions is performed locally, i.e., in each time-step, all basisfunctions \( P_i^{j+1}(x), i = 1, \ldots, N \) are newly computed.

By using sufficiently many regions \( G_i \) and \( \Delta t_j \) and by employing basis functions of sufficiently high order, the solution of (1.1) can in principle be approximated with any desired accuracy. The relatively large amount of computational
work associated with the computation of all basisfunctions in each time-step is only adequate, if the spatial flux distribution changes significantly within the time-steps. The use of direct methods is certainly uneconomical, if the spatial flux distribution does not change between time-steps, since in that case, a lot of computational work is spent to perpetually calculate identical or almost identical basisfunctions.

Besides the approximations introduced by discretisation, which are of mathematical nature, indirect methods make use of further approximations, which are justified by physical properties.

In all useful indirect methods, the physical approximations consist in a separation $\psi(x,t) = \sum A_i(t) \psi_i(x,t)$ with $\psi_i(x,t)$ being only "weakly" time dependent, relative to the time dependence of $A_i(t)$.

The complexity of space functions $\psi_i(x,t)$ varies from being constant in the whole reactor in the most simple case (point kinetics), to being a function of all 3 space variables (quasistatic method).

The propagation of the approximate solution consists only in the solution of a system of ordinary differential equations
for the determination of the amplitude functions $A_1(t)$. Changes of the space-functions $\bar{\Psi}_i(x,t)$ due to changing cross-sections are considered by exchanging the set of space functions from time to time, but in intervals which are long relatively to the integration steps for $A_1(t)$.

The most serious difficulty in the applications of indirect methods is, that it is hard to find rigid criterions which indicate the necessity to exchange the set of space functions.

The main area of application of direct methods is the analysis of events governed by localized changes of cross-sections, while indirect methods are successfully used in the analysis of events governed by global cross-section changes.

A side condition imposed by the computer hardware is, that the number of discrete variables to be stored in the fast memory is limited by ca. 200 000. For thermal reactors, this implies, that not more than 15000-20000 $G_j$'s (boxes) can be used, and this, in turn, implies that the average box size for 3d-calculations of modern LWR's has to be about $20 \times 20 \times 20 \text{ cm}^3$. 
3. Space Discretization

If \( P_i(x) = \text{const} = \psi_i \) on \( G_i \), \( i = 1, \ldots, N \), and if the spatial differential operators in \( L \) are replaced by spatial difference operators, one obtains classical FD-methods. Generally, they are described by a matrix equation.

\[
A^{n+1} \psi^{n+1} = A^n \psi^n + \cdots + A^{n-\ell} \psi^{n-\ell}
\]

If \( A^{n+1} \) is diagonal, the method is explicit, otherwise, it is implicit. Since eq. (1.1) is of second, it is unreasonable to approximate the spatial differential operator by difference operators of order higher than 2. Therefore, the commonly used difference operator is the 7-point difference operator (in 3d). The spatial coupling of the approximate solution is effected by the elements of the off-diagonal blocks. These elements are proportional to \( D/h^2 \), i.e., they disappear rapidly, as the mesh size \( h \) is increased. The elements of the diagonal block describe the local coupling of group fluxes and delayed precursors. As \( h \) is increased, these matrix entries tend toward limits which are bounded away from zero. Since the elements of the off-diagonal blocks disappear relatively to the elements of the diagonal blocks, as \( h \) is increased, the numerical property of the advancement matrix become very unfavourable for increasing \( h \).
Experience with FD-methods for LWR-calculations shows, that acceptable accuracy, with relative errors of the spatial solution less than a few percent, can only be reached with mesh size smaller than 3-4 cm. Implementation of 3d-codes employing such mesh size on present day computers is obviously impractical, since it would require the use of external storage to a large extent.

4. Coarse Mesh Methods

The only way to decrease the amount of computational time significantly is a drastic reduction of the number of unknowns by the use of so called "Coarse Mesh Methods" (CM). The first CM-methods /1-3/ used coupling coefficients which were predetermined, either empirically or theoretically, but adapted to certain typical situations. Thus, the applicability of such methods was very limited. The second generation of CM-methods /4-8/ employs higher order (2-4) basis functions, which permit an automatic computation of coupling coefficients.

The coefficients of the basis functions are either determined through global Galerkin weighting (classical Finite Element Methods (FE) /7,8/), or through integral relations and local minimal principles (Expansion Method (EM)). In any case, local operators describing the coupling of neighbouring nodes become
defined. In contrast to FD-methods, the coupling coefficients of the local operators depend not only on the leakage terms of one group flux, but on all group constants. Especially, the elements of the off-diagonal blocks do not disappear, relative to the elements of the diagonal blocks, as the mesh size is increased.

Therefore, there are no principle difficulties to be encountered with the use of box sizes which are much larger than the mean free path of neutrons. The only point of consideration in the choice of mesh size is the question of adequacy of the selected basis functions in relation to flux variation within the nodes.

Expansion method require a grid with uninterrupted grid lines (like FD method). Also the advancement of expansion methods is similar in structure to the advancement matrix of FD-methods.

Since the number of unknowns is relatively small in expansion methods (several 1000 for realistic LWR's) a direct solution of the advancement matrix equation is feasible; though it would not be an efficient method. Potentially more efficient are relaxation methods with rebalancing /6,10/, and matrix decomposition methods /5/. The latter have been applied successfully in 2d- and 3d-FD-calculations /11,12/. However, since the constancy or near constancy of the decomposed operators, which is essential for the successful application of the method, may be
severely violated in expansion methods, modifications of the basic method are required.

The implicit matrix decomposition method described in /12/ uses 2 corrector steps (in 3d-calculations) to balance the instability caused by the components of the difference operators which are treated explicitly in the predictor step. A theoretical proof of this balancing can only be given in the constant operator case. For non constant operators, it is intuitively clear, and also supported by numerous evidence, that this balance becomes very tricky and great care is required in maintaining it. This difficulty can be avoided by using stable explicit approximations in the predictor step /e.g. 11, 15/.

Coarse mesh rebalancing methods have become very popular in the past years; with \( n \) being the number of unknowns of the problem, the computational work associated with coarse mesh rebalancing methods depends on \( n \log(n) \), which is much more favourable than with conventional relaxation methods.

Finite Element Methods do not require a regular grid; especially, grid lines may be interrupted. This is of great advantage in classical applications of FE-methods, like structural analysis or fluid dynamics; however, in LWR's with their rather regular fuel-moderator structure, this offers no significant advantage. On the other hand, the advancement matrix of FD-methods is more dense than for Expansion methods of comparable accuracy. Thus,
somewhat more computing time is to be expected, relative to Expansion methods. 2d-calculations indicate about a relation of 1:4 in favour of Expansion methods /13/, where direct solution by Choleskis method is used in the FE-method. In realistic 3d-calculations, efficiency competitive with expansion methods can only be expected by application of modern relaxation methods with coarse mesh rebalancing /10, 14/. However, only insufficient experience with 3d-FE-methods is yet available /18/.

5. Conclusion

For the 3d-simulation of the time dependent behaviour of modern LWR's, CM-methods, especially Expansion method, are an adequate tool. In principle, they permit an efficient computation of transient solutions. However, further work is required to determine optimal time-integration procedures, both for FE-, and Expansion methods.
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A. Siebertz

In LMFBR's fast transient calculation, even the use of 13 energy groups (classical disjoint ones), leads to unacceptable errors in the prediction of the sodium void reactivity effect. According to some results obtained at Karlsruhe, the use of energy synthesis methods can give very good results even with as few as 3 overlapped groups. But then, there is the difficult problem of the choice of the basic spectra. Could you please comment?

L. Väth, W. Werner

We found, in fact, at Karlsruhe, that 15 energy groups had to be used with normal flux weighted collapsing for an adequate description of sodium voiding. On the other hand, we had very encouraging results for bilinear weighting and energy synthesis, but these results were arrived at using a simple 1d kinetics code with simulated feedback. It is not at all clear, for the moment, how well these methods work for 2d or 3d problems with realistic feedback; in addition, we encountered some problems with energy synthesis.

F.N. McDonnell

With the coarse-mesh method, is the spatial eigenvalue separation between the fundamental and first azimuthal mode maintained? For classical model models this is known to be not so.
W. Werner

The eigenvalue separation is maintained.
T.J. Burns / J.J. Dorning

THE PARTIAL CURRENT BALANCE METHOD: A NEW COMPUTATIONAL METHOD FOR THE SOLUTION OF MULTIDIMENSIONAL NEUTRON DIFFUSION PROBLEMS

Oak Ridge National Laboratory, Oak Ridge, Tennessee / University of Illinois, Urbana, Illinois, USA
THE PARTIAL CURRENT BALANCE METHOD: A NEW COMPUTATIONAL METHOD FOR
THE SOLUTION OF MULTIDIMENSIONAL NEUTRON DIFFUSION PROBLEMS*

T. J. Burns† and J. J. Dorning‡†

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Urbana, Illinois 61801

ABSTRACT

A new computational method for the solution of multidimensional neutron
diffusion problems which is based on local balances of partial currents is
described. After briefly motivating the ideas used in the method, the formalism
is reviewed. The technique used for the solution of the final equations via local
expansions is then described, and the resulting matrix equations are developed.
The iteration schemes which were employed in the initial calculations are
described. Computational results for two simple one-dimensional HTGR models and
for a simple two-dimensional HTGR model are reported and compared with finite
element and finite difference calculations for accuracy and computing time. In
all cases studied, the partial current balance method compared very favorably with
both these widely used methods. Some advantages of the partial current balance
formulation are discussed.

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INTRODUCTION

The partial current balance method is a coarse mesh technique based on a local integral form of the multigroup neutron diffusion equations. The method is formulated by converting the standard differential form of the neutron diffusion equation for each energy group into a local integral equation. This is done by formally using local group removal Green's functions for each of the volume elements into which the nuclear assembly is partitioned. Each volume element is coupled only to its nearest neighbors. This coupling is accomplished by the partial current continuity conditions at the volume element interfaces which naturally arise in the development of the formalism. The method has three obvious advantages which may account for its speed and accuracy. These are: it permits the use of large volume elements (a very coarse mesh) while still retaining high accuracy; it has only nearest neighbor coupling among the volume elements, which is not the case for most integral methods; the nuclear coupling parameters which are used in the iterative solution procedure are generated independently for each group and can be calculated with relative ease.

As a motivation for the formalism it is convenient to consider the actual equation which must be solved in practical neutron diffusion calculations such as multigroup source iteration calculations. This equation has the general form

$$A\Phi(r) = -\nabla \cdot D \nabla \Phi(r) + \Sigma_f \Phi(r) = S(r). \quad (1)$$

For example, an equation of this type must be solved in each inner iteration of a multigroup source iteration criticality calculation, or at each time step of an implicit space-time solution of the kinetics equations. Of course, it is generally far too difficult to invert Eq. (1) exactly for a complicated realistic reactor system. Hence, the operator in Eq. (1) is generally approximated (e.g., as in a finite difference scheme or a finite element scheme), and then the approxi-
mate operator is inverted. The inversion of this approximate operator, which is generally a large matrix operator for systems of practical interest, at each inner iteration is a time-consuming process on a digital computer. Thus we are motivated to exactly invert Eq. (1) instead of following the above procedure. As stated above, however, an exact global inversion of such an equation is not feasible. An alternative is to attempt an exact local inversion of Eq. (1) or of a closely related equation, follow this inversion by some procedure which establishes coupling of the locally inverted equations so that the overall nuclear system is again fully described, and then generate an approximate solution to the resulting system of equations. This general approach leads to the partial current balance formalism\(^1\) which is reviewed in the next section.

REVIEW OF FORMALISM

The partial current balance formalism\(^1\) is developed by first partitioning the nuclear assembly into \(K\) volume elements \(V_k\). The equation for the group flux in the volume element \(V_k\) is

\[
\nabla \cdot \mathbf{d}_g^k(r) \nabla \phi_g^k(r) - \Sigma_{g}^{r,k}(r) \phi_g(r) = -S_g^k(r)
\]

(2)

where

\[
\Sigma_{g}^{r,k}(r) = \Sigma_{g}^{a,k} + \sum_{g'=1}^{G} \Sigma_{g'g+g'}^{s,k}
\]

(3)

It is convenient at this point to decompose the group removal cross section and the group diffusion coefficient into some constant, or reference, part and a remainder which is variable due to its explicit dependence upon position within the \(k^{th}\) volume element or its implicit dependence upon position through feedback parameters and flux (for example, in a kinetics calculation).

\[
\Sigma_{g}^{r,k}(r,\phi(r)) = \Sigma_{og}^{r,k} + f_{g}^{k}(r,\phi(r))
\]

(4)
\[ D^k_g(\mathbf{r},[\phi(\mathbf{r})]) = D^k_g + h^k_g(\mathbf{r},[\phi(\mathbf{r})]) \]  \hspace{1cm} (5)

For the purposes of the present development we now take the variable part of the diffusion coefficient \( h^k_g(\mathbf{r},[\phi(\mathbf{r})]) \) to be zero. (That is, the group diffusion coefficient is taken to be constant within the \( k \)th volume element.) The effect of nonzero \( h^k_g \) upon the final equations will be stated below after the formalism is developed for the present case. The term which involves the part of the group removal cross section which is variable within the \( k \)th volume element is transferred to the right hand side of Eq. (2) and incorporated in the source term, giving

\[ \nabla \cdot D^k_g \nabla \phi^k_g(\mathbf{r}) - \Sigma^r_{og} \phi^k_g(\mathbf{r}) = -S^k_g(\mathbf{r}) \]  \hspace{1cm} (6)

where

\[ S^k_g(\mathbf{r}) = \sum_{g} f^k_{gg'} \phi^k_g(\mathbf{r}) + s^{ext,k}(\mathbf{r}) \]  \hspace{1cm} (7)

and

\[ f^k_{gg'}(\mathbf{r},[\phi(\mathbf{r})]) = \chi^k_{g}(\mathbf{r}) \phi^k_g(\mathbf{r}) + \Sigma^s_{gg'}(\mathbf{r}) - f^k_{g'}(\mathbf{r},[\phi(\mathbf{r})]) \delta_{gg'}. \]  \hspace{1cm} (8)

Equation (6) is a local equation for the group flux within the \( k \)th volume element. This equation is solved formally using a local Green's function which satisfies the equation

\[ \nabla \cdot D^k_g \nabla G^k_g(\mathbf{r}|\mathbf{r}_o) - \Sigma^r_{og} G^k_g(\mathbf{r}|\mathbf{r}_o) = -\delta(\mathbf{r}-\mathbf{r}_o) \]  \hspace{1cm} (9)

subject to the boundary condition

\[ \frac{1}{4} G^k_g(\mathbf{r}^s|\mathbf{r}_o) + \frac{1}{2} D^k_g \mathbf{n}_k \cdot \nabla G^k_g(\mathbf{r}^s|\mathbf{r}_o) = 0 \]  \hspace{1cm} (10)
on the surface of the $k^{th}$ volume element. The formal solution for the local 
group flux within the $k^{th}$ volume element is then given by

$$
\phi^k_g(r) = G^g,k_{VV} \cdot \Sigma_s^k + \sum_{\text{Surf.}} G^g,k_{VS} \cdot J_{\text{in},k}^g
$$

(11)

where

$$
G^g,k_{VV} = \int_{V_k} d^3 r_o \cdot G^k_g(r_o | r).
$$

(12)

and

$$
G^g,k_{VS} = 2 \int_{S_k} d^2 r_o \cdot G^k_g(r_o | r).
$$

(13)

Equation (6) has now been locally inverted. This local inversion which is 
given by Eq. (11) can be coupled to equations for adjacent volume elements 
by balancing the partial currents across the volume element interfaces. The 
outward partial currents from adjacent volume elements could then be eliminated 
in favor of the adjacent volume element fluxes by using Fick's Law. A system 
of coupled locally inverted equations which together describe the global system 
would then result. An approximate solution technique could then be applied to 
this set of coupled equations. However, as an alternative to this procedure 
an equation for the partial current out of the $k^{th}$ volume element across its 
surface can be developed by applying Fick's Law to Eq. (11). The result is

$$
J^{\text{out},k}_g(r_s) = G^g,k_{SV} \cdot \Sigma_s^k + \sum_{\text{Surf.}} G^g,k_{SS} \cdot J_{\text{in},k}^g
$$

(14)

where

$$
G^g,k_{SV} = \frac{1}{4} \int_{V_k} d^3 r_o \cdot [G^k_g(r_o | r_s) - 2D^k_{og} \cdot \hat{n}_k \cdot \nabla G^k_g(r_o | r_s)].
$$

(15)

and
The balance of partial currents across volume element interfaces can then be applied to these coupled equations for the group volume element flux and outward partial currents to give

\[ \phi^k_g(\mathbf{r}) = G^g_{VW} s^k_g + \sum_\ell G^g_{VS} \phi^\ell_g J^{\text{out},\ell k}, \quad k = 1, \ldots, K; \ g = 1, \ldots, G \quad (17) \]

and

\[ J^{\text{out},\ell k}(\mathbf{r}^S) = G^g_{SV} s^k_g + \sum_\ell G^g_{SS} \phi^\ell_g J^{\text{out},\ell k}, \quad k = 1, \ldots, K; \ g = 1, \ldots, G. \quad (18) \]

Here \( \ell \) and \( \ell' \) indicate adjacent volume elements. These locally inverted equations for the volume element group fluxes and outward partial currents form a coupled set which describe the global nuclear system. They represent the local inversions of Eq. (6) for each group and volume element. We now proceed to develop a straightforward approximation procedure for the solution of these exact local inverse equations.

**APPROXIMATION PROCEDURE**

The coupled set of local equations for the volume element group fluxes and outward partial currents are solved by a direct local application of the weighted residuals method. The fluxes and partial currents are treated as independent variables and expanded in separate \textit{local} expansions

\[ \phi^k_g(\mathbf{r}) = \sum_{n=1}^{N^k_g} z^k_{g,n} p^k_{g,n}(\mathbf{r}) \quad (19) \]

\[ J^{\text{out},\ell k}(\mathbf{r}^S) = \sum_{m=1}^{M^g_{\ell k}} x^k_{g,m} Q^k_{g,m}(\mathbf{r}^S). \quad (20) \]
Substitution of these local expansions into Eqs. (17) and (18), multiplication by local weight functions, and integration over volume element volumes and volume element surfaces yields coupled low order local matrix equations.

\[
[A_{g}^{k}] Z_{g}^{k} = \left[ C_{VV}^{k} \right] S_{g}^{k} + \sum_{\ell} \left[ C_{VS}^{k,\ell} \right] x_{\ell}^{k}, \quad k=1, \ldots, K; \quad g=1, \ldots, G, \tag{21}
\]

and

\[
[B_{g}^{km}] \chi_{g}^{km} = \left[ C_{SV}^{km} \right] S_{g}^{k} + \sum_{\ell} \left[ C_{SS}^{km,\ell} \right] x_{\ell}^{k}, \quad k=1, \ldots, K; \quad g=1, \ldots, G. \tag{22}
\]

Here, \( Z_{g}^{k} \), \( S_{g}^{k} \), and \( \chi_{g}^{km} \) are column vectors of expansion coefficients of the local group flux, source, and partial currents. The matrix elements of the low order matrices which appear in Eqs. (21) and (22) are given in the Appendix. These equations are the final coupled equations from which the local expansion coefficients of the group volume element fluxes and outward partial currents are determined. This is done by solving these local equations using directional iterative sweeps through the volume elements of the nuclear system. Only one iterative scheme has been employed thus far. It will be outlined in the next section.

The effect of non-zero \( f_{g}^{k} (\mathbf{r}, \Phi(\mathbf{r})) \) has been slightly obscured in the above development. Since this function was incorporated in the definition of \( f_{g}^{k} \), it appears in the terms which involve the source in both Eqs. (17) and (18).

There are two cases of non-zero \( f_{g}^{k} \) to be considered. The first, which is the one of current practical interest, is the case when \( f_{g}^{k} \) does not have explicit space dependence within the \( k \)th volume element but rather depends upon the flux through feedback parameters (e.g., as in a dynamics calculation or a static criticality calculation with feedback--at power.), and this dependence is only upon volume element averaged quantities such as \( \bar{T}_{k}, \bar{\rho}_{k} \), etc. In practice, these quantities which are obtained from a thermo-hydraulics calculation are not calculated using a finer spatial mesh than that used for the neutron diffusion...
calculation, so that more detailed dependencies than the neutron diffusion volume element averaged quantities are not available. In this case, the coefficient matrix which is used to construct the source vector \( S^k_g \) in Eqs. (21) and (22) is changed each time the cross sections change due to feedback. However, the G-matrices, whose elements are double moments of the Green's functions (see Appendix), need not be recalculated. In the second case in which \( f^k_g \) depends explicitly upon position within the \( k^{th} \) volume element, this spatial dependence must be included when the matrix elements of the G-matrices are originally constructed. The effect of the non-zero \( h^k_g(r, \Phi(r)) \) in these two cases is the following. In the first case, which is the one of current practical interest, in which \( h^k_g \) depends only upon \( k^{th} \) volume element averaged feedback parameters \( (\bar{r}^k, \bar{p}^k, \text{etc.}) \), simple multiplicative constants appear in front of each of the G-matrices in Eqs. (21) and (22). Finally, in the case where \( h^k_g \) has explicit dependence upon position within the \( k^{th} \) volume element, new terms appear on the right hand side of the volume element matrix equations. This case has not yet been studied computationally. However, these new terms may, in some cases, be large since they involve gradients of the flux. For current practical calculations, however, the dependence of the cross sections and diffusion coefficients upon volume element averaged feedback parameters is the important case, and this leads only to the very minor changes in Eqs. (21) and (22) which are described above.

**ITERATION SCHEMES**

The spatial inner iteration scheme which was used to solve Eqs. (21) and (22) for the local expansion coefficients of the volume element group fluxes and outward partial currents is schematically illustrated for slab geometry in Fig. 1. The iteration procedure begins with guesses for the volume element group fluxes (i.e., the volume element group flux expansion coefficients) and the partial currents to the right (i.e., the local expansion coefficients for the group
Fig. 1: Present Iteration Scheme
volume element outward partial currents to the right). Equation (22) for the volume element adjacent to the system surface \( k = 1 \) is then solved for the outward partial current to the left using the initial guess values for the volume element group flux and incoming partial current from the left, and the exact boundary condition zero incoming partial current from the right. This process is then repeated for the next volume element using the partial current just calculated as the incoming partial current from the right, etc. until the center of the system is reached. Then, the symmetry boundary condition is used to give the incoming partial current from the left and the sweep is reversed to determine the partial currents to the right until the outer surface is reached. The next partial current iteration \( m = 2 \) using Eq. (22) is then begun. These partial current inner iterations are repeated until partial currents consistent with the initial group fluxes are converged. Equation (21) is then used to calculate the first inner flux iteration volume element flux expansion coefficients for each volume element. The whole process is then repeated using these first iteration group flux volume element expansion coefficients. These inner flux iterations (and inner partial current iterations) are repeated until the group fluxes and partial currents are converged. Numerous other inner iteration schemes are possible, but this initial iteration scheme appeared to be satisfactory and has been the only one employed thus far. Other iteration schemes and strategies will be explored in the future.

**COMPUTATIONAL RESULTS**

The iteration scheme described above was used in the initial one- and two dimensional \( k \)-calculations done to test the method. These computations were done using simple polynomials for all expansion and weighting functions. A tabulation of some of the results of these initial PCB calculations along with
results of comparable finite difference and finite element calculations against which they were compared is shown in Tables I through III. In these tables $L/2$ is the core half-thickness, $R$ is the reflector thickness, $\varepsilon$ is the iteration convergence criterion applied to the eigenvalue, partial currents, and fluxes, $k_{fd,\infty}$ is the finite difference value for $k_{eff}$ extrapolated to an infinite number of mesh points, and $k_{ex}$ is the exact analytical value for $k_{eff}$. The $L$, $Q$, and $C$ which appear in parentheses in Tables I and II indicate that linear, quadratic, and cubic expansions, respectively, were used in the calculations. The BL and BQ in Table III indicate bilinear and biquadratic expansions.

**TABLE I**

1-DIMENSION (SLAB), 1-REGION, 1-GROUP, HTGR, $L/2 = 300$ CM, $\varepsilon = 10^{-6}$

$k_{fd,\infty} = 1.077657$; $k_{ex} = 1.077648$

<table>
<thead>
<tr>
<th>METHOD</th>
<th>NO. VOL.</th>
<th>TIME (SEC)</th>
<th>$k_{eff}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCB(L)</td>
<td>6</td>
<td>1.81</td>
<td>1.077651</td>
</tr>
<tr>
<td>FD</td>
<td>30</td>
<td>3.88</td>
<td>662</td>
</tr>
<tr>
<td>FE(L)</td>
<td>20</td>
<td>3.23</td>
<td>650</td>
</tr>
<tr>
<td>PCB(Q)</td>
<td>2</td>
<td>.85</td>
<td>655</td>
</tr>
<tr>
<td>PCB(Q)</td>
<td>3</td>
<td>1.05</td>
<td>657</td>
</tr>
<tr>
<td>FE(Q)</td>
<td>2</td>
<td>.62</td>
<td>650</td>
</tr>
<tr>
<td>FE(Q)</td>
<td>3</td>
<td>.80</td>
<td>656</td>
</tr>
<tr>
<td>FE(Q)</td>
<td>4</td>
<td>1.02</td>
<td>657</td>
</tr>
<tr>
<td>PCB(C)</td>
<td>2</td>
<td>.95</td>
<td>657</td>
</tr>
<tr>
<td>PCB(C)</td>
<td>4</td>
<td>1.50</td>
<td>657</td>
</tr>
<tr>
<td>FE(C)</td>
<td>2</td>
<td>.91</td>
<td>657</td>
</tr>
<tr>
<td>FE(C)</td>
<td>4</td>
<td>2.13</td>
<td>657</td>
</tr>
</tbody>
</table>
TABLE II

1-DIMENSION (SLAB), 2-REGION, 2-GROUP, HTGR
CORE -- L/2 = 300 CM, REFL -- R = 60 CM, \( \epsilon = 10^{-6} \)

\[ k_{fd,\infty} = 1.059993; \quad k_{ex} = 1.059975 \]

<table>
<thead>
<tr>
<th>METHOD</th>
<th>CORE NO. VOL. EL./L/2</th>
<th>REFLE. NO. VOL. EL.</th>
<th>TIME</th>
<th>( k_{eff} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCB(L)</td>
<td>10</td>
<td>2</td>
<td>10.41</td>
<td>1.059988</td>
</tr>
<tr>
<td>FD</td>
<td>50</td>
<td>10</td>
<td>24.13</td>
<td>987</td>
</tr>
<tr>
<td>FE(L)</td>
<td>40</td>
<td>8</td>
<td>21.98</td>
<td>987</td>
</tr>
<tr>
<td>PCB(Q)</td>
<td>2</td>
<td>1</td>
<td>3.00</td>
<td>988</td>
</tr>
<tr>
<td>PCB(C)</td>
<td>3</td>
<td>1</td>
<td>4.12</td>
<td>993</td>
</tr>
<tr>
<td>FE(C)</td>
<td>5</td>
<td>1</td>
<td>9.82</td>
<td>993</td>
</tr>
</tbody>
</table>

TABLE III

2-DIMENSION (SQUARE), 1-REGION, 1-GROUP, HTGR, L/2 = 300 CM, \( \epsilon = 10^{-6} \)

\[ k_{fd,\infty} = 1.063557; \quad k_{ex} = 1.063577 \]

<table>
<thead>
<tr>
<th>METHOD</th>
<th>NO. VOL. EL./QUAD.</th>
<th>TIME</th>
<th>( k_{eff} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCB(BL)</td>
<td>25(5 x 5)</td>
<td>86.04</td>
<td>1.063520 (-37)</td>
</tr>
<tr>
<td>FD</td>
<td>225(15 x 15)</td>
<td>134.64</td>
<td>592 (+35)</td>
</tr>
<tr>
<td>PCB(BL)</td>
<td>36(6 x 6)</td>
<td>131.04</td>
<td>537 (-26)</td>
</tr>
<tr>
<td>FD</td>
<td>400(20 x 20)</td>
<td>258.90</td>
<td>580 (+23)</td>
</tr>
<tr>
<td>PCB(BL)</td>
<td>49(7 x 7)</td>
<td>194.57</td>
<td>547 (-10)</td>
</tr>
<tr>
<td>FD</td>
<td>625(25 x 25)</td>
<td>424.15</td>
<td>573 (+16)</td>
</tr>
<tr>
<td>PCB(BL)</td>
<td>64(8 x 8)</td>
<td>239.49</td>
<td>552 (-5)</td>
</tr>
<tr>
<td>PCB(BL)</td>
<td>36(9 x 9)</td>
<td>304.47</td>
<td>555 (-2)</td>
</tr>
<tr>
<td>PCB(BL)</td>
<td>100(10 x 10)</td>
<td>432.96</td>
<td>557 (-0)</td>
</tr>
<tr>
<td>PCB(BQ)</td>
<td>4(2 x 2)</td>
<td>33.17</td>
<td>561 (*)</td>
</tr>
<tr>
<td>PCB(BQ)</td>
<td>9(3 x 3)</td>
<td>76.80</td>
<td>565 (*)</td>
</tr>
<tr>
<td>PCB(BQ)</td>
<td>16(4 x 4)</td>
<td>136.13</td>
<td>566 (*)</td>
</tr>
</tbody>
</table>

(*) See text.
It is clear from Tables I and II that high accuracy can be obtained for one-dimensional calculations by the proposed method for a very coarse mesh, even when only linear expansions are used for the local group fluxes. The ratio of mesh sizes for an accuracy of about $6 \times 10^{-6}$ for the one-group, one-region problem is about five when the linear PCB method is compared with the finite difference method, and about four when it is compared with the finite element method. For the two-group, two-region problem these ratios are also about five and four for the same accuracy. In this case, when a higher order (quadratic) expansion is used this ratio increases to about twenty-five when compared with the finite difference method. The results shown in Table III indicate that a coarse mesh can also be used in two-dimensional applications of the method. The ratio of the mesh sizes varies from about five to fifteen depending upon the accuracy desired, when bilinear expansion functions are used. It is about fifteen for an accuracy requirement of about $1.6 \times 10^{-5}$. Again, when a higher order (biquadratic) expansion is used this ratio is further increased, in this case to a value above one hundred.

Although the coarseness of the mesh used in a given calculation is related to the computer storage space required for that calculation, an even more important factor in determining the efficiency of a computational scheme is the time required to obtain a solution within a given (reasonable) accuracy requirement. A systematic examination and comparison of the computational results for the three test problems described in Tables I, II and III yields the following information concerning the computational speed of the proposed method. The partial current balance method (with linear expansion functions) was 3.3 and 3.8 times as fast as the finite difference method and the finite element method, respectively, for the one-dimensional, one-group, one-region problem when an accuracy of $10^{-6}$ was required. It was 12.7 and 6.7 times as fast as the finite difference method and the finite
element method, respectively, for the one-dimensional, two-group, two-region problem when an accuracy of $10^{-6}$ was required. The two-dimensional calculations show that the partial current balance method (with bilinear expansion functions) is a factor of 4.6 times as fast as the finite difference method for an accuracy specification of $10^{-5}$. The computational efficiency for both one-dimensional problems and two-dimensional problems improves further when higher order expansions are used in the partial current balance method. When a biquadratic expansion was used in the partial current balance method solution to the two-dimensional problem it was 25 times as fast and twice as accurate as the finite difference method for which the accuracy specification was $10^{-5}$. It should be noted that the two-dimensional biquadratic PCB calculations do not converge to the extrapolated finite difference value for the multiplication constant $k_{fd,\infty}$. (See bottom of Table III.) Rather, they converge to a value which is closer to the exact value $k_{ex}$. This property of the method has not yet been studied; thus for the above comparison, the accuracy cited for the $2 \times 2$ PCB (BQ) calculation was conservatively based upon a comparison with the value of $k_{fd,\infty}$. (The calculation times used in the comparisons, and tabulated above, for the partial current balance method include the time used to evaluate the required matrix element.)

The nuclear parameters for the simple initial test problems discussed above are given in Table IV and Table V.

**Table IV**

NUCLEAR PARAMETERS FOR SIMPLE HTGR TEST PROBLEMS

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>CORE REGION</th>
<th>REFLECTOR REGION</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$ (cm)</td>
<td>1.335</td>
<td>.903</td>
</tr>
<tr>
<td>$\Sigma_a$ (cm$^{-1}$)</td>
<td>$2.682 \times 10^{-3}$</td>
<td>$1.103 \times 10^{-4}$</td>
</tr>
<tr>
<td>$\Sigma_f$ (cm$^{-1}$)</td>
<td>$1.205 \times 10^{-3}$</td>
<td>---</td>
</tr>
<tr>
<td>$\nu\Sigma_f$ (cm$^{-1}$)</td>
<td>$2.929 \times 10^{-3}$</td>
<td>---</td>
</tr>
</tbody>
</table>
TABLE V
NUCLEAR PARAMETERS FOR SIMPLE HTGR TEST PROBLEMS
TWO-GROUP REFLECTED SYSTEM

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>GROUP</th>
<th>CORE REGION</th>
<th>REFLECTOR REGION</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D ) (cm)</td>
<td>1</td>
<td>1.445</td>
<td>1.065</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.152</td>
<td>0.8629</td>
</tr>
<tr>
<td>( \Sigma_a ) (cm(^{-1}))</td>
<td>1</td>
<td>1.383 \times 10^{-3}</td>
<td>1.945 \times 10^{-6}</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>5.394 \times 10^{-3}</td>
<td>1.436 \times 10^{-4}</td>
</tr>
<tr>
<td>( \Sigma_f ) (cm(^{-1}))</td>
<td>1</td>
<td>1.878 \times 10^{-4}</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>3.328 \times 10^{-3}</td>
<td>0</td>
</tr>
<tr>
<td>( \nu \Sigma_f ) (cm(^{-1}))</td>
<td>1</td>
<td>4.577 \times 10^{-4}</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>8.088 \times 10^{-3}</td>
<td>0</td>
</tr>
<tr>
<td>( \chi )</td>
<td>1</td>
<td>1.0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>2</td>
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<td>0</td>
</tr>
<tr>
<td>( \Sigma_{gg'} )</td>
<td>1</td>
<td>2.420 \times 10^{-3}</td>
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</tr>
<tr>
<td></td>
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</table>

**SUMMARY**

The partial current balance formalism which is reviewed in the second section of this paper is reasonably straightforward and incorporates very simple intuitive physically appealing concepts. These characteristics lead to both physical and computational advantages such as local neutron balances, nearest neighbor coupling, etc. Since Eq. (1) which was used in the introduction as a motivation for the formalism is a *local* equation for the energy dependence in the neutron diffusion problem (because it represents an inner iteration equation for a particular energy group), and the partial current balance formalism incorporates a *local* inversion of Eq. (1) in the space variables, the formalism results in an integral formulation of the multigroup neutron diffusion problem which is both *local*
in energy (within group), and *local* in space (within volume element). This leads to several apparent advantages. The final equations represent an integral formulation without long range coupling (nearest neighbor coupling, only). No large matrices are directly involved. (See Appendix for the dimensions of the various matrices which appear in the final matrix equations.) The matrix elements are calculated separately for each group (*local* in energy); hence, multigroup equations need not be solved to construct the matrix elements. The number of local expansion functions can be varied with volume element and with a group. Either low order or high order approximations can be used. Low and high order approximations can be combined. Little additional coding effort is required for higher order calculations. The method naturally accommodates exact diffusion theory boundary conditions, interface conditions, and symmetry conditions. Finally, the method is potentially useful on parallel array machines.

It is important, at this point, to note that in many cases it is not actually necessary to evaluate the Green's functions to construct the required matrix elements. Rather, when polynomial expansion and weighting functions are used, as in all of the calculations done so far, the matrix elements which are then double moments of the Green's functions can be evaluated directly. This is important in multidimensional calculations since the series representations of the matrix elements have far better convergence properties than the series representations of the Green's functions.

It is also important to note that the elements of the matrices can also be calculated directly (e.g., via transport theory, Monte Carlo, etc.) without employing Green's functions at all, simply by noting and using the physical meanings of the matrix elements. For example, the various matrix elements correspond to: the constant component of the outward partial current across a surface due to a linear partial current input across a surface in the diffusion-removal problem
described by the left hand side of Eq. (6), the linear component of the outward partial current due a quadratic-quadratic volume source, etc.

An approximate method for directly generating the matrix elements which is based upon their physical meanings and which utilizes a variational principle has also been developed, and tested in one-dimensional calculations.\textsuperscript{2}

The apparent advantages suggested above have been shown, by the test problem results reported here, to lead to gains in actual computational efficiency over standard finite difference and finite element methods. These gains have, of course, only been confirmed for the simple test problems which have been studied. It is clear that extensive calculations in which the method is applied to far more complicated reactor models must be done to verify its potential advantages for practical reactor calculations. However, the results obtained thus far are encouraging. They indicate that it is very much worthwhile to apply the method to more elaborate benchmark problems, as well as to extend it to three-dimensional problems and reactor kinetics problems and to test these extensions by three-dimensional neutron kinetics benchmark studies and by calculations for actual power reactor models used in safety analyses.

REFERENCES


APPENDIX

The expressions for the matrix elements of the matrices which appear in Eqs. (21) and (22), the low order \textit{local} matrix equations for the solution vectors
of local expansion coefficients for the volume element group fluxes and outward partial currents, are given below. The dimensions of the matrices are also indicated.

\[
(G_{VV})_{ij} = \int d^3 r \ u^k_{g,i} (r) \int d^3 r_0 \ G^k_{g,r} (r_0) p^k_{g,j} (r_0),
\]

\[
\text{dim} [G_{VV}^{k,k,g}] = [N^k_g \times N^k_g], \tag{A-1}
\]

\[
(G_{VS})_{ij} = \frac{1}{2} \int d^3 r \ u^k_{g,i} (r) \int d^2 r_0 G^k_{g,r} (r_0) q^k_{g,j} (r_0),
\]

\[
\text{dim} [G_{VS}^{k,2k,g}] = [N^k_g \times M^{2k}_g], \tag{A-2}
\]

\[
(G_{SV})_{ij} = 2 \int d^2 r \ v^{km}_{g,i} (r_0) \int d^3 r_0 G^k_{g,r} (r_0) p^k_{g,j} (r_0),
\]

\[
\text{dim} [G_{SV}^{km,k,g}] = [M^{km}_g \times N^k_g], \tag{A-3}
\]

\[
(G_{SS})_{ij} = \int d^2 r_0 \ v^{km}_{g,i} (r_0) \int d^3 r_0 G^k_{g,r} (r_0) - \delta (r_0) q^k_{g,j} (r_0),
\]

\[
\text{dim} [G_{SS}^{km,2k,g}] = [M^{km}_g \times M^{2k}_g], \tag{A-4}
\]

\[
(A^k_g)_{ij} = \int d^3 r \ u^k_{g,i} (r) p^k_{g,j} (r), \text{dim} [A^k_g] = [N^k_g \times N^k_g], \tag{A-5}
\]

and

\[
(b^{km}_g)_{ij} = \int d^2 r \ v^{km}_{g,i} (r_0) q^{km}_{g,j} (r_0), \text{dim} [b^{km}_g] = [M^{km}_g \times M^{km}_g]. \tag{A-6}
\]
Here $p_{g,j}^k (r)$ is the $j$th expansion function for the $g$th group flux in the $k$th volume element, $w_{g,i}^k (r)$ is the $i$th weighting function for the $g$th group over the $k$th volume element, $q_{g,j}^{km} (r_s)$ is the $j$th expansion function for the $g$th group outward partial current across the $km$ interface, and $v_{g,i}^{km} (r_s)$ is the $i$th weighting function for the $g$th group over the $km$ interface surface.

The matrices $[A^k_g]$ and $[B^{km}_g]$ become identity matrices if orthonormal expansion and weighting functions are used, and diagonal matrices if orthogonal functions are used. In any case, the dimensions of these matrices are small, and they are only inverted once, at the beginning of the calculation when the $G$-matrices are constructed, and are incorporated in the $G$-matrices from then on. Hence, the computing time associated with the $A$-, and $B$-matrices is insignificant.

The $N^k_g$ and the $M^{km}_g$ are the numbers of expansion functions used in the local expansions of the fluxes and partial currents. Generally these are quite small (e.g., two to four in one-dimensional calculations, and four to nine in two-dimensional calculations).

As indicated in the last section of the main text, it is important to note that in many cases it is not actually necessary to evaluate the Green's functions to construct the matrix elements of the $G$-matrices. Rather, numerous other more efficient methods, some of which are described there, can be employed to generate these matrix elements.
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A CONSISTENT NODAL METHOD FOR THE ANALYSIS OF SPACE-TIME EFFECTS IN LARGE LWR

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A Consistent Nodal Method for the Analysis of Space-Time Effects in Large LWR's*

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Abstract
The solution method of the computer code IQSBOX is discussed. IQSBOX solves the time dependent multidimensional neutron diffusion equation by a combination of nodal methods with weighted residual techniques. This nodal technique relies on 1D diffusion calculations for determining the spatial coupling coefficients. The 1D diffusion equations are solved by polynomial expansion. For this reason, the method has been called Nodal-Expansion-Method (NEM). Several results for static and dynamic problems are discussed which demonstrate the accuracy and computational efficiency of the method.


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I. Introduction

This paper discusses the solution method of the computer program IQSBOX and some numerical examples run with this code. The IQSBOX program solves the time dependent multidimensional neutron diffusion equation by a combination of nodal methods with weighted residual techniques. For this reason, the method has been called Nodal-Expansion-Method (NEM).

Recently several improved coarse mesh methods were proposed \( (1, 2, 3, 4, 5) \) in an attempt to overcome two basic drawbacks of most nodal techniques presently used, namely insufficient accuracy in deriving the spatial coupling coefficients and the lack of information about the flux distribution inside the nodes. The various approaches are similar in that they combine multidimensional coarse mesh with auxiliary calculations, the purpose of which is to obtain the coupling coefficients. In the method described in \( (1, 2) \) these calculations reduce to a direct elimination of surface fluxes whereas in the so called nodal synthesis method \( (3, 4) \) (NSM) one dimensional (1D) fine-mesh diffusion calculations are performed through all channels for each space direction. In \( (5) \) a Green's function is used to eliminate the spatial differential operators in the equations for each element of the nuclear system.

Since separability of the flux distribution in the nodes has proven to be a reasonable assumption for deriving accurate coupling coefficients \( (3, 4) \) it is also used in the nodal expansion method. This nodal technique is similar to NSM in that it relies on 1D diffusion calculations for determining spatial coupling coefficients, but in contrast to NSM no complete 1D channel sweeps are performed to improve the
spatial coupling coefficients. Instead inhomogeneous 1D diffusion equations are solved for each box and space direction such that the coupling coefficients can be updated during the nodal iterational process. Furthermore, the 1D diffusion equations are solved by polynomial expansion, the expansion coefficients being determined by the Galerkin method. In this way a strong coupling between 1D and 3D calculations can be achieved which is the reason for the good convergence properties of the method. Another important property of the nodal expansion method is that the polynomial expansion coefficients need not be stored. Only the coarse mesh variables, average fluxes and partial currents or spatial coupling coefficients, must be kept in storage. One of the great advantages of this improved nodal technique is its convergence to the exact solution of the diffusion equation for finer mesh sizes.

In Sec. II, the method is formulated for the multigroup neutron diffusion equation. Sec. III discusses the application of the method to the two group diffusion equation. A set of equations is obtained which is formally identical to the one used in the well known nodal collision probability method \((6, 7)\). Some numerical results using the nodal expansion method for both static and dynamic problems are presented in Sec. IV.
II. General Representation of the Nodal Expansion Method

The starting point for the derivation of the method is the set of multigroup neutron diffusion equations in $P_1$-form (8)

\[
\frac{1}{V_g} \frac{\partial \psi_g(r, t)}{\partial t} + \nabla \cdot j_g(r, t) + (\Sigma_{ag}(r, t) + \sum_{g'=1}^{G} \Sigma_{g'g}(r, t)) \phi_g(r, t) = \sum_{g=1}^{G} \Sigma_{gg}(r, t) + \frac{1}{\lambda} \sum_{j=1}^{J} (1 - \beta^j) \chi^j_{pg} \nabla \cdot \Sigma_{fg'}(r, t) \phi_g(r, t) \\
+ \sum_{i=1}^{l} \chi^i_{dg} \lambda_i C_i(r, t) + S_{eg}(r, t)
\]

\[
\vec{j}_g(r, t) + D_g(r, t) \nabla \psi_g(r, t) = 0
\]

\[
\frac{\partial C_i(r, t)}{\partial t} + \lambda_i C_i(r, t) = \frac{1}{\lambda} \sum_{g'=1}^{G} \sum_{j=1}^{J} \beta^j \nabla \cdot \Sigma_{fg} \phi_g(r, t)
\]

$\psi$ and $\vec{j}$ are the flux and current, respectively, in each energy group $g$.

$\chi_p$ and $\chi_d$ are the fission spectra of prompt and delayed neutrons, respectively.
\( \nu \sum_{fg}^{j} \) is \( \nu \) times the fission cross section of fissionable isotope \( j \) in energy group \( g \)

\( 1/\nu_g \) is the reciprocal speed in energy group \( g \)

\( \Sigma_{ag} \) is the macroscopic absorption cross section in group \( g \)

\( \Sigma_{g'g} \) is the scattering cross section for neutrons of initial energy \( g \)

\( D_g \) is the diffusion constant in energy group \( g \)

\( \beta_i \) and \( \lambda_i \) are the delay fraction and decay constant, and \( C_i \) is the concentration of delayed neutron precursor type \( i \); \( \beta^i = \sum_{i=1}^{1} \beta_i \)

\( S_{eg} \) is the external source in energy group \( g \)

The eigenvalue \( \lambda \) is unity for a physically critical reactor. Equations (1a, b) and (2) are to be solved subject to the boundary condition that \( \phi (\tilde{r}, t) \) be everywhere continuous and that the components perpendicular to internal surfaces of the current vector \( \tilde{j}_g \) be continuous across these surfaces. Along the exterior boundary of the reactor the incoming current vanishes. An initial distribution must be specified. As shown in (2) it is a simple matter to obtain formally exact coarse mesh equations. We integrate the Eqs. (1a) and (2) over the box volume \( V^m = (a_x \cdot a_y \cdot a_z)^m \) and (1b) over the six surfaces in order to define appropriate averaged quantities.
\[ \phi_g^m(t) = \frac{1}{V^m} \int_{V^m} \phi_g(\vec{r},t) \, dV \]

\[ \Sigma_g^m(t) = \frac{1}{V^m \phi_g^m} \int_{V^m} \Sigma_g(\vec{r},t) \phi_g(\vec{r},t) \, dV \]

\[ \frac{1}{V^m} \int_{A_u^m} j_{gur} \cdot \hat{n} \, dA = \frac{1}{a_u^m} \left( j_{gur}^+ - j_{gur}^- \right) \]

\[ \frac{1}{V^m} \int_{A_u^m} j_{gul} \cdot \hat{n} \, dA = \frac{1}{a_u^m} \left( j_{gul}^- - j_{gul}^+ \right) \]

\[ (u = x, y, z) \]

\[ C_i^m(t) = \frac{1}{V^m} \int_{V^m} C_i(\vec{r},t) \, dV \]

\[ S_{eg}^m(t) = \frac{1}{V^m} \int_{V^m} S_{eg}(\vec{r},t) \, dV \]

\( A_u^m \) denotes the surface of box \( m \), the normal of which points into the positive or negative \( u \)-direction \((u = x, y, z)\).

\( j_{gus}^+ \) and \( j_{gus}^- \) represent average partial currents on the right \((s = r)\) or left \((s = l)\) surface of box \( m \).

The result is the set of nodal equations.
\[
\frac{1}{\nu_g} \frac{d \Phi^m_g}{d t} + \sum_{u=x,y,z} \frac{1}{A^m_u} \left[ (j^-_{gu} + j^+_{gu}) - (j^+_{gu} + j^-_{gu}) \right] \\
+ \left( \sum_{ag} \Sigma_{g=1}^G \Sigma_{g'}^m \Phi^m_g \right) \\
= \sum_{g=1}^G \left( \sum_{g=1}^G \gamma^m_{pg} - \frac{1}{\lambda} \sum_{j=1}^J (1 - \beta^j_{pg}) \chi^j_{pg} \nu \Sigma^m_{g'} \Phi^m_{g'} \right) \\
+ \sum_{i=1}^I \chi^i_{dg} \lambda^m_i C^i_m + S_{eg} 
\]

\[
D^m_g \frac{\partial \psi^m_{gu}}{\partial u} \bigg|_S + (j^+_{gus} - j^-_{gus}) = 0 
\quad (s = l,r; \quad u = x,y,z) 
\]

\[
\frac{d C^m_i}{d t} + \lambda^m_i C^m_i = \frac{1}{\lambda} \sum_{g=1}^G \sum_{j=1}^J \beta^j_{pg} \nu \Sigma^m_{g'} \Phi^m_{g'} 
\quad (s = l,r; \quad u = x,y,z) 
\]

In (3b) the derivative is to be interpreted as

\[
D^m_g \frac{\partial \psi^m_{gu}}{\partial u} \bigg|_S = \frac{1}{A^m_u} \int D^m_g \frac{\partial \psi^m_{gu}(r,t)}{\partial u} \bigg|_S dA 
\quad (s = l,r; \quad u = x,y,z) 
\]
Conventional nodal methods define spatial coupling coefficients by the relationship (2)

\[ C_{gu}^{m}(u) = j_{gu}^{m} / (a_u \phi_g^m) \]

\[ C_{gu}^{m,1}(u) = j_{gu}^{m} / (a_u \phi_g^m) \]

\( (u = x, y, z) \)

If these coupling coefficients can be determined by subsidiary calculations and/or by applying fitting procedures Eq. (3b) is superfluous. Another way of dealing with the problem is to determine the spatial dependence of \( \psi_g^m(u, t) \) by concomitant auxiliary calculations (4). For this purpose, \( \varphi_g(r, t) \) is approximated in each time interval \( t_n < t \leq t_{n+1} \) by

\[ \varphi_g(r, t) = \Phi_g^m(t) \prod_{u=x,y,z} f_{gu}^m(u) \] \( (5) \)

The shape functions \( f_{gu}^m(u) \) are normalized to unity

\[ \frac{1}{a_u^m} \int_0^{a_u^m} f_{gu}^m(u) \, du = 1 \]

Substituting Eq. (5) into Eqs. (1a) and (2) and integrating over two space directions of box \( m \) we obtain
\[
(\frac{1}{V_g} \cdot \frac{1}{\phi^m_g} \cdot \frac{d\phi^m_g}{dt} + \sum a_g + \sum_{g=1}^G \sum_{g'=1}^m g_{g'}^{m}) \psi_{gu} \\
- D_{g}^m \frac{\partial^2 \psi_{gu}^m}{\partial u^2} + \sum_{v \neq u}^m \frac{1}{a_{v}^m \phi^m_g} \left[ (j_{gvi}^{-m} + j_{gvi}^{m}) - (j_{gvi}^{m} + j_{gvi}^{-m}) \right] \psi_{gu}^m \\
= \sum_{g=1}^G \left( \sum_{g'=1}^m g_{g'}^m + \frac{1}{\lambda} \sum_{j=1}^J (1 - \beta_j^i) \chi_{gj}^i \psi_{fg}^j \psi_{fg}^j \right) \psi_{gu}^m \\
+ S_{gu}^m(u, t) + S_{egu}(u, t)
\]

(\text{u = x, y, z}) \tag{6}

The third term on the left hand side of Eq. (6) describes the transverse leakage.

\(S_{gu}^m(u, t)\) denotes the source of delayed neutrons

\[
S_{gu}^m(u, t) = \sum_{i=1}^I \chi_{dg}^i \lambda_i \left[ C_{iu}^m(u, t_0) e^{-\lambda_i(t-t_0)} \right. \\
+ \frac{1}{\lambda} \sum_{g=1}^G \sum_{j=1}^J \beta_j^i \int_{t_0}^t e^{-\lambda_i(t-\tau)} \psi_{fg}^j \psi_{gu}^j(u, \tau) d\tau \\
= \sum_{i=1}^I \chi_{dg}^i \lambda_i S_{ui}^m(u, t) \\
S_{ui}^m(u, t_0) = \frac{1}{\lambda} \sum_{g=1}^G \sum_{j=1}^J \beta_j^i \psi_{fg}^j(u, t_0) / \lambda_i
\]
If we now introduce the diffusion theory expression

\[ \psi^m_{\text{gus}} = 2 \left( j^m_{\text{gus}} + j^{-m}_{\text{gus}} \right) \quad (s = l, r) \]  

(7)

the auxiliary one dimensional diffusion problem (6, 7) for the determination of \( \psi^m_{\text{gus}} (u, t) \) is completely defined. The Eqs. (3, 4) and (6, 7) constitute a coupled system of ordinary and partial differential equations which can be solved simultaneously. The assumption of separability (5) had to be introduced in order to be able to derive an expression for transverse leakage. Of course, the assumption of separability is also of use if one wants to consider simple spatial dependence of cross sections as given f. i. by partial insertion of control rods into boxes.
III. Reduction to Two Neutron Groups.
Approximation Procedure

The underlying idea of the method as described in the foregoing paragraph is that an approximate calculation of spatial coupling coefficients suffices to obtain accurate spatial mean values of reaction rates. For this reason it is not necessary and even not desirable to calculate an exact solution of Eq. (6). Therefore, we approximate the solution of (6) by an expansion in known functions. Taking into account normalization and boundary conditions we have

\[
\psi_{g u}^m (u, t) = \psi_{g u}^m + \left[ \psi_{g u}^m - \psi_{g u}^m \right] \frac{u}{a_u^m} \\
+ 3 \left[ 2 \phi_g^m (t) - \psi_{g u}^m - \psi_{g u}^m \right] \frac{u}{a_u^m} \left( 1 - \frac{u}{a_u^m} \right) \\
+ \sum_{i=1}^n C_{i+2, g, u} h_{i+2} \left( \frac{u}{a_u^m} \right) \\
\quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \ qua
approximation is a poor one when applied to the nodal expansion method. At least \( n = 1 \) is required for an accurate determination of the coupling coefficients. This is to be expected, because for \( n = 0 \) the properties of the node as given by Eq. (6) get lost. The expansion functions \( h_{i+2} \) have to be chosen such that

\[
\int_{0}^{1} h_{i+2}(v) \, dv = 0
\]

\( h_{i+2}(0) = h_{i+2}(1) = 0 \)

To facilitate the calculation of the expansion coefficients \( C_{i+2}^m \), \( g, u \), it is advisable to orthogonalize the expansion functions. Thus we get for the first two functions:

\[
h_3(v) = v(1-v)(v-1/2)
\]

\[
h_4(v) = v(1-v)(v^2-v+1/5)
\]

The expansion coefficients can be determined by applying the Galerkin scheme (10) to Eq. (6). In a two group representation we get for each box \( m \) and space direction \( u \)

\[
\begin{align*}
\int_{0}^{1} h_1 \left[ (\frac{\omega_1^m}{v_1} + (D_1 B_{1u}^2) + \Sigma_{a1}^m + \Sigma_{21}^m) \psi_1^m \
- D_1^m \frac{\partial \psi_1^m}{\partial u^2} - \frac{1}{\lambda} \sum_{j=1}^{J} (1 - \beta_j) (v \sum_{f1}^{jm} \psi_{1u}^m + v \sum_{f2}^{jm} \psi_{2u}^m) \right] \\
- \sum_{i=1}^{J} \lambda_i (S_{u_i}^m (u,t_n) e^{-\lambda_i (t_{n+1} - t_n)} + \\
\frac{1}{\lambda} \sum_{j=1}^{J} \beta_j \int_{t_n}^{t_{n+1}} e^{-\lambda_i (t_{n+1} - \tau)} \left[ \sum_{g=1}^{G} v \sum_{f1}^{jg} \psi_{g}^m (u,\tau) \, d\tau \right] - S_{e_1 u}] \, du = 0
\end{align*}
\]
\[ q_m^u \int_{0}^{h_1} \left[ (\frac{w_m^2}{v_2} + (D_2 B_{2u}^2)^m + \Sigma_{a2}^m) \psi_{2u} \\
- D_2^m \frac{\partial^2 \psi_{2u}}{\partial u^2} S_{e2u} (u, t_{n+1}) \right] du = 0 \] \hspace{1cm} (9b)

\( l = 3, 4, \ldots \)

\( \omega_{g}^m \) is the local reciprocal period of the box average flux

\[ \omega_{g}^m = \frac{1}{\Phi_{g}^m} \frac{d \Phi_{g}^m}{dt} \bigg|_{t = t_{n+1}} \]

\( (D, B_{gu}^2)^m \) is a short notation for the transverse leakage term

\[ (D, B_{gu}^2)^m = \sum_{v+u} \frac{1}{a_v^m \Phi_{g}^m} \left[ j_{gvr}^- m \psi_{gvr}^- (j_{gvl}^m + j_{gvt}^m) \right]_{t = t_{n+1}} \]

\( u = x, y, z \)

The treatment of the time dependence of Eq. (6) corresponds to a fully implicit time differencing scheme.

At this point a further approximation is introduced. In order to keep storage requirements low the spatial shape of the precursor concentration is assumed to be proportional to the instantaneous fission source. In the auxiliary 1D calculations \( S_{ui}^m \) is replaced by

\[ S_{ui}^m (u, t_n) = \frac{k_i}{\lambda} \sum_{j=1}^{J} \beta_j \sum_{g=1}^{G} \Sigma_{fg}^{jm} \psi_{gu}^m (u, t_{n+1}) \]

where \( k_i \) denotes a properly chosen proportionality constant. Further investigations must show if this simplification is generally adequate.
The solution of Eqs. (9a, b) is now a simple matter. For \( n = 1 \) (G\(_1\)-approximation) the expansion coefficients are the solution of a 2 x 2 matrix system for each space direction. For \( n = 2 \) (G\(_2\)-approximation) the 4 x 4 system degenerates into two 2 x 2 systems so that the additional cost is tolerable. The G\(_2\)-approximation is presently the standard option of the computer code IQSBOX.

With the solution of (9a) and (9b) at hand, Eq. (3b) can be solved for outgoing currents in terms of average fluxes, incoming currents and the expansion coefficients which are themselves implicit functions of the various cross sections, average fluxes and partial currents.

The outgoing currents can be eliminated from the neutron balance equation by substituting (3b) into (3a). Formally, the following set of equations has to be solved for each box \( m \)

\[
\frac{1}{V} \frac{d\Phi}{dt} = A\Phi + BJ^{in} + f \tag{10a}
\]

\[
J^{out} = D\Phi + EJ^{in} + g \tag{10b}
\]

In two group theory the balance equation (10a) is a 2 x 2 system, whereas the equation for the outgoing currents (10b) split into three 2 x 2 systems. Nodes are coupled by the condition that outgoing currents are the incoming currents of adjacent boxes.
In summary, the iterative solution procedure is as follows

1. Determine expansion coefficients (Eq. 9a, b) by using last known values of fluxes, currents and cross sections

2. Determine average fluxes by solving Eq. (10a)

3. Solve Eq. (10b) for outgoing currents.

Steps 1 to 3 have to be followed for each box \( m \) and must be repeated until convergence. Several acceleration techniques are used in combination: overrelaxation is used during a mesh sweep, coarse mesh rebalancing \((11, 12)\) after each mesh sweep, and asymptotic extrapolation \((13)\) every time the iterative solution has adopted an asymptotic behaviour.
IV. Numerical Results

A. Static Problems

Being a spatial approximation technique, NEM has been tested extensively in static problems. The solution of the IAEA Benchmark problem (14) was compared with results obtained by finite difference (FDM) and finite element methods (FEM). The upper part of Fig. 1 shows results for the IAEA-2D problem for various orders of approximation \((G_0, G_1, G_2)\). It can clearly be seen that there is a substantial improvement of the solution by going from \(G_0\) to \(G_1\) and \(G_2\). In the lower part of the figure a NEM-solution, using a \(G_2\)-approximation (mesh size 20 cm) is compared with a FDM-solution (mesh size 1 cm). The agreement is considered satisfactory. Although there are considerable local deviations from the reference solution in those parts of the solution where the separability assumption is strongly violated, the maximum error of the average power density per fuel element is less than 4 %. In Tables 1a, b solutions obtained with various approximation methods are compared. Clearly, NEM is computationally more efficient than NSM and FEM (15) and yields better results for very large mesh sizes. This fact becomes even more important for dynamic 3D problems. Table 2 shows the initial distribution of the LRA-2D Benchmark problem (16) for different mesh sizes. In this problem the maximum error for a mesh size of 15 cm is also below 4 %. Fig. 2 and Fig. 3 show the traverse of maximum power density for this problem.
B. Dynamic Problems

In addition to 2D and 3D static calculations, a number of 1D, 2D and 3D dynamic problems have also been set up and run. The first problem to be discussed here is an ANS benchmark problem for 1D space-time kinetics (17). The reactor in this problem has three regions; a low enrichment central region and two identical high-enrichment end sections. Decreasing the thermal absorption cross section in region 1 leads to a delayed super-critical transient. Fig. 4 compares the results for the initial distribution with the published reference solution. The results are strongly dependent on the boundary condition. The "natural" boundary condition in IQSBOX is \( J^{\text{in}} = 0 \), whereas conventional diffusion codes frequently use \( \phi = 0 \). This leads to a difference in \( k_{\text{eff}} \) of about 1% in this example. The differences in regional power fractions and in the time behaviour of the solution (Tables 3, 4) are even more pronounced. Table 5 shows the results for a subcritical transient calculated with time dependent and constant spatial coupling coefficients. The results for both cases demonstrate once more that transient calculations cannot be performed with coupling coefficients derived for the initial state. Indeed, a continuous deterioration of the solution can be observed with diminishing accuracy of coupling coefficients. Table 6 compares the results of the delayed super-critical transient for different sets of coupling coefficients. The reference solution is obtained with completely converged coupling coefficients. In the other cases the iterative procedure for the calculation of coupling coefficients is terminated when two successive values differ by less than a specified parameter \( \varepsilon_c \). A considerable amount of computing time can be saved if the calculation of coupling coefficients can be stopped before the nodal iterative procedure has come to the end.
However, this strategy is somewhat dangerous. The next two test cases are 3D problems taken from a paper by FERGUSON and HANSEN (18). The first case is a simple delayed super-critical transient caused by a step change in reactivity in a bare homogeneous reactor (test case 1 of (18)). Table 7 compares the result with the published solution.

The last case to be considered here (test case 4 of (18)) is a spatially dependent problem. It represents an attempt to simulate the withdrawal of control rods from two adjacent subassemblies in a pressurized water reactor. In (18) the rod withdrawal was simulated by linearly decreasing the thermal absorption cross section over three successive time zones of 0.08-sec. length. During the first zone, only the bottom third of the subassembly was perturbed. The middle and upper thirds followed successively in the next two time zones. In IQSBOX the perturbation was introduced by linearly decreasing the thermal absorption cross section box by box over the time interval $0 \leq t \leq 0.24$. For this reason the results of 3DKIN (18) and IQSBOX are not completely comparable. There are at least two other reasons for expecting different results for the two codes. Because of storage limitations the mesh sizes could not be chosen identically (Table 8). Further, the different spatial approximations produce different initial states (Table 9). With this in mind one should look at the results displayed in Tables 10, 11 and 12. The results of IQSBOX are obtained with a time step size of $\Delta t = 0.01$ sec which is 10 times longer than that used in 3DKIN. As expected, the largest discrepancies between the two solutions can be observed at those mesh points (1, 21) where the rods are moved. Nevertheless, the general agreement between the solutions is considered satisfactory.
V. Conclusions

This paper has almost exclusively dealt with the spatial approximation method of the space-time kinetics code IQSBOX. It has been shown that the nodal expansion method is a useful variant of those nodal methods which generate spatial coupling coefficients during the solution process. The method is characterized by high accuracy and computational efficiency.

The time integration of the nodal equations is presently performed by the backwards-difference algorithm (8). In view of the flexibility of the method as to the iterative procedure other time integration schemes will probably be more efficient. This is one of the problems which remain for further investigations.
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Bonn 1971

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Comparison of Different NEM-Approximations

Nodal Expansion Method
- G2 Approximation
--- G1 Approximation
----- G0 Approximation
mesh size: 20 cm

Normalized thermal flux

FDM versus NEM

PDQ Finite Difference, mesh size: 1 cm
- G2 Approximation, mesh size: 20 cm

2D IAEA Problem, Radial Traverse, y=0  Fig. 1
Table 1a

IAEA 2D Problem (14)
COMPARISON OF DIFFERENT METHODS

Fuel element size: 20 x 20 cm

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<thead>
<tr>
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<td>0.473</td>
<td>0.689</td>
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<td>IQSBOX</td>
<td>20 cm</td>
<td>0.460</td>
<td>0.702</td>
<td>0.603</td>
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<td>FEM2D</td>
<td>1/2 Fuel</td>
<td>0.496</td>
<td>0.698</td>
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<td>1.301</td>
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<td>1.321</td>
<td>1.081</td>
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<td>1.264</td>
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<td>1.033</td>
<td>0.978</td>
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Table 1b: 2D IAEA PROBLEM: Average Power Density per Fuel Element

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<th>NEM</th>
<th>NSM</th>
<th>FEM (15)</th>
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<td>20.0</td>
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<td>10^-5</td>
<td>10^-6</td>
<td>10^-6</td>
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Table 2

LRA-2D Problem (16)

Average Power Densities

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<tr>
<th>Mesh Size</th>
<th>Solution 1</th>
<th>Solution 2</th>
<th>Solution 3</th>
<th>Solution 4</th>
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</thead>
<tbody>
<tr>
<td>15.0 cm</td>
<td>2.195</td>
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<td>7.5 cm</td>
<td>2.174</td>
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</tr>
<tr>
<td>3.75 cm</td>
<td>2.162</td>
<td>1.628</td>
<td>0.842</td>
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NEM Solutions for Different Mesh Sizes. Traverse of Maximum Power Density is Marked by Heavy Lines

<table>
<thead>
<tr>
<th>Mesh Size</th>
<th>Solution 1</th>
<th>Solution 2</th>
<th>Solution 3</th>
<th>Solution 4</th>
</tr>
</thead>
<tbody>
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<td>1.884</td>
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<td>3.75 cm</td>
<td>1.853</td>
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<td>1.677</td>
<td>0.970</td>
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Average Power Densities

<table>
<thead>
<tr>
<th>Mesh Size</th>
<th>Solution 1</th>
<th>Solution 2</th>
<th>Solution 3</th>
<th>Solution 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>15.0 cm</td>
<td>0.868</td>
<td>1.147</td>
<td>1.335</td>
<td>1.432</td>
</tr>
<tr>
<td>7.5 cm</td>
<td>0.866</td>
<td>1.151</td>
<td>1.338</td>
<td>1.427</td>
</tr>
<tr>
<td>3.75 cm</td>
<td>0.865</td>
<td>1.151</td>
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Average Power Densities

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<th>Solution 3</th>
<th>Solution 4</th>
</tr>
</thead>
<tbody>
<tr>
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Average Power Densities

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<th>Solution 3</th>
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Average Power Densities

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Average Power Densities

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<td>0.509</td>
</tr>
<tr>
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<tr>
<td>3.75 cm</td>
<td>0.614</td>
<td>0.441</td>
<td>0.414</td>
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</table>
2-D-LRA-Case: Traverse of Maximum Power Density

Fast, Thermal Flux × 10^7 cm⁻²
Descriptive Title: 1D 2-group Neutron Diffusion Problem in Thermal Reactor (17)

Initial Power Fractions:

<table>
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<tr>
<th>Region</th>
<th>Initial Distribution ( J_{\text{in}} = 0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Region 1</td>
<td>.2790 \quad .2788 \quad .3022</td>
</tr>
<tr>
<td>Region 2</td>
<td>.4421 \quad .4424 \quad .3956</td>
</tr>
<tr>
<td>Region 3</td>
<td>.2790 \quad .2788 \quad .3022</td>
</tr>
</tbody>
</table>

\( k_{\text{eff}} \) values:
- RAUMZEIT: .901551
- IQSBOX: .901626
- \( J_{\text{in}} = 0 \): .910293

Fig. 4
Table 3

ANS 1D Benchmark Problem:
Delayed Super-critical Transient \(17\)

\[ \Delta \Sigma_{a2} \text{ (Region 1)} = -0.0018 \text{ cm}^{-1} \text{ in 1.0 sec} \]

Total Power versus Time \( \Delta x = 10 \text{ cm} \)

<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>ANS Reference Solution (\phi=0)</th>
<th>IQSBOX (\phi=0)</th>
<th>IQSBOX (J_{in}=0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>0.1</td>
<td>1.029</td>
<td>1.029</td>
<td>1.032</td>
</tr>
<tr>
<td>0.2</td>
<td>1.063</td>
<td>1.063</td>
<td>1.070</td>
</tr>
<tr>
<td>0.5</td>
<td>1.205</td>
<td>1.207</td>
<td>1.234</td>
</tr>
<tr>
<td>1.0</td>
<td>1.743</td>
<td>1.748</td>
<td>1.929</td>
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<td>1.5</td>
<td>1.960</td>
<td>1.969</td>
<td>2.260</td>
</tr>
<tr>
<td>2.0</td>
<td>2.167</td>
<td>2.181</td>
<td>2.586</td>
</tr>
</tbody>
</table>
Table 4

ANS 1D Benchmark Problem:

Delayed Super-critical Transient (17)

\[ \Delta \Sigma_{a_2}(\text{Region 1}) = -0.0018 \text{ cm}^{-1} \text{ in } 1.0 \text{ sec} \]

Relative Regional Power versus Time

<table>
<thead>
<tr>
<th>Time</th>
<th>Program</th>
<th>Region 1</th>
<th>Region 2</th>
<th>Region 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>ANS Ref IQSBOX ( \phi = 0 )</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td></td>
<td>&quot; ( J_{in} = 0 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>ANS Ref IQSBOX ( \phi = 0 )</td>
<td>2.440</td>
<td>1.703</td>
<td>1.108</td>
</tr>
<tr>
<td></td>
<td>&quot; ( J_{in} = 0 )</td>
<td>2.450</td>
<td>1.709</td>
<td>1.109</td>
</tr>
<tr>
<td>2.0</td>
<td>ANS Ref IQSBOX ( \phi = 0 )</td>
<td>3.217</td>
<td>2.114</td>
<td>1.119</td>
</tr>
<tr>
<td></td>
<td>&quot; ( J_{in} = 0 )</td>
<td>3.242</td>
<td>2.128</td>
<td>1.202</td>
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<tr>
<td></td>
<td></td>
<td>4.068</td>
<td>2.518</td>
<td>1.188</td>
</tr>
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</table>
Table 5

ANS 1D Benchmark Problem:

Sub-critical Transient \((17)\)

\[ \Delta \Sigma_{a2} \text{ (Region 1)} = 0.0054 \text{ cm}^{-1} \text{ in 1.0 sec} \]

Total Power versus Time \(\Delta x = 10 \text{ cm}\)

| Time (sec) | ANS Reference Solution \(\phi=0\) | IQSBOX \(J^{in}=0\) | IQSBOX \(J^{in}=0\) *
<table>
<thead>
<tr>
<th></th>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>0.1</td>
<td>0.9300</td>
<td>0.9237</td>
<td>0.9274</td>
</tr>
<tr>
<td>0.2</td>
<td>0.8735</td>
<td>0.8646</td>
<td>0.8675</td>
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<tr>
<td>0.5</td>
<td>0.7598</td>
<td>0.7499</td>
<td>0.7410</td>
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<tr>
<td>1.0</td>
<td>0.6589</td>
<td>0.6522</td>
<td>0.6197</td>
</tr>
<tr>
<td>1.5</td>
<td>0.6433</td>
<td>0.6380</td>
<td>0.5992</td>
</tr>
<tr>
<td>2.0</td>
<td>0.6307</td>
<td>0.6266</td>
<td>0.5824</td>
</tr>
</tbody>
</table>

*Spatial coupling coefficients taken from initial Distribution
Table 6

ANS 1D Benchmark Problem:

Delayed Super-critical Transient (17)

\[ \Delta \Sigma_{a2} \text{ (Region 1)} = -0.0018 \text{ cm}^{-1} \text{ in 1.0 sec} \]

Dependence of the Solution on Accuracy of Coupling Coefficients \( \varepsilon_c \)

Total Power versus Time, mesh size \( \Delta x = 20 \text{ cm} \)

<table>
<thead>
<tr>
<th>Time sec</th>
<th>IQSBOX Reference Solution</th>
<th>IQSBOX ( \varepsilon_c = 10^{-5} )</th>
<th>IQSBOX ( \varepsilon_c = 5 \cdot 10^{-5} )</th>
<th>IQSBOX ( \varepsilon_c = \infty )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>0.1</td>
<td>1.0318</td>
<td>1.0293</td>
<td>1.0288</td>
<td>1.0278</td>
</tr>
<tr>
<td>0.2</td>
<td>1.0695</td>
<td>1.0646</td>
<td>1.0627</td>
<td>1.0598</td>
</tr>
<tr>
<td>0.5</td>
<td>1.2323</td>
<td>1.2221</td>
<td>1.2136</td>
<td>1.1819</td>
</tr>
<tr>
<td>1.0</td>
<td>1.9225</td>
<td>1.8864</td>
<td>1.8764</td>
<td>1.5251</td>
</tr>
<tr>
<td>1.5</td>
<td>2.2452</td>
<td>2.2269</td>
<td>2.2207</td>
<td>1.6255</td>
</tr>
<tr>
<td>2.0</td>
<td>2.5658</td>
<td>2.5423</td>
<td>2.5393</td>
<td>1.7158</td>
</tr>
<tr>
<td>3.0</td>
<td>3.3153</td>
<td>3.2696</td>
<td>3.2647</td>
<td>1.8877</td>
</tr>
<tr>
<td>4.0</td>
<td>4.2463</td>
<td>4.1784</td>
<td>4.1635</td>
<td>2.0577</td>
</tr>
<tr>
<td>CPU sec</td>
<td>50.6</td>
<td>23.7</td>
<td>21.6</td>
<td>8.6</td>
</tr>
</tbody>
</table>

\( * \) Spatial coupling coefficients derived for the initial state
<table>
<thead>
<tr>
<th>Program</th>
<th>3DKIN $\Delta t = 0.01$</th>
<th>3DKIN $\Delta t = 0.001$</th>
<th>IQSBOX $\Delta t = 0.01$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time sec</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>0.816</td>
<td>0.816</td>
<td>0.816</td>
</tr>
<tr>
<td>0.05</td>
<td>0.920</td>
<td>1.127</td>
<td>1.121</td>
</tr>
<tr>
<td>0.1</td>
<td>1.151</td>
<td>1.407</td>
<td>1.399</td>
</tr>
<tr>
<td>0.15</td>
<td>1.454</td>
<td>1.660</td>
<td>1.651</td>
</tr>
<tr>
<td>0.2</td>
<td>1.782</td>
<td>1.890</td>
<td>1.881</td>
</tr>
<tr>
<td>0.3</td>
<td>2.383</td>
<td>2.289</td>
<td>2.280</td>
</tr>
<tr>
<td>0.4</td>
<td>2.840</td>
<td>2.622</td>
<td>2.613</td>
</tr>
</tbody>
</table>
TEST CASE 4 (Ferguson - Hansen, (18))

Meshsize: 10 × 10 × 30 Core
           10 × 10 × 15 Reflector

Perturbation:
withdrawal of control rod in mesh m (material 1)

Table 8
<table>
<thead>
<tr>
<th>Table 9</th>
<th>Material Properties:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Group 1</td>
</tr>
<tr>
<td><strong>Material 1</strong></td>
<td></td>
</tr>
<tr>
<td>$\Sigma_{tr}$ cm$^{-1}$</td>
<td>0.2246</td>
</tr>
<tr>
<td>$\Sigma_a$ cm$^{-1}$</td>
<td>0.009434</td>
</tr>
<tr>
<td>$\nu$</td>
<td>2.571</td>
</tr>
<tr>
<td>$\Sigma_f$ cm$^{-1}$</td>
<td>0.002437</td>
</tr>
<tr>
<td>$\Sigma_{J\rightarrow J+1}$ cm$^{-1}$</td>
<td>0.01872</td>
</tr>
<tr>
<td><strong>Material 2</strong></td>
<td></td>
</tr>
<tr>
<td>$\Sigma_{tr}$ cm$^{-1}$</td>
<td>0.2264</td>
</tr>
<tr>
<td>$\Sigma_a$ cm$^{-1}$</td>
<td>0.009223</td>
</tr>
<tr>
<td>$\nu$</td>
<td>2.584</td>
</tr>
<tr>
<td>$\Sigma_f$ cm$^{-1}$</td>
<td>0.002236</td>
</tr>
<tr>
<td>$\Sigma_{J\rightarrow J+1}$ cm$^{-1}$</td>
<td>0.01893</td>
</tr>
<tr>
<td><strong>Material 3</strong></td>
<td></td>
</tr>
<tr>
<td>$\Sigma_{tr}$ cm$^{-1}$</td>
<td>0.1971</td>
</tr>
<tr>
<td>$\Sigma_a$ cm$^{-1}$</td>
<td>0.0001984</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.0</td>
</tr>
<tr>
<td>$\Sigma_f$ cm$^{-1}$</td>
<td>0.0</td>
</tr>
<tr>
<td>$\Sigma_{J\rightarrow J+1}$ cm$^{-1}$</td>
<td>0.03010</td>
</tr>
<tr>
<td><strong>Material 4</strong></td>
<td></td>
</tr>
<tr>
<td>$\Sigma_{tr}$ cm$^{-1}$</td>
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</tr>
<tr>
<td>$\Sigma_a$ cm$^{-1}$</td>
<td>0.0003288</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.0</td>
</tr>
<tr>
<td>$\Sigma_f$ cm$^{-1}$</td>
<td>0.0</td>
</tr>
<tr>
<td>$\Sigma_{J\rightarrow J+1}$ cm$^{-1}$</td>
<td>0.0</td>
</tr>
</tbody>
</table>

**Initial Condition:**

Critical $k_{eff}$: 1.28041608 (3DKIN)
1.276504 (IQSBOX)
<table>
<thead>
<tr>
<th>Program</th>
<th>IQSBOX</th>
<th>3DKIN</th>
<th>IQSBOX</th>
<th>3DKIN</th>
</tr>
</thead>
<tbody>
<tr>
<td>z-plane</td>
<td>$(3+4)$</td>
<td>5</td>
<td>$(3+4)$</td>
<td>5</td>
</tr>
<tr>
<td>Time sec</td>
<td>Point</td>
<td></td>
<td>Point</td>
<td></td>
</tr>
<tr>
<td>0.0</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>0.04</td>
<td>1.012</td>
<td>1.027</td>
<td>1.206</td>
<td>1.268</td>
</tr>
<tr>
<td>0.08</td>
<td>1.062</td>
<td>1.076</td>
<td>1.591</td>
<td>1.694</td>
</tr>
<tr>
<td>0.12</td>
<td>1.162</td>
<td>1.158</td>
<td>1.936</td>
<td>1.948</td>
</tr>
<tr>
<td>0.16</td>
<td>1.289</td>
<td>1.309</td>
<td>2.231</td>
<td>2.385</td>
</tr>
<tr>
<td>0.20</td>
<td>1.402</td>
<td>1.426</td>
<td>2.466</td>
<td>2.639</td>
</tr>
</tbody>
</table>

Table 10  Test Case 4  (Ferguson-Hansen, (18))
Results, z-Plane 5  (18)
<table>
<thead>
<tr>
<th>Program</th>
<th>IQSBOX</th>
<th>3DKIN</th>
<th>IQSBOX</th>
<th>3DKIN</th>
</tr>
</thead>
<tbody>
<tr>
<td>z-plane</td>
<td>(6+7)</td>
<td>10</td>
<td>(6+7)</td>
<td>10</td>
</tr>
<tr>
<td>Time sec</td>
<td>Point</td>
<td>Point</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(1,4)</td>
<td>(1,5)</td>
<td>(1,19)</td>
<td>(1,21)</td>
</tr>
<tr>
<td>0.0</td>
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<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
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<td>1.009</td>
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<td>1.017</td>
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<tr>
<td>0.08</td>
<td>1.051</td>
<td>1.059</td>
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<tr>
<td>0.12</td>
<td>1.144</td>
<td>1.143</td>
<td>1.524</td>
<td>1.532</td>
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<tr>
<td>0.16</td>
<td>1.274</td>
<td>1.291</td>
<td>2.088</td>
<td>2.260</td>
</tr>
<tr>
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<td>1.395</td>
<td>1.413</td>
<td>2.442</td>
<td>2.561</td>
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</table>

Table 11 Test Case 4 (Ferguson-Hansen, (18)) Results, z-Plane 10 (18)
<table>
<thead>
<tr>
<th>Program</th>
<th>IQSBOX</th>
<th>3DKIN</th>
<th>IQSBOX</th>
<th>3DKIN</th>
</tr>
</thead>
<tbody>
<tr>
<td>z plane</td>
<td>(9+10)</td>
<td>16</td>
<td>(9+10)</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Time sec</td>
<td>Point</td>
<td>Point</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(1,4)</td>
<td>(1,5)</td>
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<td>0.16</td>
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</table>

Table 12  Test Case 4 (Ferguson-Hansen, (18)) Results, z-Plane 16 (18)
DISCUSSION

F.N. McDonnell

What are the relative computing efficiencies between the conventional finite difference (3DKIN) method and your coarse-mesh method (IQSBOX)?

H. Finnemann

Using the same mesh size, the computing cost per time step is of course lower in conventional finite difference methods. Taking into account accuracy and computing cost, the proposed nodal method is much more efficient. You gain a factor of at least 3 to 5 for each space direction. In fact, only by using coarse-mesh methods 3-D space-time calculations become feasible.

G. Williams

How do you intend to develop your nodal programme in the future? What improvements do you have in mind?

H. Finnemann

Up to now, the efforts were concentrated on an accurate spatial approximation. The time integration is performed by the simple backwards difference algorithm. Perhaps other integration methods will be more efficient. Together with the problem of an efficient time integration, the implementation of thermal hydraulic feedback has high priority. At present, only prompt feedback is considered.
A.F. Henry

Since you are neglecting certain cross terms in the polynomial expression for the flux, would it not be somewhat more meaningful to use a product of cubic functions with 10 cm mesh rather than quartic functions with 20 cm mesh?

H. Finnemann

Because of storage limitations, it is necessary to use boxes of approximately 20 x 20 x 20 (30) cm$^3$ in 3-D calculations. For these large meshes, quartic functions yield generally far better results than cubic functions.

One advantage of the proposed nodal method is that these expansion coefficients need not be stored. This means that using quartic functions instead of a cubic approximation results in cost increase of about 10 %, whereas halving the mesh size increases cost and storage requirements by a factor 8.
S. Langenbuch, W. Maurer, W. Werner

SIMULATION OF TRANSIENTS WITH SPACE-DEPENDENT FEEDBACK BY COARSE MESH FLUX EXPANSION METHOD

Laboratorium für Reaktorregelung und Anlagensicherung, Technische Universität München, Germany
1. Introduction

For the simulation of the time-dependent behaviour of large LWR-cores, even the most efficient Finite-Difference (FD) methods require a prohibitive amount of computing time in order to achieve results of acceptable accuracy.

In /1/ a Coarse Mesh (CM) method was introduced, which requires significantly fewer unknowns without appreciably increasing the complexity of the calculations, thus achieving a drastic reduction of computing costs. In /2/ and /3/ it is substantiated that static CM-solutions computed with mesh-size corresponding to the fuel element structure (about 20 cm) are at least as accurate as FD-solutions computed with about 5 cm mesh-size. For 3d-calculations this results in a reduction of storage requirements by a factor 60 and of computing costs by a factor 40, relative to FD-methods. These results have been obtained for pure neutronic calculations, where feedback is not taken into account.

In this paper it will be demonstrated that the method retains its accuracy also in kinetic calculations, even at the presence of strong space dependent feedback.
2. Coarse Mesh Flux Expansion Method (FEM)

Basis of the FEM is the spatially integrated multi-group neutron diffusion equation:

$$\frac{\partial}{\partial t} \int_{V_j} \psi \, dV = \int_{V_j} L \psi \, dV, \quad j = 1, \ldots, M$$

$$\bigcup_{i=1}^{M} V_i = \text{Volume of reactor, } V_i \cap V_j = \emptyset, \quad i \neq j$$

$$\psi = (\varphi, c)^T$$

In order to numerically advance the solution from time layer $n$ to $n+1$, time differencing

$$\int_{V_j} (I - \alpha \Delta t \mathbf{L}) \psi^{n+1} \, dV = \int_{V_j} (I + (1-\alpha) \Delta t \mathbf{L}) \psi^n \, dV$$

is used.

In order to evaluate the integrals in (I), polynomial expansion:

$$\vec{x} \in [x_j - \gamma_2, x_j + \gamma_2] : \quad \tilde{\phi}^\gamma (\vec{x}) = \phi_j^\gamma \prod_i \tilde{G}_{ji}^\gamma (x_i)$$

is introduced.
Variables in the problem are the function values \( \ldots, \phi_{j-1}, \phi_j, \phi_{j+1}, \ldots \) at the center points \( \ldots, x_{j-1}, x_j, x_{j+1}, \ldots \) of the nodes \( \ldots, v_{j-1}, v_j, v_{j+1}, \ldots \) The function values \( \ldots, \phi_{j-1/2}, \phi_{j+1/2}, \phi_{j+3/2}, \ldots \) at the centers of the surfaces of the nodes ("half points") serve as auxiliary variables. (Compare the 1-dimensional illustration in fig. 1).

![Figure 1](image)

Points of support of \( G_{ji} \): \( x_{i,j-1/2}, x_{i,j}, x_{i,j+1/2} \)

Among the many possible choices of the polynomials \( G_j(x) \), the following have been studied:

i) Quadratic Taylor Polynomial (QUABOX)

\[
G_j(x) = 1 + \frac{\phi_{j+1} - \phi_j}{\phi_j} x + 2 \frac{\phi_{j+1} + \phi_j - 2 \phi_j}{\phi_j^2} x^2
\]

or Quadratic Lagrange Polynomial
ii) Higher order Polynomials determined by minimal principle

e.g.

\[ G_j(x) = 1 + \beta_j (x-x_j) + \gamma_j (x-x_j)^2 + \delta_j (x-x_j)^3 \]

(CUBBOX)

\[
\begin{align*}
G_j(-\frac{\beta_j}{2} + x_j) &= \phi_j - \frac{\gamma_j}{2} \\
G_j(+\frac{\beta_j}{2} + x_j) &= \phi_j + \frac{\gamma_j}{2} \\
G_j(x_j) &= \phi_j
\end{align*}
\]

\[ G_j(x) = 1 + \left[ (\frac{\phi_j + \gamma_j - \phi_j - \gamma_j}{2\delta_j})(x-x_j) \right]^2 + \delta_j (x-x_j)^3 \]

\[(iii)\]

\[ d_j \text{ is determined from minimization of} \]

\[
\int_{V_j} \left( L G_j \right)^2 dV
\]
$d_j^{(1)}$ and $d_j^{(2)}$ become functions of
\[
\frac{\phi_{j+i_1}^{(1)} - \phi_{j-i_1}^{(1)}}{\epsilon_j} \quad \frac{\phi_{j+i_2}^{(2)} - \phi_{j-i_2}^{(2)}}{\epsilon_j}
\]
and of all group constants (explicit expressions).

The evaluation of the integrals in (I) yields for case (i), Quadratic Taylor Polynomial:

\[
\int \phi(x) dV = \frac{V_i}{6} \left( \phi_{i+i_2} + \phi_{i-i_2} + \phi_{j+i_2} + \phi_{j-i_2} + \phi_{j+i_1} + \phi_{j-i_1} \right)
\]

\[
\int \nabla \phi \cdot ds = 2V_i \left\{ \frac{\beta_{ij}}{\epsilon_j} \left( \phi_{i+i_2} + \phi_{i-i_2} - 2\phi_j \right) + \frac{\beta_{ij}}{\epsilon_{i-j}} \left( \phi_{i+i_2} + \phi_{i-i_2} - 2\phi_j \right) + \frac{\beta_{ij}}{\epsilon_{i-j}} \left( \phi_{j+i_1} + \phi_{j-i_1} - 2\phi_j \right) \right\}, \quad \beta_{ij} = \frac{2\rho_{ij}}{\epsilon_{i-j}}, \quad i = 1, 2, 3
\]
With the explicitly known integration formulae, eq. (I) constitutes for each $V_j$ a relation $R$ between fluxes $\phi_j$ at the center of $V_j$ and fluxes $\phi_{j-1/2}$, $\phi_{j+1/2}$ ... at the 6 centerpoints of the surfaces of $V_j$, for time layers $n$ and $n+1$.

For the elimination of the "Halfpoints" $\phi_{j-1/2}$, $\phi_{j+1/2}$ ... continuity of flux and current across interfaces is exploited.

For each energy group $j$ and each coordinate direction $i$ the equation

$$\frac{\partial}{\partial x_i} \phi_j = \frac{\partial}{\partial x_i} \phi_{j+1}$$

yields for case (i) Quadratic Taylor Polynomial

$$\frac{2\phi_j}{\partial x_i} \left( \frac{3}{2} \phi_{j+1} + \frac{1}{2} \phi_{j-1} \right) = \frac{2\phi_{j+1}}{\partial x_i} \left( -\frac{3}{2} \phi_{j+1} + 2 \phi_{j+1} - \frac{1}{2} \phi_{j+1} \right)$$

which is a tridiagonal matrix equation for each energy group and each coordinate direction.
for case (ii) Cubic Polynomial (minimal principle):

Due to dependence of coefficients \( d \) (eq. II) on derivatives of both group fluxes, matrix equation becomes pentadiagonal (1 equation for both groups) for each coordinate direction.

By rearranging the continuity condition for currents, the "Halfpoints" can be expressed by "Centerpoints":

\[
\phi_{j+\frac{1}{2}} (\beta_j + \beta_{j+1}) = \frac{4}{3} \left( \beta_j \phi_j (1 - \ell_j) + \beta_{j+1} \phi_{j+1} (1 - \ell_{j+1}) \right)
\]

\[
\ell_j = \frac{1}{4} \frac{\phi_j - \nu_j}{\phi_j}, \quad \ell_{j+1} = \frac{1}{4} \frac{\phi_{j+\frac{1}{2}}}{\phi_{j+1}}
\]

(IV)

Substitution of (IV) into coupling-relation (R) yields a coupling-relation (R') between ..., \( \phi_{j-1} \), \( \phi_j \), \( \phi_{j+1} \), ....

The structure of the advancement matrix is very similar to FD-matrices, however, the coupling coefficients depend on all nuclear cross-sections, and (through relation IV), on the neutron fluxes.

For the time integration, a modification of the Matrix Decomposition Scheme described in /4/ is presently used.
3. Numerical Examples

For a model LWR, a static solution without feedback, a static solution with strong space dependent feedback, and a dynamic solution are computed. All calculations have been performed with 20 cm mesh width, which corresponds to the size of fuel elements, and with 10 cm mesh size. In addition, the static calculations have also been performed with 5 cm mesh width. Feedback effects which act on group constants are considered by using the box-average of the feedback quantities to compute the change of cross-sections within the box. Thus, an additional discretization effect is introduced into the numerical results.

Fig. 2 shows a horizontal cross-section of a quarter of the model reactor. The numerals inside the heavily lined boxes refer to the numbering of boxes in tables 1 and 2.

Static Calculations

Table 1 shows relative power densities in boxes 1, ..., 6 along A-C for a static solution without feedback. The solutions were obtained with mesh sizes of 5, 10 and 20 cm mesh size, resp. In the lower part of table 1 the relative deviations of the 10 cm-, resp. 20 cm-solution from the 5 cm solutions are shown.

Table 2 shows relative power densities at the same locations for a solution with space dependent temperature- and xenon-feedback for the hot reactor (average power density: 300 W/ccm). Again, the same three mesh sizes have been used. The deviations of the 10 cm-, resp. 20 cm-solution from the 5 cm-solution are shown in the lower part of table 2.
The deviations between 5 cm- and 10 cm-solution are less than 1% everywhere, and also the 20 cm-solution shows very good agreement with the 5 cm-solution.

Since there is no significant difference between the relative deviations in tables 1 and 2, resp., it can be concluded, that the global treatment of feedback within the individual boxes does not appreciably affect the accuracy of the method, relative to calculations without feedback.

**Dynamic Calculations**

In the dynamic calculations only doppler-feedback is considered. Because of the short duration of the transient, adiabatic heatup of fuel elements is assumed.

For reasons of economy, only 10 cm- and 20 cm-solutions have been calculated. This seems to be justified by the excellent agreement between 5 cm- and 10 cm-solutions in the static case.

As an example, a superprompt critical excursion is presented, which is caused by a fast withdrawal of one of the 2 absorber rods (fig. 2). Both the 10 cm- and 20 cm-solution have been calculated with identical time step sizes.

For both mesh sizes, fig. 3 shows the time-history of average power. The excursion starts out at a power level of 250 W/ccm. Thus, feedback effects are significant already at the beginning of the calculation.

Time to peak (of average power) agrees within .4 %, and the power maxima differ by 1.4 %.

Table 3 shows the relative power densities in 20 cm boxes of the core for 10 cm-, resp. 20 cm-solutions. The 3rd
line in each box indicates the relative deviations between 10 cm- and 20 cm-solutions. Again, these deviations are not appreciably different from the deviations found for static solutions without feedback.

Conclusion

The accuracy of the coarse mesh flux expansion method QUABOX/CUBBOX reported for static calculations without feedback is retained also for situations with strong space dependent feedback, even when feedback effects are considered only by box-averages. At present, there seems to be no need to go into a more elaborate treatment of feedback effects, e.g. by a subdivision of boxes into subboxes to which are associated different cross-sections /5/.
Fig. 2: Horizontal Cross-Section of Quarter of Model Reactor
<table>
<thead>
<tr>
<th>Mesh Width</th>
<th>Mesh Relative Power Density along Section A-B</th>
<th>Width</th>
<th>Box 1</th>
<th>Box 2</th>
<th>Box 3</th>
<th>Box 4</th>
<th>Box 5</th>
<th>Box 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 cm</td>
<td>2.062</td>
<td>1.849</td>
<td>1.181</td>
<td>1.315</td>
<td>1.135</td>
<td>0.6997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10 cm</td>
<td>2.072</td>
<td>1.860</td>
<td>1.174</td>
<td>1.322</td>
<td>1.136</td>
<td>0.7004</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20 cm</td>
<td>2.113</td>
<td>1.870</td>
<td>1.157</td>
<td>1.328</td>
<td>1.170</td>
<td>0.7246</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Relative Deviation (%) from 5 cm-Solution

<table>
<thead>
<tr>
<th>Mesh Width</th>
<th>Relative Deviation (%) from 5 cm-Solution</th>
<th>Width</th>
<th>Box 1</th>
<th>Box 2</th>
<th>Box 3</th>
<th>Box 4</th>
<th>Box 5</th>
<th>Box 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 cm</td>
<td>+0.48</td>
<td>+0.59</td>
<td>-0.59</td>
<td>+0.53</td>
<td>+0.09</td>
<td>0.10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20 cm</td>
<td>+2.5</td>
<td>+1.1</td>
<td>-1.9</td>
<td>+0.99</td>
<td>+3.1</td>
<td>+3.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Static Solution for Cold Reactor

<table>
<thead>
<tr>
<th>Mesh Width</th>
<th>Mesh Relative Power Density along Section A-B</th>
<th>Width</th>
<th>Box 1</th>
<th>Box 2</th>
<th>Box 3</th>
<th>Box 4</th>
<th>Box 5</th>
<th>Box 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 cm</td>
<td>1.950</td>
<td>1.763</td>
<td>1.154</td>
<td>1.304</td>
<td>1.137</td>
<td>0.7070</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10 cm</td>
<td>1.960</td>
<td>1.773</td>
<td>1.147</td>
<td>1.312</td>
<td>1.138</td>
<td>0.7070</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20 cm</td>
<td>2.001</td>
<td>1.784</td>
<td>1.133</td>
<td>1.319</td>
<td>1.169</td>
<td>0.7300</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Relative Deviation (%) from 5 cm-Solution

<table>
<thead>
<tr>
<th>Mesh Width</th>
<th>Relative Deviation (%) from 5 cm-Solution</th>
<th>Width</th>
<th>Box 1</th>
<th>Box 2</th>
<th>Box 3</th>
<th>Box 4</th>
<th>Box 5</th>
<th>Box 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 cm</td>
<td>+0.51</td>
<td>+0.57</td>
<td>-0.58</td>
<td>+0.64</td>
<td>+0.11</td>
<td>0.00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20 cm</td>
<td>+2.6</td>
<td>+1.2</td>
<td>-1.8</td>
<td>+1.2</td>
<td>+2.9</td>
<td>+3.3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2: Static Solution with Temperature- and Xenon Feedback for Hot Reactor (Average Power Density: 300 W/ccm)
Fig. 3: Comparison of Average Power Density for superprompt Critical Excursion

Table 3: Comparison of Relative Power Densities for Dynamic Calculations with 10 cm and 20 cm Mesh Width (at Time of Peak of Mean Power)

<table>
<thead>
<tr>
<th></th>
<th>10 cm</th>
<th>10 cm</th>
<th>10 cm</th>
<th>10 cm</th>
<th>10 cm</th>
<th>10 cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 cm</td>
<td>0.789</td>
<td>0.609</td>
<td>0.805</td>
<td>0.624</td>
<td>1.102</td>
<td>0.909</td>
</tr>
<tr>
<td>20 cm</td>
<td>1.302</td>
<td>1.076</td>
<td>1.317</td>
<td>1.090</td>
<td>1.302</td>
<td>1.076</td>
</tr>
</tbody>
</table>

Table 3: Comparison of Relative Power Densities for Dynamic Calculations with 10 cm and 20 cm Mesh Width (at Time of Peak of Mean Power)
References

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/3/ S. Langenbuch, W. Werner:
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Reaktortagung des DatF (1974), S. 49-52

/4/ A. Birkhofer, W. Werner:
Fully Implicit Matrix Decomposition Method for Space Time Kinetics,
ANS Transactions, 15, 789 (1972)

/5/ L.O. Deppe, K.F. Hansen:
NSE 54 (456) 1974
DISCUSSION

A.F. Henry

Have you any running time comparisons between this method and that described by Dr. Finnemann in the previous paper?

W. Werner

Running time comparisons are available for LRA Benchmark problems.

For QUABOX, we have a running time per space point and time step which is about 5 to 6 times slower than that for the simplest explicit FD-method.

J. Devooght

1) What was the value of $\varphi$?
2) What was the value of $\Delta t$?

W. Werner

1) $\varphi$ is determined by exponential fitting. (Padé 1,1)
2) Time step: $\sim 10^{-4}$
O. Norinder

THE BITNOD METHOD OF REACTOR COARSE MESH CALCULATIONS

AB Atomenergi, Studsvik, Sweden
The BITNOD Method of Reactor Coarse-Mesh Calculations

By
Olov Norinder, AB Atomenergi, Studsvik, Sweden

Abstract

A new methodology is described for accurate determination of flux distributions in coarse-mesh calculations. Principles, results of a first test phase and development status are noted.

Revised edition of a paper presented at NEACRP/CSNI Specialists' Meeting on New Developments on Three-Dimensional Kinetics, Garching, Munich, 1975-01-22--24

RF-75-7087
1975-02-06
1. Introduction

This paper describes methods for accurate and with regard to computer effort economical calculations of reactor core power distributions. The name BITNOD is selected as an acronym from "Buckling ITeration NODal".

The fundamental simplification in the method is that the nuclear cross sections are treated as constant in comparatively large regions; in the following called nodes. This simplification is in general suitable in power reactor calculations, where each fuel assembly mostly is divided in a small number of nodes.

In thermal reactor 3D calculations one often uses a fast and a thermal neutron flux group and this case is especially treated below.

Considerations and calculations make evident the important fact that the neutron current between two nodes with one common surface fundamentally depends on the properties of both nodes.

Most of the ideas described have been stated in a technical Memo [1] and particularly a later Memo [2]. In connection with the BITNOD development only restricted literature surveys have been made. At the presentation of the paper published work [5] describing a similar approach to obtain nodal equations was pointed out [4].

2. BITNOD principles of solution

The neutron flux is described with a fast and a thermal group.
In each node the general solution of the two-group equations is used. Due to the approximation of constant cross sections, it is possible to identify asymptotic and transient parts of the solution. The buckling of the asymptotic solution is closely related to the material buckling of elementary reactor theory.

The asymptotic buckling $B^2$ is in the usual way split into three parts corresponding to the Cartesian coordinates of the node. With self-explanatory notation one then has

$$B_x^2 + B_y^2 + B_z^2 = B^2$$

In BITNOD the asymptotic buckling is treated as an anisotropic quantity. The necessity and convenience of this approach has also been recognized elsewhere [3]. The asymptotic buckling may also have anisotropy [6].

Consider two nodes with a common boundary surface. The asymptotic and transient parts of the solutions in each node must combine to make fast and thermal neutron flux and current continuous. The transient part must decrease nearly exponentially away from the surface. If the components of the asymptotic bucklings normal to the boundary surface are known, the flux may be represented with well-known solutions for the asymptotic parts, in the plane case cos, sin, cosh, sinh, and exponentials for the transient parts. Some node surfaces border reflectors. Arguments similar to the foregoing make it possible to write down the appropriate expressions also for this case.

The anisotropic distribution of the asymptotic buckling is in general not known initially. Iterative methods will be used for the solution of the flux distribution. The iterations will be started with a trial distribution for both the neutron source and the anisotropic buckling. In
connection with investigations related to [5] it was found [4] that it was in many cases difficult to iteratively determine the buckling distributions in the nodes. Other comments [6] also pointed to the possibility of difficulties with the buckling iterations.

For subsets of the iterations only the average asymptotic fast flux of the nodes will be treated as variable. Between these subsets the buckling distribution and the cross sections will be updated from current values of the leakages of the solution, effective neutron multiplication or power - cross section interaction.

As was realized at an early stage of the BITNOD deliberations, BITNOD will not give the true solution in the limit of small nodes. In the 1D case the true solution is obtained in the limit of large nodes.

3. Detailed solution

For every internodal surface the selected general solution contains for each of the two nodes three coefficients, that multiply cos (cosh), sin (sinh) and an exponential decreasing away from the surface. The four boundary conditions and desired values of fast asymptotic fluxes give six equations that determine the coefficients.

The choice of average asymptotic fast flux as retained variable is important as this quantity is easily identified from every surface bounding a node.

To simplify the formulation of the equations for the interaction of all nodes two elementary solutions are found for each internodal surface, the first with average asymptotic fluxes 1 and 0, the second with 0 and 1 about the surface. For a surface bordering a reflector only the solution with unit fast asymptotic flux is determined.
The solutions are obtained through manipulation of a few matrices of the order two as is evident from Appendices 1 and 2.

The set of elementary solutions for each internodal and nodal-reflector surface together with the two-group cross sections and diffusion coefficients make possible formulation of a neutron balance for each node with average asymptotic fast fluxes of the node and its neighbors as unknowns.

The neutron balances contain large contributions from the asymptotic part of the solutions and smaller contributions from the transient parts. Diffusion to other nodes and to the reflector is represented by comparatively large terms in the sink sides of the balances. The source sides of the balances include small contributions from the asymptotic fluxes of neighboring nodes. The latter contributions can be canceled by adjustment of terms in the sink sides.

4. Optional simplifications

Node-reflector interactions should be calculated with full representation of both flux groups.

For calculation of node-node interactions a formal reduction to one-group flux was attempted by collapsing the flux for each node according to the asymptotic spectrum. This simplification gave rise to large errors in the gross power distribution in systems with dimensions corresponding to half or full light water reactors.

In test calculations it was observed that the transients in the fast flux were small except near reflector boundaries. For that reason equations representing continuity of fast flux and fast neutron current were tested. In a representative
set of different cases this approach approximated well the true two-group solutions. As one might expect, the approximation deteriorated somewhat when there were control rods in the system. This is probably not a serious disadvantage of the described simplificated method.

The advantage of the fast-flux approach is that the calculation of the elements of the neutron balance matrices is simplified and that the nuclear properties of the nodes can be described by a reduced number of parameters. The latter circumstance is a significant advantage when interaction between power distribution and cross sections leads to much updating of cross sections. The equations of the fast-flux approximation are noted in Appendix 3.

5. Extension of BITNOD methods

The described principles can with some complications be extended to more than two neutron groups. Some deterioration of the approximation will follow from the smaller modulus of the transient bucklings, which for each node will be one less than the number of groups. The BITNOD methods can be modified to RZ geometry and to hexagonal geometry.

6. Status of development

One-dimensional codes have been made and used for test purposes. Most of the essential features of BITNOD except the anisotropic buckling iteration have been tested. A code for XY geometry will be made and especially the buckling iteration investigated. If acceptable iterative schemes can be found for the buckling determination codes for RZ and probably also XYZ will be made.
7. Summary of advantages with the BITNOD methods

. The solution lies near the exact two-group solution.

. Nodes and reflectors of arbitrary and varying size can be used.

. Accurate treatment of reflectors. Calculations can be extended to several reflector zones.

. In the fast-flux simplification reduced number of parameters for description of node nuclear properties.

. Conveniently testable against experiments in both smaller and large systems.

. Solution expandable so that details in nodes can be rather well demonstrated.

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   A nodal approach to solve few region neutron diffusion problems
   Energia Nucleare, 17:7 p 429-435, July 1970

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Equations for an internodal surface

In the derivations below conventional, easily identified or equation-defined notation is used.

Consider two nodes with a common YZ-boundary at x=0 in a 3D nodal system (XYZ). The nodes are designated as left (l) and right (r).

For the flux collapsed in the YZ-dimensions of the nodes, the following equations are assumed.

\[
\phi_l^l = c_1 g \cos(B_l x) + c_3 \frac{l}{D_1} g \sin(B_l x) + c_5 \exp(-B_l x)
\]  

(1)

\[
\phi_r^l = c_2 g \cos(B_r x) + c_4 \frac{l}{D_1} g \sin(B_r x) + c_6 \exp(B_r x)
\]  

(2)

\[
\phi^l_2 = c_1 c \cos(B_l x) + c_3 \frac{c}{D_1} g \sin(B_l x) + c_5 c \exp(-B_l x)
\]  

(3)

\[
\phi^r_2 = c_2 c \cos(B_r x) + c_4 \frac{c}{D_1} g \sin(B_r x) + c_6 c \exp(B_r x)
\]  

(4)

The gcos and gsin functions are defined as

\[
B > 0: \ gcos(Bx) = \cos Bx, \ gsin(Bx) = \frac{1}{B} \sin Bx
\]  

(5)

\[
B = 0: \quad 1, \quad x
\]  

\[
B < 0: \ gcos(Bx) = \cosh Bx, \ gsin(Bx) = \frac{1}{B} \sinh Bx
\]  

(6)

For the total asymptotic buckling \(B^2_s\) and the transient buckling \(B^2_{ts}\) (s=l or r) one has the determinant equation

\[
\phi_l^l \phi_r^l - \phi_l^r \phi_r^r = 0
\]
For the coupling factors one has

\[ c_s = \frac{\Sigma_s^R}{D_2^{s}B^{s} + \Sigma_2^{as}} \quad , \quad c_t = \frac{\Sigma_t^R}{D_2^{t}(B_t^{s})^{2} + \Sigma_2^{as}} \]  

(9)

The asymptotic buckling is treated as an anisotropic quantity.

\[ B_s^{2} = (B_x^{s})^{2} + (B_y^{s})^{2} + (B_z^{s})^{2} \]

(10)

\[ B_s^{t} = \sqrt{(B_t^{s})^{2}} \quad , \quad (B_t^{s})^{2} > 0 \]

(10)

\[ B_d^{s} = -\sqrt{(B_d^{s})^{2}} \quad , \quad (B_d^{s})^{2} < 0 \]

(10)

For construction of the fundamental solutions the following integrals are used

\[ g_1 = \int_{-h_x^{l}}^{0} g \cos(B_x^{l}x)dx \quad , \quad g_3 = \frac{1}{D_1^{s}} \int_{-h_x^{l}}^{0} g \sin(B_x^{l}x)dx \]

(11)

\[ g_2 = \int_{0}^{h_x^{r}} g \cos(B_x^{r}x)dx \quad , \quad g_4 = \frac{1}{D_1^{r}} \int_{0}^{h_x^{r}} g \sin(B_x^{r}x)dx \]

(12)
The first fundamental solution should have unit mean asymptotic fast flux in the left node and zero in the right node. The second fundamental solution should have zero mean asymptotic fast flux in the left node and unit in the right node. The boundary and the stated conditions are conveniently expressed in the following matrix equations.

\[
\begin{pmatrix}
1 & -1 \\
C_l & -C_r
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2
\end{pmatrix}
= \begin{pmatrix}
-1 & 1 \\
-C_l & C_r
\end{pmatrix}
\begin{pmatrix}
c_5 \\
c_6
\end{pmatrix}
\]

(13)

\[
\begin{pmatrix}
1 & -1 \\
d_l & -d_r
\end{pmatrix}
\begin{pmatrix}
c_3 \\
c_4
\end{pmatrix}
= \begin{pmatrix}
e_l & e_r \\
d_l & d_r
\end{pmatrix}
\begin{pmatrix}
c_5 \\
c_6
\end{pmatrix}
\]

(14)

\[
\begin{pmatrix}
g_1 & 0 & g_3 & 0 \\
0 & g_2 & 0 & g_4
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2 \\
c_3 \\
c_4
\end{pmatrix}
= \begin{pmatrix}
h_x^l \\
0
\end{pmatrix}
or
\begin{pmatrix}
h_x^r
\end{pmatrix}
\]

(15)

\[
d_s^s = \frac{D_s^s}{D_1^s} C^s
\]

(16)

\[
e_t^s = D_1^s B_t^s
\]

(17)

\[
d_t^s = C_t^s D_2^s B_t^s
\]

(18)

By (13) and (14) express \( c_1 \) etc in \( c_5 \) and \( c_6 \). Insertion in (15) gives two equations for \( c_5 \) and \( c_6 \) for each fundamental. Solve for \( c_5 \) and \( c_6 \) and get \( c_1 -- c_4 \) from their expressions in \( c_5 \) and \( c_6 \).

The set of \( c \)-values enters in an obvious way into the neutron balances of the left and right nodes.
**Equations for a node-reflector interface**

Let the node be to the left and the reflector to the right. With mostly notation similar to that of Appendix 1 one then has

\[
\phi_1^k = c_1 \cos (B^k x) + c_2 \exp (-B^k x) + c_3 \frac{1}{D_1^k} \sin (B^k x) \quad (21)
\]

\[
\phi_1^r = c_4 \sinh B^r (x - h^r_x) \quad (22)
\]

\[
\phi_2^k = c_1 C^k \cos (B^k x) + c_2 C^k \exp (-B^k x) + c_3 \frac{C^k}{D_1^k} \sin (B^k x) \quad (23)
\]

\[
\phi_2^r = c_4 C^r \sinh B^r (x - h^r_x) + c_5 \sinh B^r_t (x - h^r_x) \quad (24)
\]

\[
B^2_r = - \frac{\Sigma^a_r + \Sigma^r_r}{D_1^r}, \quad (B^r)^2_t = - \frac{\Sigma^a_r}{D_2^r} \quad (25)
\]

\[
B^r = - \sqrt{-B^2_r} \quad , \quad B^r_t = - \sqrt{-B^2_t} \quad (26)
\]

Many quantities are used as they are defined in Appendix 1. Some new quantities are used

\[
s_1 = \sinh (-B^r_x h^r_x) \quad , \quad s_2 = \sinh (-B^t_x h^r_x) \quad (27)
\]

\[
t_1 = D_1^r B^r \cosh B^r_x h^r_x \quad , \quad t_2 = D_2^r B^t \cosh B^t_x h^r_x \quad (28)
\]

The wanted solution should have unit mean asymptotic fast flux in the left node. This leads to the following matrix equations.
By (29) and (30) express $c_1$, $c_2$ and $c_3$ in $c_4$ and $c_5$. The two expressions for $c_2$ must be equal. This and (31) make it possible to determine $c_4$, $c_5$, $c_1$, $c_2$ and $c_3$. $c_1$, $c_2$ and $c_3$ enter into the neutron balance of the left node.
The fast flux approximation

On the internodal surface continuity of fast neutron flux and fast neutron current is obtained with the following expressions

\[ \phi^f_1 = c_1 \cos(B_x^f x) + c_2 \frac{1}{D_1^f} \sin(B_x^f x) \quad (41) \]

\[ \psi^r_1 = c_1 \cos(B_x^r x) + c_2 \frac{1}{D_1^r} \sin(B_x^r x) \quad (42) \]

For the flux-level equations the following integrals are used

\[ g^f_1 = \int_{-h_x^f}^{0} \cos(B_x^f x) dx \quad , \quad g^r_1 = \int_{0}^{h_x^r} \cos(B_x^r x) dx \quad (43) \]

\[ g^f_2 = \frac{1}{D_1^f} \int_{-h_x^f}^{0} \sin(B_x^f x) dx \quad , \quad g^r_2 = \frac{1}{D_1^r} \int_{0}^{h_x^r} \sin(B_x^r x) dx \quad (44) \]

The fundamental solutions are obtained from

\[
\begin{pmatrix}
  g^f_1 & g^f_2 \\
  r^f_1 & r^f_2
\end{pmatrix}
\begin{pmatrix}
  c_1 \\
  c_2
\end{pmatrix}
=
\begin{pmatrix}
  h^f_x \\
  h^r_x
\end{pmatrix}
\quad \text{or}
\begin{pmatrix}
  0 \\
  0
\end{pmatrix}
\quad (45)
\]

For the writing-down of neutron balances one observes that the thermal flux is \( C \) times the fast flux. (\( C \) from Eq. (9) (APPENDIX 1)). The total neutron current to use in the balances should be \( d = 1 + C (D_2 / D_1) \) times the fast current. Node-reflector interfaces should get full two-group treatment as described in APPENDIX 2.
Session III

EVALUATION OF MULTIDIMENSIONAL CALCULATIONS

Chairman: W. Werner, Germany

A.R. Dastur, D.B. Buss
SPACE-TIME KINETICS OF CANDU SYSTEMS
Atomic Energy of Canada Limited, Missisauga, Ontario, Canada

J.K. Fletcher, M.A. Perks
THE SPATIAL KINETICS PROGRAM SPARK AND ITS APPLICATION TO FAST REACTOR TRANSIENTS
UKAEA, Risley, Warrington, United Kingdom

G. Dubois
THE IMPORTANCE OF FLUX SHAPE CHANGES IN SPACE-TIME KINETICS CALCULATIONS
Ecole Polytechnique de Montreal, Quebec, Canada
A.R. Dastur, D.B. Buss

SPACE-TIME KINETICS OF CANDU SYSTEMS

Atomic Energy of Canada Limited, Missisauga, Ontario, Canada
Characteristics of CANDU systems which affect space dependent neutron transients have been studied. Major factors have been found to be neutronic decoupling of reactor segments due to deliberate flattening of the power distribution; retardation of the power shape transient due to delayed neutron holdback; photoneutron production in heavy water; asymmetric insertion of reactivity devices. A full scale excursion analysis in 3-dimensions is presented to show the degree and manner in which these characteristics contribute to produce the overall spatially-dependent neutron transients when a detailed model of the system is used in the simulation.
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1.4 Photoneutron Production in Heavy Water 5
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INTRODUCTION

Space dependent neutron transients in CANDU systems result from a combination of:

1. neutronic decoupling of reactor segments due to deliberate flattening of the power distribution,
2. significant retardation of the power shape transient due to delayed neutron holdback, and
3. asymmetric insertion of reactivity devices.

In Section 1 of this study the above points are illustrated by transients calculated using the Improved Quasistatic Method. The models used are relatively simple but are designed to exhibit the spatial characteristics of the CANDU system as regards neutronic decoupling, shutdown system configuration and prompt subcriticality. Wherever possible without loss of system characteristics, static flux shapes, i.e. solutions of the time-independent equations, are used to illustrate certain points. The use of static flux shapes is justified when similar differences can be shown to exist between dynamic flux shapes, the latter being solutions of the time-dependent equations.

In Section 2, results of an excursion analysis carried out for a 750 MWe system are presented. The power excursion is a result of LOC from the primary coolant circuit followed by tripping of the shutdown systems. These results are presented to show the degree and manner in which the characteristics described in Section 1 contribute to produce the overall spatially-dependent neutron transient when a detailed model of the system is used in the simulation. A method of grouping reactivity devices with adjacent fuel channels into supercells is described. This allows significant reduction in problem size without loss of accuracy.

In Section 3 conclusions regarding the characteristics of CANDU systems which affect space dependent neutron transients are summarized.
1. Characteristics of CANDU Systems that Affect Spatially Dependent Neutron Transients

1.1 Neutronic Decoupling

In CANDU reactors decoupling of reactor segments is increased by deliberate flattening of the flux distribution in order to maximize power output. This is illustrated in Table 1.1.1 where reactivities associated with coupling are compared for 600 MWe systems with flattened and unflattened flux shapes. The figures indicate the increase in reactivity required to make each segment critical on its own, i.e. it is completely decoupled from the rest of the system. Any perturbation applied to a decoupled segment does not affect the rest of the system.

The effect that neutronic decoupling can have on power shapes encountered during shutoff rod insertion is shown in Figure 1.1.1 for a 600 MWe system. The powers were calculated from flux distributions obtained by solving the time-independent (static) two group neutron diffusion equation in 3-dimensions. Integrated powers for 12 radial planes are given as a function of axial position. Twenty-eight shutoff rods located symmetrically with respect to axial position are worth -84.2 milli-k when inserted into a flattened power distribution and -82.0 milli-k when inserted into an unflattened power distribution. Omission of two shutoff rods from one segment results in a decrease in worth of -25.0 milli-k for the unflattened power distribution as compared with -36.8 for the flattened power distribution. This difference results from the change in flux shape (and hence of shutoff rod importance) being higher for the system with higher neutronic decoupling due to flux flattening. The same effect is observed when comparing dynamic flux shapes (obtained as solutions of the time dependent diffusion equation) but to a lesser degree due to the presence of delayed neutron precursors as shown below.

The effect of neutronic decoupling on space dependent power transients has been calculated to show its importance in CANDU space-time kinetics. A 3-D model of a 600 MWe system was used in the calculations. Two power
<table>
<thead>
<tr>
<th>Reactor Segment</th>
<th>Coupling Reactivity (millik)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Flattened Flux Distribution</td>
<td>Unflattened Flux Distribution</td>
</tr>
<tr>
<td>Radial Plane</td>
<td>-16.1</td>
<td>-21.2</td>
</tr>
<tr>
<td>Radial Plane</td>
<td>-44.3</td>
<td>-50.1</td>
</tr>
<tr>
<td>Axial Plane</td>
<td>-23.5</td>
<td>-31.5</td>
</tr>
<tr>
<td>SHUTOFF RODS</td>
<td>REACTIVITY (MK)</td>
<td></td>
</tr>
<tr>
<td>------------------------------</td>
<td>-----------------</td>
<td></td>
</tr>
<tr>
<td>(FLATTENED CORE)</td>
<td>-47.42</td>
<td></td>
</tr>
<tr>
<td>(UNFLATTENED CORE)</td>
<td>-57.21</td>
<td></td>
</tr>
<tr>
<td>(FLATTENED CORE)</td>
<td>-84.2</td>
<td></td>
</tr>
<tr>
<td>(UNFLATTENED CORE)</td>
<td>-82.0</td>
<td></td>
</tr>
</tbody>
</table>

**Figure 1.1-1** EFFECT OF NEUTRONIC DECOUPLING DUE TO POWER FLATTENING

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transients were obtained by solving the time-dependent neutron diffusion equations using the IQS method.

In model A (see Fig. 1.1.2) the flux shape was deliberately flattened along one direction as compared to Model B where the flux shape was unflattened in all directions. When segmented into two halves across the direction of flattened flux shape Model A exhibited a coupling reactivity of 7.6 milli-k (obtained from the solution of the static diffusion equations) as compared with 14.5 milli-k for Model B.

The reactivity transient due to loss-of-coolant and subsequent asymmetric insertion of reactivity devices was approximated by a linear increase up to 0.5% in neutron yield per fission for 1 sec in both segments and subsequent linear ramps amounting to 25% increase in absorption cross-section over one segment for 2 secs, as illustrated in Figure 1.1.2.

Six delayed neutron groups and two energy groups were used. Delayed neutron data used is listed in Fig. 1.1.2. The method used for collapsing 33 delayed neutron precursors into six groups is discussed in Section 1.3.

The total power and segment power transients are shown in Fig. 1.1.2. Since negative reactivity insertion is restricted to one segment the power transient in the unpoisoned segment is affected by the neutronic coupling of the segments. The energy produced in the unpoisoned segment is \( \approx 50\% \) higher in Model A which has less neutronic coupling than in Model B. This difference is reflected in the total energy produced which is \( \approx 20\% \) higher in Model A than in Model B.

1.2 Asymmetric Insertion of Reactivity Devices

Shutoff rod failure is a consideration in shutdown system design. In CANDU systems, the limiting case, i.e. one which dictates the final design,
PHOTONEUTRONS INCLUDED

<table>
<thead>
<tr>
<th>$\lambda$ SEC$^{-1}$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.013786</td>
<td>0.0072562</td>
</tr>
<tr>
<td>0.0305098</td>
<td>0.00819557</td>
</tr>
<tr>
<td>0.1336881</td>
<td>0.01041406</td>
</tr>
<tr>
<td>0.3155434</td>
<td>0.0033520</td>
</tr>
<tr>
<td>1.2252777</td>
<td>0.00579031</td>
</tr>
<tr>
<td>3.147497</td>
<td>0.00225563</td>
</tr>
<tr>
<td>TOTAL $\beta$</td>
<td>0.00572738</td>
</tr>
</tbody>
</table>

APPLIED REACTIVITY TRANSIENT

FIGURE 1.1-2 EFFECT OF NEUTRONIC DECOUPLING ON POWER PULSE
involves failure of adjacent rods leaving an asymmetric configuration. Considering the 600 MWe system with a flattened power distribution, failure of 2 shutdown rods from a total of 28 as shown in Figure 1.2 results in a decrease of -36.8 milli-k in shutdown system worth. As shown in Section 1.1, the effects of asymmetric reactivity perturbations are accentuated by neutronic decoupling. The effects on power shape are shown in Figure 1.2.1. The power produced in the segment with unfailing rods is < 10% of the total, whereas symmetric insertion results in segments producing equal power. The same effects are observed when considering dynamic flux shapes but to a lesser degree due to the presence of delayed neutron precursors (see Sections 2.3 and 2.4).

1.3 Delayed Neutron Holdback

For a major part, the reactivity transients encountered in CANDU systems are prompt sub-critical. This characteristic is the combined effect of the reactivity transient associated with loss-of-coolant and with shutdown system operation. Hence the shape of the delayed source distribution significantly affects the transient power shapes and reactivity.

The effect of delayed source shape is illustrated by selected results of a 3-D space-time kinetics calculation for a 750 MWe system using the IQS method. Six delayed groups and two energy groups were used. Results selected are at 60 sec following initiation of LOC, i.e. well after coolant voiding and reactivity device insertion is complete. Subcritical multiplication of the delayed source produces the power shape shown in Figure 1.3.1. The shape of the delayed source is similar to the pre-event power shape. Its effect on the present power shape is seen by reducing the delayed source term to an insignificant level and re-solving the flux shape equations. The resulting power shape is shown in Figure 1.3.1. The resulting change in neutron importance of the reactivity devices increases the system reactivity from -91.8 milli-k to -55.0 milli-k.
FIGURE 1.2.1 POWER SHAPES RESULTING FROM ASYMMETRIC SHUTOFF ROD CONFIGURATION
Figure 1.3.1 Effect of Delayed Source Shape on Power Shape

### Table 1.3.1

<table>
<thead>
<tr>
<th>$\lambda$ (sec$^{-1}$)</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01261</td>
<td>0.000329</td>
</tr>
<tr>
<td>0.03051</td>
<td>0.001003</td>
</tr>
<tr>
<td>0.1200</td>
<td>0.000856</td>
</tr>
<tr>
<td>0.3209</td>
<td>0.002319</td>
</tr>
<tr>
<td>1.262</td>
<td>0.000587</td>
</tr>
<tr>
<td>3.239</td>
<td>0.000206</td>
</tr>
</tbody>
</table>

### Table 2.3.1

<table>
<thead>
<tr>
<th>$\rho$ (mk)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-55.013</td>
</tr>
<tr>
<td>2</td>
<td>-91.777</td>
</tr>
<tr>
<td>3</td>
<td>-55.017</td>
</tr>
</tbody>
</table>

**Figure 1.3.1** Effect of Delayed Source Shape on Power Shape

- **TIME = 60.0 SEC AFTER LOCA**
  - 1 Static Simulation
  - 2 Dynamic Simulation
  - 3 Dynamic Simulation (Precursors Eliminated)
  - 4 Total Precursors
In the case of prompt super-critical transients, delayed source shape is similar to the transient power shape due to the predominance of precursors formed during the transient at high power levels.

The significant effect of delayed source shape emphasizes adequate representation of delayed neutron sources in the simulation model for CANDU systems. Proper representation would involve 24 neutron precursors (six from each of the fissioning isotopes U235, Pu239, Pu241 and U238) and nine groups of gamma precursors which produce photoneutrons in heavy water. These are given in reference (4). Various methods of collapsing the 33 groups are available. In order to demonstrate the effect these may have on the analysis, two methods have been used to produce data for a space-time simulation. In method A, the 24 neutron precursors were collapsed into six groups. The average delayed neutron fraction for each of the six groups was obtained by weighting with the fission rates for each of the four fissioning isotopes and dividing the weighted sum by the total fission rate. The average decay constant was obtained by weighting with the delayed source produced by each isotope and dividing the weighted sum by the total source. The nine gamma precursors were collapsed into two groups and included by modifying groups one and four. In method B the total decay transient of the 33 precursors was approximated by the sum of six exponential decay terms. The coefficients of the terms were obtained by a least square fit. The collapsed data obtained by the two methods is listed in Figure 1.3.2.

The data produced by the two methods was used in the simulation of a transient designed to accentuate spatial effects. The simulation model is described in Section 1.4.

The effect on power shape following completion of the perturbation ramp is shown in Figure 1.3.2. The simulation using data from method B shows larger variations in flux shape following completion of the applied perturbations. Method B favours the slower decaying precursors as compared with method A, which results in effectively larger delayed neutron holdup. After removal of the faster decaying precursors the flux shape is closer to
FIGURE 1.3.2 VARIATIONS IN FLUX SHAPE DUE TO PRECURSOR DECAY

CASE C: 33 GROUP DATA FROM REF. (4)

<table>
<thead>
<tr>
<th>CASE A</th>
<th>CASE B</th>
</tr>
</thead>
<tbody>
<tr>
<td>WITH PHOTONEUTRONS</td>
<td>WITH PHOTONEUTRONS</td>
</tr>
<tr>
<td>$\lambda, \text{SEC}^{-1}$</td>
<td>$\beta$</td>
</tr>
<tr>
<td>0.0137856</td>
<td>0.0034103</td>
</tr>
<tr>
<td>0.0305098</td>
<td>0.0019496</td>
</tr>
<tr>
<td>1.336881</td>
<td>0.0051184</td>
</tr>
<tr>
<td>0.3154234</td>
<td>0.0013296</td>
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<tr>
<td>1.225077</td>
<td>0.0019300</td>
</tr>
<tr>
<td>3.147497</td>
<td>0.0021930</td>
</tr>
</tbody>
</table>

($\Delta t = 0.00579$)

($\Delta t = 0.0072738$)
the pre-event shape and subsequently a larger variation in shape is necessary to reach the asymptotic shape.

For comparison, the results of the simulation using the uncollapsed 33 group data are also given in Fig. 1.3.2. After removal of the faster decaying precursors, the variation in shape is negligible on the time scale shown. Fifteen percent of the photoneutrons precursors have decay constants ranging between $4.81 \times 10^{-3}$ and $6.20 \times 10^{-7}$ sec$^{-1}$. These lie outside the ranges of the six decay constants of the collapsed groups. The retardation in flux shape is increased when using 33 groups as both methods of collapsing favour the faster decaying precursors.

1.4 Photoneutron Production in Heavy Water

Approximately 17% of the delayed source in CANDU systems is due to photoneutron production in heavy water. The effect of delayed source on power shape and reactivity has been illustrated in Section 1.3. The contribution of photoneutrons to these effects has been calculated to demonstrate their significance to CANDU space-time kinetics.

A 3-D model of a 600 MWe system was used in the calculations. Reactivity transient due to loss-of-coolant and subsequent asymmetric insertion of reactivity devices was represented as discussed in section 1.1 (See Figure 1.4-1 and 1.4-2).

Six delayed neutron groups and two energy groups were used. Delayed neutron data used is listed in Figure 1.4.1. Photoneutrons were included by modifying data for groups 1 and 4. The changes to parameters for groups 1 and 4 due to photoneutrons were obtained by collapsing the nine group photoneutron data given in reference (4). The methods used for collapsing are discussed in Section 1.3. Power pulses calculated with and without the photoneutron source are compared in Figure 1.4.1. The peak powers in the two cases differ by 25%. Excluding photoneutrons changes the system from prompt sub to prompt-supercritical during the transient.
FIGURE 1.4.1 EFFECT OF PHOTONEUTRONS ON POWER PULSE
FIG. 1.4.2  EFFECT OF PHOTONEUTRONS ON POWER SHAPE

- 226 -
The effect on power shape following completion of the perturbation ramp is illustrated in Figure 1.4.2. The values plotted vs time for each point is the deviation from the average of all points. The points are located on an axis chosen to demonstrate maximum shape change. The case with photoneutrons included shows larger variation in flux shape subsequent to completion of the applied perturbations. The increase in delayed neutron source due to photoneutrons results in a shape that is closer to the pre-event shape and subsequently a larger variation in shape is necessary to reach the asymptotic shape. On the time scale shown, the major contribution to this effect is from group 1 which has a decay constant of \(0.0138 \text{ sec}^{-1}\).

1.5 Static Modeling

The dependence of the results on the simulation model is accentuated by neutronic decoupling. In particular, larger flux gradients are encountered in a system with higher neutronic decoupling which increases the number of mesh lines required for calculation of the flux gradients to a given degree of accuracy. In order to reduce mesh size without loss of accuracy, fuel channels with adjacent reactivity devices are grouped into supercells. Cross-sections to be used in supercells are obtained by solution of the static diffusion equations using precalculated internal boundary conditions to represent the fuel and reactivity devices. The supercell method is described in Section 2 - 2.2. It allows significant reduction in problem size by elimination of the mesh lines required to simulate the large flux gradients encountered near the surface of reactivity devices.

Large flux gradients in the heavy water reflector make the results particularly sensitive to the mesh structure in that vicinity. This is illustrated by comparing power shapes and reactivities obtained from solutions of the static diffusion equations for two reflector models with a 600 MW\(e\) system. In Figure 1.5.1 the integrated power of 12 radial planes is shown as a function of axial position with 26 shutoff rods inserted asymmetrically as discussed in Section 1.1.1. The difference in flux shape due to the removal of four mesh lines in the radial plane accompanied with the change in the representation of the reflector produces significant changes in static reactivities and power distributions.
FIGURE 1.5-1  EFFECT OF STATIC MODELING ON POWER SHAPE

<table>
<thead>
<tr>
<th>REACTIVITY WORTH OF 26 SHUT-OFF RODS</th>
<th>ORIGINAL MODEL</th>
<th>SIMPLIFIED MODEL</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-4:05 (mk)</td>
<td>-44.40 (mk)</td>
</tr>
</tbody>
</table>

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DEC., 1974
The dependence of calculated space-dependent power transients on static modelling is illustrated in Fig. 1.5.2. The models used in the calculations are described in section 1.1. Model C is identical to Model A of section 1.1. Model D is identical to Model C except for the mesh structure; the number of mesh lines in the direction of flux flattening has been increased in Model D.

Total power and segment power transients are shown in Fig. 1.5.2. The calculated gradients and neutronic decoupling are larger in Model D. This leads to a higher power transient in the poisoned segment which is further reflected in the total power.
FIGURE 1.5-2  EFFECT OF STATIC MODELING ON POWER PULSE

PHOTONEUTRONS INCLUDED

<table>
<thead>
<tr>
<th>$\Delta$ SEC$^{-1}$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0137856</td>
<td>0.00072662</td>
</tr>
<tr>
<td>0.0305998</td>
<td>0.000819557</td>
</tr>
<tr>
<td>0.1336981</td>
<td>0.001044106</td>
</tr>
<tr>
<td>0.3155434</td>
<td>0.00233520</td>
</tr>
<tr>
<td>1.2725077</td>
<td>0.000579031</td>
</tr>
<tr>
<td>3.147497</td>
<td>0.000225563</td>
</tr>
</tbody>
</table>

TOTAL $\beta = 0.00572738$

APPLIED REACTIVITY TRANSIENT

MODEL D
(FINE MESH)
- $\times$ SEGMENT 1
- $\Delta$ SEGMENT 2
- $\gamma$ TOTAL

MODEL C
(COARSE MESH)
- $\times$ SEGMENT 1
- $\Delta$ SEGMENT 2
- $\gamma$ TOTAL

FIGURE 66:0110049
DEC. 1974
2. Application of the IQS Method to Excursion Analysis

The accuracy of the Improved Quasistatic Method has been adequately discussed in reference (1). The method has been used to simulate the space-dependent neutron transient in a 750 MWe system due to loss-of-coolant from the fuel channels and operation of two shutdown systems.

2.1 Simulation Model

The reactor consists of 480 horizontal fuel channels, each with 12 fuel bundles having 37 natural UO\(_2\) fuel pencils sheathed in Zircaloy. The fuel bundles are placed in a Zirconium-Niobium pressure tube (inner radius = 5.169 cm, outer radius = 5.588 cm) which completes the fuel channel. The channels are arranged in a square lattice on a 28.575 cm pitch. The heavy water moderator is contained in a stainless steel cylindrical reactor vessel (calandria) (inner radius = 422.9 cm, wall thickness = 3.175 cm) and is thermally insulated from the pressure tubes by an 0.86 cm wide annulus of CO\(_2\) which is provided by a Zircaloy calandria tube (inner radius = 6.448 cm, outer radius = 6.587 cm), the latter being an integral part of the calandria. The size of the reactor vessel is such as to provide a \(\approx\) 65 cm radial heavy water neutron reflector outside the outermost ring of fuel channels. In order to conserve heavy water, the reflector is omitted at either end of the reactor length, where its neutron importance is low, by providing a 47.5 cm long notch in the calandria. The channel arrangement and calandria is shown in Figure 2.1.1. The fuel bundle geometry is shown in Figure 2.1.2.

Two shutdown mechanisms are provided in this system. Thirty vertical shutoff rods, each consisting of a 0.0914 cm thick cylindrical cadmium shell sandwiched in stainless steel (outer radius = 5.78 cm) are arranged as shown in Figure 2.1.4. The rods are normally parked with their lower ends outside the calandria shell. During insertion they travel in between the fuel channels through Zircaloy guide tubes filled with heavy water. On complete insertion the rods are symmetric with respect to the horizontal diametral plane of the calandria. In the present model, shutoff rod insertion was initiated 0.43 sec. after coolant started to void due to failure of the inlet header.
FIGURE 2.1-1 REACTOR ASSEMBLY
FIGURE 2.1-2  37-ELEMENT FUEL BUNDLE

1 ZIRCALOY BEARING PADS
2 ZIRCALOY FUEL SHEATH
3 ZIRCALOY END SUPPORT PLATE
4 URANIUM DIOXIDE PELLETS
5 INTER ELEMENT SPACERS
6 PRESSURE TUBE
The second shutdown mechanism consists of seven horizontal injection nozzles placed between fuel channels through which a concentrated solution of gadolinium nitrate in heavy water is injected into the moderator at high pressure. Each nozzle is connected to a storage tank of poison and each tank is connected to a common reservoir of helium maintained at a pressure of 1200 psia. The injection nozzles have four rows of 0.159 cm radii holes along its length and each row extends over 16 lattice pitches (458 cm). In the present model poison injection was initiated 0.53 sec. after coolant started to void.

Two shutoff rods and one poison injection nozzle were assumed unoperational in the analysis. The locations of the omitted reactivity devices is shown on Figure 2.1.4.

The relatively long cooling time of the UO₂ fuel (time constant \( \approx 0.125 \text{ sec}^{-1} \)) compared with the time taken for reactivity device insertion (\( \approx 1.5 \text{ sec} \)) results in, at most, a weak effect of the power transients on the rate at which the coolant is lost from the core. The coolant voiding is, therefore, mainly a pressure driven phenomenon which allows pre-calculation of the voiding transient which is used as input to the IQS method.

The variation of the thermal neutron cross-sections with fuel temperature is influenced by the presence of plutonium isotopes. The average fuel composition in the core during nominal operating conditions is such that the negative reactivity coefficient of fuel temperature due to doppler broadening of the U238 resonances is largely compensated by the positive reactivity coefficient of fuel temperature due to the temperature dependence of all other isotopes. In this analysis the fuel temperature change corresponding to a 100% increase in power gave rise to a total reactivity change of -3 milli-k. This change is considered small compared with the worth of the reactivity devices. Furthermore, the cooling time of the fuel (time constant = 0.125 sec^{-1}) is relatively long compared with the time taken for reactivity device insertion. For these reasons temperature effects were excluded from the model.
FIGURE 2.1-3 INJECTION NOZZLE CONFIGURATION
FIGURE 2.14  SHUTDOWN DEVICE LOCATIONS
The voiding of the coolant and movement of reactivity devices is simulated by changing various neutron cross-sections in space and time. The cross-section changes produced by coolant voiding are calculated using empirical lattice recipes which have been correlated with various lattice measurements. The cross-section changes produced by reactivity device movement are obtained for regions termed as 'supercells' which include the fuel channels adjacent to the shutdown device. The method used in this calculation is outlined below.

2.2 Static Modeling

As shown in Section 1.5 the mesh line distribution in the simulation model affects the flux shape and reactivity. The number of mesh lines required for negligible effect increases in regions of high flux gradients. In particular, at the shutoff rod surface mesh spacings of ~ 0.5 cm are necessary for explicit representation of the shutoff rod in the simulation model. In order to reduce the size of the numerical computation to within practical limits the flux shape is calculated in two stages. The flux in the region adjacent to reactivity devices including the neighboring fuel channels is pre-calculated for various degrees of reactivity device insertion.

1. Internal boundary conditions are used to represent the surfaces of fuel and reactivity devices. There are two options available for calculating these. If the absorber rod is in the form of a black tube filled with heavy water, the method of reference (2) is used. If the absorber material is highly scattering or is grey, then the method of reference (3) is used. In both cases the extrapolation distance for fast neutrons is obtained by assuming that neutrons thermalized within the rod are absorbed if the rod is black. Poison injected into the moderator is represented in the supercells by surfaces experimentally observed in out-of-core test rigs. Resonance absorption in the fuel is included by modifying the fast extrapolation distance.
2. A 3-D model of the supercell is set up in rectangular geometry. The absorber rod and fuel are represented by an equivalent surface such that the net current integrated over the surface is the same as in actual geometry. Pressure, calandria and guide tubes are included in the model. (See Fig. 2.2.1)

3. The thermal flux distribution within the cell is obtained by solving the inhomogeneous 2 group diffusion equation with a fixed source assuming that the fast flux is flat outside the absorber rod and fuel regions. The calculated extrapolation distances are used as internal boundary conditions. Reflection boundary conditions are used on the outer surfaces of the cell.

4. From the thermal flux shape and reaction rates (including leakage rates in absorber rod and homogenized region) calculated in 3 average supercell cross-sections are obtained.

5. Using these cross-sections a check is made on the neutron spectrum used in 2 to obtain the cross-sections and extrapolation distances. If a large enough discrepancy is found due to spectral hardening, the cross-sections are recalculated and procedures (1) to (5) repeated.

6. The average cell cross-sections are used to model the absorber rods in the total system and a macroscopic flux distribution is obtained by solving the time-independent neutron diffusion equations in 3-dimensions.
INTERNAL BOUNDARY CONDITIONS
FOR FUEL AND ABSORBER

\[ \int (J^- - J^+) ds = \int (J^- - J^+) ds \]

surface in cylindrical
supercell surface
pre-calculated using
methods of ref. (2) and (3).

FIGURE 2.2.1 TYPICAL SUPERCELL MODEL
7. The macroscopic flux shape at the surface of the supercells representing the absorber rod is used to check the boundary condition used in (3) on the outer surface of the supercell. If the reflection boundary conditions are grossly incorrect, they are replaced by the ones obtained from the macroscopic flux shape and procedures (3) to (7) repeated.

For all shutoff rod simulations we have so far found it unnecessary to repeat (3) with the inhomogeneous boundary conditions on the outer surfaces of the supercell.

The simulation model consisted of 26,136 regions of which 2,539 were supercells. Two energy groups and six delayed neutron groups shown in Figure 1.3.1 were used. The six delayed neutron groups were obtained by collapsing 33 neutron precursors, 9 of which were photoneutrons (see Section 1.3).

During reactivity device insertion the flux shape was calculated at intervals ranging from 0.1 to 0.4 secs. Relatively slow variations in flux shape before and after reactivity device insertion allowed use of larger time intervals in the shape calculation. In particular when the delayed source was comprised mainly of photoneutrons time steps of 30 to 50 secs were adequate.

2.3 Static and Dynamic Reactivities

As illustrated in Section 1, the degree of neutronic decoupling encountered in CANDU systems accentuates the effect of the delayed neutron source on the space-time behaviour of the system. The effect on reactivity (defined here as the excess neutron production over loss) is produced through the influence on dynamic flux shape and hence on the importance of the reactivity devices. The system reactivity transient is shown in Figure 2.3.1. For comparison the static reactivity obtained by solution of the time-independent equations is
FIGURE 2.3-1 DYNAMIC REACTIVITY
indicated when voiding and reactivity device movement is complete. The static and dynamic reactivity definitions are identical. In each case the neutron balance is taken with the balancing term of the equations excluded, i.e. the time derivatives of the flux shape and amplitudes in the dynamic case and the adjustment to the neutrons per fission in the static case. As illustrated in Section 2.4 the effect of the delayed source is to retard the change in flux shape produced by the reactivity devices which invariably increases their importance and reactivity worth. As precursor decay progresses the dynamic shapes and reactivities approach their static values. The time scale of this process is determined by the slowest decaying photon-neutron precursors and is of the order of minutes.

The above results indicate that solutions of time-independent diffusion equations are inadequate for the design of the reactivity device configurations in CANDU systems.

2.4 Shape Transient Retardation

Figures 2.4.1 to 2.4.6 show flux shapes at various times along three axes all passing through the reactor centre. The static flux shapes are given for times > 9 sec. For times greater than 9 secs the change in flux shape is due to precursor decay alone. The approach to the asymptotic shape and the extent to which the shape transient is retarded by the delayed neutron holdback is clearly seen.

2.5 Total Power Transient

The total power pulse is shown in Figure 2.5.1. The system remains prompt sub-critical during the transient as seen in Figure 2.3.1. The values shown in Figure 2.5.1 are for neutron power. Power produced by radiation from decay of fission products predominates after 20 sec and is not included.
FIGURE 2.4-1 VARIATIONS OF FLUX SHAPE WITH TIME
FIGURE 2.4-2  VARIATIONS OF FLUX SHAPE WITH TIME

DISTANCE (cm) -- MESH NUMBER ALONG AXIS

GROUP 2 FLUX SHAPE (NORMALIZED TO MAX. = 1.0)

PLOT
AXIS

Y-AXIS

0.0 SEC
△ 1.41 SEC
× 1.81 SEC
● 2.45 SEC

DEC., 1974
FIGURE 2.4-3 VARIATIONS OF FLUX SHAPE WITH TIME

GROUP 2 FLUX SHAPE (NORMALIZED TO MAX. = 1.0)

DISTANCE (cm)

MESH NUMBER ALONG AXIS

Z-AXIS

PLOT AXIS

1.0

Z-AXIS

0.0

0.1

0.2

0.3

0.4

0.5

0.6

0.7

0.8

0.9

1.0

0.0

1.0

2.0

3.0

4.0

5.0

6.0

7.0

8.0

9.0

10.0

11.0

12.0

13.0

14.0

15.0

16.0

17.0

18.0

19.0

20.0

21.0

22.0

23.0

24.0

23.8 152.9 301.0

23.8 152.9 301.0 578.2

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

0.0 SEC

△ 1.41 SEC

X 1.81 SEC

○ 2.45 SEC

66.01100 58
DEC., 1974
FIGURE 2.4.4  VARIATIONS OF FLUX SHAPE WITH TIME
FIGURE 2.4.5  VARIATIONS OF FLUX SHAPE WITH TIME
FIGURE 2.4.6  VARIATIONS OF FLUX SHAPE WITH TIME
<table>
<thead>
<tr>
<th>$\lambda;\text{SEC}^{-1}$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01261</td>
<td>0.000329</td>
</tr>
<tr>
<td>0.03051</td>
<td>0.001003</td>
</tr>
<tr>
<td>0.12000</td>
<td>0.003856</td>
</tr>
<tr>
<td>0.32090</td>
<td>0.002319</td>
</tr>
<tr>
<td>1.26200</td>
<td>0.000583</td>
</tr>
<tr>
<td>3.23900</td>
<td>0.000206</td>
</tr>
</tbody>
</table>

$\beta\;\text{(TOTAL)} = 0.0053$

**Figure 2.5-1 Total Power Transient**

Power (Arbitrary Units) vs. Time (SEC)
3. Conclusions

3.1 Space dependent neutron transients in CANDU systems result from a combination of:

a) asymmetric insertion of reactivity devices,

b) neutronic decoupling of reactor segments produced partially by deliberate flattening of flux distribution,

c) increased effect of delayed source distribution due to mainly prompt sub-critical transients.

3.2 Neutronic decoupling accentuates the effect of asymmetric insertion of reactivity devices. As shown in Section 1.1 increased neutronic decoupling due to power flattening significantly reduces the reactivity worth of shutdown devices.

3.3 Photoneutrons have a significant effect on the magnitude of the total power transient and on the variation of the power distribution due to precursor decay. In some simulations when photoneutrons were included peak powers were 25% lower and flux shape variation following completion of applied perturbations increased by 100% due to excess retardation.

3.4 Neutronic decoupling accentuates the effect of the delayed source distribution on flux (power) distribution and reactivity. The retardation of the flux shape during the approach to the asymptotic flux shape increases the importance and hence the worth of the reactivity devices by as much as 80%. Solutions of the time-dependent diffusion equations with adequate representation of delayed neutron precursors are required for the design of reactivity device configurations.
ACKNOWLEDGEMENTS

Thanks are due to L. Pease, and A. A. Pasanen for helpful discussion; Special thanks are due to D. E. Meneley for detailed guidance on the improved quasistatic method and on all aspects of space-time kinetics; to G. Kugler for providing up-to-date delayed neutron and photoneutron data; to M. H. Guenzel, J. Howieson and T. L. Tang for modeling and input preparation for the CERBERUS code, to F. Sheldrake for typing and to the Computation Section for assistance in development and execution of the CERBERUS code.
REFERENCES


DISCUSSION

A. Siebertz

I have two questions:

1) What do you mean by "neutronic decoupling of reactor segments due to deliberate power flattening"?

2) What time integration methods do you use for the solution of the amplitude equation, for the shape equation and for the thermohydraulic feedback equation? What is the order of magnitude of the corresponding time steps?

A.R. Dastur

1) The coupling reactivity of a segment may be defined as the fraction of neutrons born in the segment which result from fissions produced by neutrons that were born outside the segment in the previous generation. Power flattening reduces this quantity.

2) The amplitude equation is solved by expansion of the term giving the time dependence of the flux and precursor concentrations into matrix series.

3) The shape equation is solved using a finite difference formulation.

4) There is no thermalhydraulic feedback included in the model.
5) The size of the time step varies during the transient depending on the size of the shape variation. During reactivity device insertion, the shape is calculated approximately every 0.1 sec. During precursor decay (after all "external" perturbations are complete) it can be as large as 30 sec. The time step for the amplitude calculation is usually 1/100 of that used in the shape calculation.

G. Williams

Is there any governing philosophy which limits the cost of a study even though the study is in support of a safety case to the Regulatory Authority?

A.F. Henry

Machine running time is one practical limitation.

Very few computing machines will run for twenty straight hours without a fault. For an iterative procedure, such a fault will require that the problem will have to begin its convergence process over again.

Aside from that, it seems to me some sort of cost benefit analysis must be brought into consideration in deciding how much money should be spent for safety calculations.

H. Küsters

This morning, we heard that large effort is being spent to improve the calculational time without loss of too much accuracy. You have presented a full Candu-reactor representation within a 3dimensional improved quasi-static method. Even without the inclusion of feedback, what is the amount
of time to produce the complete input (including cell calculation) and the amount of computing time, getting this way a figure from which we may learn what can be gained by approximate methods for 3d cases?

A.R. Dastur

1) To prepare the complete input, which consists of a) normal lattice calculations, b) supercell calculations and c) reactor configuration in space and time, it would require between 2 and 3 weeks of professional time.

2) For the problem described (25 000 mesh points, 2500 supercells, 6 delayed neutron groups and 2 energy groups), it would require 200 sec of CP time on the CDC 6600 per shape calculation.
J.K. Fletcher, M.A. Perks

THE SPATIAL KINETICS PROGRAM SPARK AND ITS APPLICATION TO
FAST REACTOR TRANSIENTS

UKAEA, Risley, Warrington, United Kingdom
The Spatial Kinetics Program SPARK and its Application to Fast Reactor Transients

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M A Perks
UKAEA, Risley, Warrington, England

Introduction

This paper describes the one, two and three-dimensional fast reactor kinetics code SPARK with space and energy dependence of the neutron flux. The solution of the equations is discussed and then a description of the neutronics, heat transfer and feedback formulation is presented.

The program was used to calculate the two-dimensional fast reactor benchmark problem, the results of which are being presented at the conference. The program has also been used to study several types of transients leading to can failure or fuel melting and some typical examples are presented.

Discussion of the Method

Solutions used in other computer programs fall roughly into three groups:

a. Synthesis in which the time and space dependent behaviour is obtained from a series of precalculated spacial flux distributions.

b. Splitting techniques where the flux is expressed as the product of two factors, one time dependent only, the other called the shape function which is space dependent with a comparatively small time variation. These are usually called quasistatic methods.

c. Methods in which the flux is derived as $e^{\int Hdt}$ where $H$ is a matrix, $t$ the time and approximation methods are used to evaluate the exponential.

The SPARK program was based on (b) because use could be made of existing programs and feedback could be incorporated fairly easily, also by increasing the number of shape function calculations the exact solution of the equations can be approached.

Synthesis procedures have difficulty with temperature feedback and accuracy estimates and some iteration and recalculation of the base functions may be necessary.

Method (c) is new and makes use of sophisticated mathematics which may prove not to be suitable for practical problems especially if $H$ depends on $t$.

Neutronics Solution

The multigroup space and time dependent diffusion equations are

$$\frac{1}{v_g} \frac{\partial \phi_g}{\partial t} = D \nabla^2 \phi_g - \sigma_r \phi_g + \sum_m \sum_{g'} (1 - \beta_m) \nu_{fmg'} \phi_{g'} \chi_g$$

$$+ \sum_{g'} \sigma_{g'g} \phi_{g'} + \sum_n \lambda_n \chi_n \quad g = 1, \text{NG}$$
\[ \frac{\partial \phi_n}{\partial t} + \nabla \cdot \left( \sum_{m, n} \beta_{nm} \nu_{nmg} \phi_m \right) = -\lambda_n \phi_n \quad n = 1, N \quad \cdots \quad (1) \]

where \( \phi_n \) is the space and time dependent flux, \( C_n \) the precusor concentration for delayed neutron group \( n \).

\( D, \sigma_r, \sigma_s \) are the diffusion coefficient, removal and scatter cross-sections, \( \nu_{nmg} \) the nu-fission cross-section for material \( m \), \( \lambda_n \) is the time constant for delayed group \( n \), \( \beta_{nm} \) the delayed fraction for material \( m \) and delayed group \( n \). \( \chi_g \) and \( \chi_{ng} \) are the spectra for prompt delayed fission neutrons and \( V_g \) the group velocity. Also

\[ \beta_n = \sum_n \beta_{nm} \]

Consider the steady state adjoint equation

\[ \psi = D_{g} \psi_{g} + \nu_{nmg} \psi_{nmg} + \sum_{g'} \sigma_{g} \chi_{g} \psi_{g} \]

\[ + \sum_{g'} \beta_{ng} \phi_{ng} + \sum_{n} \lambda_n \psi_{ng} \psi_{g} \cdots \quad (2) \]

where \( \psi_{g} \) is the adjoint flux for group \( g \).

Multiply (1) by \( \psi_{g} \), (2) by \( \psi_{g} \) subtract, integrate over volume and sum over \( g \) then,

\[ \sum_{g} \int_{V} \frac{\partial \psi_{g}}{\partial t} dV = \sum_{g} \int_{V} \nu_{nmg} \psi_{nmg} dV - \sum_{g} \int_{V} \sigma_{g} \chi_{g} \psi_{g} dV \]

\[ + (1 - \frac{1}{k}) \sum_{g'} \sum_{m} \nu_{nmg} \psi_{g'} \chi_{g} \psi_{g} \]

\[ - \sum_{g} \beta_{ng} \psi_{ng} \psi_{g} \]

\[ + \sum_{n} \lambda_n \psi_{ng} \psi_{g} \]

but

\[ \int_{V} D_{g} \psi_{g} \psi_{g} dV - \sum_{g} \int_{V} \sigma_{g} \chi_{g} \psi_{g} dV = \int_{V} \nu_{nmg} \psi_{nmg} dV \]

\[ = \int_{V} (\psi_{g} \nu_{nmg} \psi_{nmg} - \nu_{g} \psi_{g} \psi_{nmg}) dV \]

\[ = \int_{V} (\psi_{g} \nu_{nmg} \psi_{nmg} - \nu_{g} \psi_{g} \psi_{nmg}) dV \]

\[ = \int_{S} \psi_{g} \nu_{nmg} \psi_{nmg} dS - \nu_{g} \psi_{g} \psi_{nmg} dS \]

\[ as D_{g} \psi_{g} \psi_{g} = -\lambda \psi_{g} \quad and \quad D_{g} \psi_{g} = \lambda \psi_{g} \quad on \quad the \quad boundary. \]

Let \( \phi_{g} = N_{g} \psi_{g} \) and \( C_{n} = \alpha C_{n} \), where \( \alpha \) and \( N \) depend only on time.
\[
\sum \int \frac{g^*}{g} \cdot \frac{\partial}{\partial t} (N_g) \, dv = \sum \int (1 - \frac{1}{k}) \sum \nu f_m g^* N g' \chi g \phi g^* \\
- \sum \beta_m \nu f_m g' N g' \chi g \phi g^* + \alpha \sum C_n \chi g g^* \, dv
\]

Also from (1)

\[
\sum g^* \frac{d}{dt} (C_n \alpha) = \int \sum \beta_{nm} \nu f g' m g' \chi g \phi g^* - \lambda_n C_n \sum \chi g g^* \, dv
\]

let \(l = \sum \int \frac{g^*}{g} \, dv\)

\[
\beta_n = \sum g \sum \beta_{nm} \nu f \chi g \phi g^* \, dv
\]

\[
\beta = \sum \beta_n, \quad \rho = \int (1 - \frac{1}{k}) \sum \nu f g' \chi g \phi g^* \, dv
\]

\[
\gamma_n = \sum g \sum C_n \chi g g^* \, dv
\]

Then neglecting \(\frac{\partial \psi}{\partial t}\) and \(\frac{\partial \alpha'}{\partial t}\)

\[
1 \frac{dN}{dt} = (\rho - \beta)N + \Sigma \lambda_n \alpha_n \gamma_n \\
\]

\[
\gamma_n \frac{d\alpha_n}{dt} = \beta_n N - \lambda_n \gamma_n \alpha_n \quad \text{for} \quad n = 1, N
\]

(The difference between delayed spectra and prompt spectrum has been neglected).

The above are the well known point kinetics equations. If the time derivative is taken to first order then (3) becomes in difference form.

\[
1 \left( \frac{N_{i+1} - N_i}{\delta t} \right) = (\rho - \beta) N_{i+1} + \Sigma \lambda \gamma_n \alpha_n, i+1
\]
\[
\frac{(\alpha_{n,i+1} - \alpha_{n,i})}{\delta t} = \beta_n N_i - \lambda_n \gamma_n \alpha_{n,i+1}
\]

where \( \delta t \) is the time step at interval \( i \).

\[
\alpha_{n,i+1} = \frac{\beta_n N_i \delta t + \alpha_{n,i} \gamma_n}{\gamma_n (1 + \lambda_n \delta t)}
\]

\[
N_{i+1} = \frac{1N_i + \sum \lambda_n \gamma_n \alpha_{n,i+1} \delta t}{(1 - (\rho - \beta) \delta t)}
\]

Since it has been assumed that \( \psi_g \) and \( C'_n \) are slowly changing in time the above equations can be solved over some time interval \( \Delta t \) and then \( \psi_g \) can be re-calculated in the following manner. From (1)

\[
\frac{\partial C}{\partial t} = \sum\sum \beta_{nm} \nu_{fgm} \psi_g N - \lambda C_n
\]

\[
\frac{\partial}{\partial t} (e_n C_n) = e_n \left( \sum\sum \beta_{nm} \nu_{fgm} \psi_g N \right)
\]

ie

\[
C_{n,t+\Delta t} - C_n = e^{-\lambda \Delta t} \sum\sum \beta_{nm} \nu_{fgm} \psi_g \int_0^{\Delta t} Ne \lambda t dt
\]

New values of \( \psi_g \) are obtained from

\[
\frac{1}{V_g} \left( \psi \frac{dN}{dt} + N \frac{\partial \psi}{\partial t} \right) = N \left( \delta_g \nabla^2 \psi_g - \sigma \psi_g + \sum_g \sum_m (1 - \beta_m) \nu_{fgm} \psi_{g,g'} + \sum_g \sigma_{g,g'} \psi_{g,g'} \right) + \sum_n C_n \lambda_n \chi_{ng}
\]

where \( \frac{dN}{dt} \) is taken from the last \( \delta t \) time step in the equation 4

\[
\frac{\partial \psi}{\Delta t} = \frac{\psi_{t+\Delta t} - \psi_t}{\Delta t}
\]

Solving for \( \psi_{t+\Delta t} \) is in fact just solving the steady state diffusion equation with a source term. SPARK uses the forward substitution backward difference method in ID and the PDQ method in higher dimensions.
It will be noticed that in the solution for \( N \) and \( \psi_g \) the right hand sides have all been calculated with the value of \( i+1 \) for \( N \) and \( t+\Delta t \) for \( \psi_g \). This eliminates build up of rounding errors caused by 1. For fast reactors 1 is of the order of \( 10^{-7} \) and in a forward difference scheme would divide the previous estimate of \( N \) so that any error in \( N \) is increased by a factor of \( 10^7 \) and very small steps in \( \Delta t \) (\( 10^{-8} \)) have to be used. As can be seen from (4), 1 multiplies \( N_i \) and hence errors are diminished by \( 10^7 \) so that larger \( \Delta t \) values related to the change in \( N \) rather than elimination of rounding errors can be used. (\( 10^{-4} \) for \( \Delta t \) is usually used in SPARK).

The method is in effect a point kinetics solution with periodic recalculation of the flux shape. Because of the inclusion of the \( \frac{\partial \psi}{\partial t} \) term in equation (5), if the frequency of flux calculations is \( \Delta t \) then a full backward difference solution is obtained. This is sometimes called the improved quasi-static method.

**Feedback and Incidents**

The steady state equation is first solved giving the precursor concentrations and equilibrium fluxes. Then one of the following four incidents as specified in the data is initiated:

i. Insertion of reactivity over the whole system by adding a constant multiplied by time to \( \rho \) in equation 3.

ii. Localised variation of reactivity by linear variation with time of \( \nu \) in a given region.

iii. Control rod movement at a given speed. This can be made to correspond to the incident of sodium voiding fairly obviously by removing sodium at a given rate.

iv. Sodium flow rundown.

Reactivity feedbacks for expansion of fuel, sodium and sodium density change are allowed for.

Temperature variation from heat transfer calculations is reflected in changes to cross-sections in (1). The temperature calculation will be described in the next section but can be performed at specified intervals (but more often than \( \psi_g \)). When the cross-sections have changed the subtraction procedure of equations (1) and (2) gives a residual term

\[
\sum_g \int \phi_g^+ \partial \psi_g^+ + \frac{\partial \psi_g^+}{\partial \Delta t} - \sum_g \sum_m \psi g f m g' \phi_g^+ \phi_g^+ \Delta g' \frac{\partial \Delta g'}{\partial \Delta t} d\psi_g
\]

After each temperature calculation the above sum is added to \( \rho \) and at each \( \psi_g \) recalculation the temperature modified cross-sections are used.

Cross-sections are tabulated for several temperatures and a \( T^k \) interpolation is used where \( T \) is the temperature at the mesh point.
Heat Transfer and Temperature Equations

For the purpose of calculating reactivity feedback arising from temperature changes, the reactor is considered to be composed of a number of axial channels each of which is divided into a number of discrete thermal regions.

If the flux calculation is in slab (Z) geometry then a single reactor channel is used and thermal regions correspond one-to-one with the mesh-boxes defined for the flux calculation.

If the flux calculation is in cylindrical (R) geometry then a number of axial reactor channels overlay the radial flux-channel, and a fixed axial power profile is defined for each reactor channel.

The equations determining the behaviour of material temperatures in each thermal region are presented in Appendix 1. Thermal capacities and heat transfer coefficients for each thermal region are defined by items of input data: the power distribution \( P(i,j) \) is obtained, in the slab (Z) case, directly from the flux calculation, or, in the cylindrical (R) case, by a synthesis of the results of the radial flux calculation together with the axial power profiles defined as input data.

A flow rundown disturbance may be specified which acts directly on the temperature equations via the coolant axial heat transport term \( G \) and the can/coolant and structure/coolant heat transfer coefficients.

Time Step Selection

It is assumed that the amplitude is the fastest changing variable followed by the temperature and flux shape respectively. In SPARK a time step is selected for the point kinetics (usually \( 10^{-4} \)) then in the data the number of time steps per temperature calculation and number of temperature calculations per shape function is specified (these could obviously both be 1). The selection of these is left to the user at present as there does not seem to be any time saving method of automatic adjustment.

SPARK is flexible in that after doing say 100 time steps between temperature calculations and 20 temperature calculations between shape functions these can be altered to 50 and 2 after a specified number of shape functions and so on.

Solution of Temperature Equations

The thermal equation for a general material \( i \) may be written as

\[
\frac{dT_i}{dt} = aP + bT_{i-1} - cT_i + dT_{i+1} + e
\]

where \( a, b, c, d \) and \( e \) are known and positive. In finite-difference form, this is

\[
\frac{T_i^{n+1} - T_i^n}{\Delta t} = (1 - \theta) \left( aP^n + bT_{i-1}^n - cT_i^n + d T_{i+1}^n + e \right) + \theta \left( a P^n + b T_{i-1}^n - c T_i^n + d T_{i+1}^n + e \right)
\]

where \( \theta \) is an integration parameter whose value is a matter of choice.
If \( T_{i-1}^{n}, T_{i}^{n}, T_{i+1}^{n}, p_{i}^{n} \) and \( p_{i+1}^{n} \) are known, the finite-difference equation may be re-arranged to yield a relationship between the unknowns \( T_{i-1}^{n+1}, T_{i}^{n+1} \) and \( T_{i+1}^{n+1} \). In the particular case of \( \theta = 1 \) ('forward differencing'), the coefficients of \( T_{i-1}^{n+1} \) and \( T_{i+1}^{n+1} \) are zero and \( T_{i}^{n+1} \) is determined explicitly. More generally, if there are \( N \) materials in each thermal-region then the finite-difference formulation of their \( N \) thermal equations yields a tri-diagonal \( N \times N \) matrix whose inversion is necessary to obtain \( T_{i}^{n+1}, i = 1, 2, \ldots, N \). Other frequent choices of \( \theta \) are \( \frac{1}{2} \) ('central differencing') and \( 0 \) ('backward differencing').

**Forward differencing (\( \theta = 1 \))**

\[
T_{i}^{n+1} = a \times \Delta t \times p_{i}^{n} + (b \times \Delta t) T_{i-1}^{n} + (1 - c \Delta t) T_{i}^{n} + (d \Delta t) T_{i+1}^{n} + e \Delta t
\]

**Central differencing (\( \theta = \frac{1}{2} \))**

\[
\begin{align*}
-b \times \frac{\Delta t}{2} T_{i-1}^{n+1} + (1 + c \times \Delta t) T_{i}^{n+1} + (-d \times \frac{\Delta t}{2}) T_{i+1}^{n+1} &= a \times \Delta t \times p_{i}^{n+1} + p_{i}^{n} \\
+ (b \times \frac{\Delta t}{2}) T_{i-1}^{n} + (1 - c \times \Delta t) T_{i}^{n} + (d \times \frac{\Delta t}{2}) T_{i+1}^{n} &= a \times \Delta t \times p_{i}^{n} + p_{i}^{n+1} + e \times \Delta t
\end{align*}
\]

**Backward differencing (\( \theta = 0 \))**

\[
\begin{align*}
-b \times \Delta t T_{i-1}^{n+1} + (1 + c \times \Delta t) T_{i}^{n+1} + (-d \times \Delta t) T_{i+1}^{n+1} &= a \times \Delta t \times p_{i}^{n+1} + p_{i}^{n} + e \times \Delta t
\end{align*}
\]

The apparent superiority of forward differencing arising from its simplicity may well be outweighed by the fact that a very small time increment \( \Delta t \) is necessary to satisfy stability criteria. Moreover, central differencing, which is not thus restricted, has a truncation error only of order \((\Delta t)^3\) compared to the order \((\Delta t)^2\) of forward and backward differencing. A disadvantage of central differencing arises from the extra arithmetic necessary in setting up the coefficients of the matrix.

An intermediate difference scheme, a compromise between the classical forward and backward difference methods, is obtained by writing

\[
\frac{T_{i}^{n+1} - T_{i}^{n}}{\Delta t} = a p_{i}^{n+1} + b T_{i-1}^{n+1} - c T_{i}^{n+1} + d T_{i+1}^{n+1} + e
\]

yielding

\[
\begin{align*}
-b \times \Delta t T_{i-1}^{n+1} + (1 + c \times \Delta t) T_{i}^{n+1} &= a \times \Delta t \times p_{i}^{n+1} + T_{i}^{n} + d \Delta t T_{i+1}^{n} + e \times \Delta t
\end{align*}
\]
The method does not have the instability disadvantage of forward-differencing, and gains over backward-differencing in that the matrix obtained is now lower-diagonal and may be solved simply by forward substitution.

Another possibility arises from the observation that, on integrating across a time-step in which the true temperature derivative is of constant sign, the errors, when compared to the true solution, of the forward difference solution and the backward difference solution are of opposite sign and similar magnitude. Thus the application of backward difference and forward difference methods in alternate time steps results in some cancellation of errors, yielding a solution method more accurate and faster than simple backward differencing and less liable to stability difficulties than forward differencing.

All five one-step difference methods (forward, central, backward, intermediate and alternate backward/forward) are available in the present version of SPARK. The choice of method, and the time-step employed in the one-step methods, are user-options. It is hoped that experience gained in using the program will lead to empirical rules to guide the user in his choice of solution method. A time-step algorithm may also be an advantage.

Programming Details and Running Times

The program is written completely in FORTRAN IV. There are no fixed dimensions so that problem size is limited only by the amount of fast store available in the computer.

In order to reduce the running time, as little use as possible is made of peripheral storage. In one and two dimensions disc storage is used for the finite difference coefficients in the shape function calculation. In three dimensions some data transfers are used so that practical problems can be run. During the shape function calculation the adjoint, initial temperatures and point precursor values are put onto disc and read back for the amplitude calculation.

A one dimensional nine group problem takes about five minutes and ten minutes without and with shape functions respectively. Two dimensional problems take about 60 minutes in 6 energy groups with shape function recalculation. Only a small problem in three dimensions has been done taking twenty minutes (900 mesh points three groups).

Future Developments

Up to now SPARK has been used to predict the onset of fuel melting, can failure or coolant boiling in a variety of transients, some examples of which are given later in this paper. It is hoped to extend the program to deal with situations arising after coolant boiling and gross fuel movement have occurred. This will necessitate the incorporation of sub routines dealing with detailed failure criteria, coolant expulsion, fuel movement before and after clad failure and molten fuel-coolant interaction. Typical examples of these are already available in the whole core accident code FRAX currently under development in the UK.

Application of SPARK Program to Fast Reactor Transients

The program has been used to study several types of transient in large fast reactors leading to can failure or fuel melting. The results presented in this paper are for the following incidents:
1. A range of localised reactivity ramp insertions in three sizes of fast reactor (by changing $v$) - cylindrical geometry.

2. The effect of control rod ejection (by movement of absorber) - RZ geometry.

3. The effect of channel voiding (by progressive removal of coolant) - RZ geometry.

4. The effect of multinode representation of the fuel pin for fast reactivity ramps and coolant voiding - RZ geometry.

Test problems in three dimensions (XYZ geometry) have been successfully run for a flow run-down incident and a localised ramp (change of $v$). Some graphical results will be presented at the conference.

Local Ramp Insertion of Reactivity

A comparison has been made of the effect of local ramp insertion of reactivity in three sizes of fast reactor. Details of the reactor models used, representative of fast power reactors of 250 MW(E), 1,000 MW(E) and 2,000 MW(E), are given in Table 1. One-dimensional (cylindrical) geometry was used and in each model there is an annular region containing absorber. There are two zones of differing $u + Pu$ fractions with absorber region situated within the inner zone. The fuel is oxide and the absorber natural boron carbide. For the largest reactor (type 3) the fraction of absorber was lower than for the other two in order to produce about the same flux depression in the steady state.

Transients were induced by changing $v$ for every fuel isotope linearly with time in the absorber region only. Calculations were made using an appropriate 9 energy group condensation of the FD4 data set. For types 2 and 3 the rates of change of $v$ were selected to give reactivity ramps varying between 1 and 100 $$/sec. For type 1 a ramp of 50 $$/sec only was considered. All the transients were calculated using both the point kinetics and spatial kinetics options of SPARK.

Typical results for fuel temperature for a ramp rate of 50 $$/sec in type 2 are shown in Fig 1. Similar results were found for type 3 but for type 1 the differences between point and spatial kinetics were small. The effect of the range of ramp rate is shown in Figs 2 and 3 where the time for the maximum fuel temperature to rise from 2,100$^\circ$K (steady state) to 3,000$^\circ$K (approximate melting point) is given for types 2 and 3. It can be seen that the difference between point and spatial kinetics is largely independent of ramp rate but is much larger for reduced power.

The effect of the range of reactor sizes is shown in Fig 4 where the peak fuel temperature and power are given for a ramp of 50 $$/sec. The general conclusion to be drawn from this study is that it is difficult to induce spatial effects in reactors of the 250 MW(E) size but that they can be significant in reactors of 1,000 MW(E) size and large in reactors of 2,000 MW(E) size. This conclusion refers to a comparison between spatial kinetics and point kinetics using the steady state flux and adjoint distributions to calculate reactivity feedback. The obvious inadequacy of using point kinetics in this way when significant flux changes are anticipated can be avoided by the methods used in the next example.

Control Rod Ejection

The model used for this work was in RZ geometry with a core radius of 142 cm and height 100 cm. The two zone fuel Pu fractions were 0.176 and 0.220. Both 3 group
and 9 group condensations of the FD4 data set were used and also a 3 group conden-
sation of the FD5 data set.

The calculations were concerned with the ejection of a central control rod of
natural boron carbide. Three speeds of removal were considered - 1,000 cm/sec, 
100 cm/sec and 10 cm/sec. Calculations were made using the material movement
facility of SPARK to change 'rod in' composition to 'rod out' composition in a
central 7.6 cm radius region. For a power of approximately 3,000 MW(H) the maximum
fuel temperature in the steady state (rod in) was 1,700°K occurring in the outer
core zone.

Steady state and kinetics calculations of the reactivity change due to control rod
movement at 100 cm/sec in 3 groups and in 9 groups showed little difference so sub-
sequent calculations were restricted to 3 groups. Steady state calculations gave
the worth of the central control rod as 0.50% or 1.6 $\%$.

Kinetics calculations were made using SPARK in both the point mode (no flux shape
recalculations) and the spatial mode (usually employing about 10 flux shape re-
calculations). Typical results (for rod speed of 100 cm/sec) for the reactivity
and maximum fuel temperature are shown in Figs 5 and 6. Significant differences
are seen to exist between the two modes of calculation.

The main reason for these differences was assumed to be that in the point mode
SPARK uses the steady state (rod in) flux and adjoint to calculate reactivity
changes. To test this the reactivity change between different steady state situations
as the rod was withdrawn was calculated using three methods with the program
MARC:

a. direct $k_{\text{eff}}$ calculations

b. first order perturbation theory

c. exact perturbation theory for rod out (using adjoint flux with rod out).

The results are given in Fig 7 and show the same sort of difference between methods
(a) and (b) as between point and spatial modes (Fig 5 - until significant Doppler
feedback occurs).

The test was taken a stage further by setting up a point kinetics case with the
program FUTURE-2 using the steady state $k_{\text{eff}}$ curve of Fig 7 as a reactivity vari-
ation for a rod speed of 100 cm/sec. The Doppler constant, effective delayed frac-
tion and prompt reaction lifetime used were obtained from 3 group MARC calculation
for the rod in condition. The resulting transient reactivity and fuel temperature
are shown in Figs 5 and 6. These are seen to agree well with the SPARK spatial
kinetics calculations.

Results for rod speeds of 1,000 cm/sec and 10 cm/sec showed similar trends to those
for 100 cm/sec, ie the fuel temperature rise calculated using the point mode was
about half that using the spatial mode, but the use of FUTURE-2 with direct $k_{\text{eff}}$
reactivity data gave results within 100°C of the spatial mode ones.

For the rod speed of 100 cm/sec calculations were also made at 10% power and flow.
Results obtained using the above (improved point kinetics) method were in poorer
agreement with the SPARK spatial mode one. For this transient can failure (about
1,200°K) occurs at about 2 sec (well before fuel melting). Although the time to
reach this failure criterion was within 0.3 sec for the spatial kinetics and the
improved point kinetics methods, the temperature distributions were different. The variation of can temperature with radius at 2 sec is shown in Fig 8, from which it can be seen that most of the channels in the inner core are within 70K of failure when this occurs in the outer core, whereas in the improved point kinetics case these channels are 200K to 600K below failure.

Coolant Voiding

Calculations have been made of the effect of progressive loss of coolant in a radial channel in RZ geometry. The reactor model used was type 2 of table 1 (without absorber region) with a core height of 100 cm and axial blanket thickness of 45 cm. The boundary between 'sodium in' and 'sodium' regions moves linearly with time starting from a specified height. When the boundary is between two mesh points an arithmetic average of composition is used in that mesh box. A 9 group condensation of FD4 data was used with appropriate spectra for the voided and unvoided volumes.

Two cases were considered in which central regions of the core were voided at 1,000 cm/sec from the bottom of the core. In the first case the radius of the region was 42.5 cm (one eighth of the core) and in the second case the radius was 85 cm (one half of the core - all the inner zone).

The resulting reactivity variations gave maximum rates of reactivity addition of 32 $/sec and 61 $/sec for the two cases. The difference between point and spatial kinetics was small. The variation of peak fuel temperature is shown in Figs 9 and 10 which show temperature differences between point and spatial kinetics of up to 200°K for the first case and up to 1,000°K for the second case.

In an accident code context where the progress of voiding cannot easily be predetermined the method of improving point kinetics used before is more difficult to apply and the effects found may be significant.

Multinode Representation of the Fuel Pin

In all the foregoing three studies the fuel pin was represented by a single mean temperature only. The effect of using several nodes in the pin has been considered for a reactivity ramp insertion of 100 $/sec and for a case of coolant voiding. For this work the model described previously for the control rod ejection study was used.

For a uniform fast ramp of 100 $/sec cases with 1, 3 and 10 nodes in the fuel pin were considered. It was found that there was negligible difference in the mean fuel temperature (across the pin) throughout the transient. However the peak fuel temperature, shown in Fig 11, reveals considerable difference between 1 and 3 nodes but little between 3 and 10 nodes. The effect of the latent heat of melting at 3,040°C is clear.

Next a non-uniform ramp equivalent to 100 $/sec was applied over an annular region between radii 8 cm and 29 cm by changing $v$. The cases were restricted to 1 and 3 nodes and the results for fuel temperature are shown in Fig 12. It can be seen that the error in using 1 node compared to 3 nodes is of similar magnitude to that in using point kinetics compared to spatial kinetics.

The case of coolant voiding considered with multinode pin representation was the progressive removal of coolant from the whole of the inner core zone at 1,000 cm/sec starting at the bottom of the core. Fuel melting was found to start after about 40 msec and in Fig 13 is shown the fraction of cross-sectional area molten in the
hottest pin. Cases with no flux recalculation (point kinetics) were run with 1, 3 and 10 nodes and show a difference mainly between 1 and 3 nodes. Cases with 5 flux recalculations (up to a molten fraction of unity) were run with 1 and 3 nodes only.

In this case it can be seen that the error in using 1 node compared to 3 is of less significance to that in using point kinetics.

Conclusions

The improved quasistatic method as used in SPARK has proved to be very suitable for development and programming into a one, two and three-dimensional spatial kinetics system for fast reactor transients.

No difficulties in running the program have been experienced over a wide range of transients. There are no restrictions on number of mesh points or energy groups other than those imposed by the size of computer store available. Running times are reasonable considering the early stage of development.

The transients considered have shown that spatial effects will be significant in the larger commercial fast reactors currently under consideration. Although an improved point kinetics scheme in which the reactivity input is pre-calculated can be used to obtain accurate results for power level, it has also been shown that detailed temperature distributions can not be well calculated without a spatial kinetics capability.

The inclusion of SPARK into a whole core accident code is regarded as important in order to be able to cope with the unpredictable reactivity and flux shape changes which are associated with events such as coolant voiding and fuel motion which occur under whole core accident conditions.
APPENDIX 1

Equations for a thermal region \((i, j)\) - The suffices \((i, j)\) are omitted for clarity.

**Fuel:**

\[
\frac{dT_{f3}}{dt} = \pi_{f3} \times P - H_{fc3} (T_{f3} - T_{f2})
\]

\[
\frac{dT_{f2}}{dt} = \pi_{f2} \times P - H_{fc3} (T_{f2} - T_{f3}) - H_{fc2} (T_{f2} - T_{f1})
\]

\[
\frac{dT_{f1}}{dt} = \pi_{f1} \times P - H_{fc2} (T_{f1} - T_{f2}) - H_{fcl} (T_{f1} - T_{c})
\]

**Can:**

\[
\frac{dT_c}{dt} = - H_{fc1} (T_c - T_{f1}) - W^h \times Hcd (T_c - T_d)
\]

**Coolant:**

\[
\frac{dT_d}{dt} = - W^h \times H_{cd} (T_d - T_c) - W^h \times H_{sd} (T_d - T_s) - G
\]

**Structure:**

\[
\frac{dT_s}{dt} = - W^h \times H_{sd} (T_s - T_d) - H_{sdo} (T_s - T_{do})
\]

**Stagnant sodium:**

\[
\frac{dT_{do}}{dt} = - H_{sdo} (T_{do} - T_s)
\]

**Material 1:**

\[
\hat{\tau}_1 = \left[ M_1 + (T_1 - T_{ref}) \mu_1 \right] \rho_1 \times A_1 \times Z \quad 1 = f_3, f_2, f_1, c, d, s, do
\]

\[
G = \left[ M_d + (T_d - T_{ref}) \mu_d \right] \times W \times \Omega_w \times (T_{out} - T_{in})
\]

\[
T_{in} (\text{region } k) = T_{out} (\text{region } k - 1) \quad or \quad \text{reactor inlet temperature if start of a new channel.}
\]

\[
T_{out} = 2T_d - T_{in}
\]

\[
\pi_e = \frac{A_{fe}}{A_{f1} + A_{f2} + A_{f3}} \quad , \quad e = 1, 2, 3
\]

\[P = \text{power of region } (i,j)\]

\[W = \text{normalised flow rate}\]
Region-dependent data specified as input

1. Material specific heats $m_1(i,j)$ at reference temperature
   \[ (J/gm \, ^0K) \]
   \[ l = f, c, d, s, do \]

2. Gradient of material specific heats $m_1(i,j)$
   \[ (J/gm \, {^0K} \times {^0K}) \]
   \[ l = f, c, d, s, do \]

3. Cross-sectional area of material $A_1(i,j)$
   \[ (cm^2) \]
   \[ l = f_3, f_2, f_1, c, d, s, do \]

4. Density of material $\rho_1(i,j)$
   \[ (gm/cm^3) \]
   \[ l = f, c, d, s, do \]

5. Height of region $S(i,j)$
   \[ (cm) \]

6. Heat transfer coefficients $H_{lm}(i,j)$
   \[ (watts/cm^2K) \]
   \[ l, m = f_2, f_1, c, d, s, do \]

7. Coolant flow rate in steady state $\Omega_w(i,j)$
   \[ (gm/sec) \]

Other parameters in the equations

1. Reference temperature $T_{ref}$ for specific heats
   \[ (^0K) \]

2. Index in can/coolant heat transfer correlation $h$

3. Reactor inlet temperature \[ (^0K) \]
FIG 2  TIME TO MELT FOR TYPE R
FIG 4  Ramp of 50 $/sec by changing $\nu$ in Annular Region
Reactivity (%) vs. Distance of control rod from bottom of core (cm)

FIG 7  STEADY STATE CALCULATIONS OF REACTIVITY
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(Point kinetics case with reactivity input from statics Cals.)
Fig 9: Voiding of inner one eighth of Core from bottom at 1000 cm/sec.
Fig 10: Voiding of inner half of Core from bottom at 1000 cm/sec
Fig 11. Uniform ramp of 100% sec. Multinode results
Fig 12: Non-uniform ramp of 100 °C sec 1 node and 3 node
A.F. Henry

How many energy groups are required for accurate spectrum representation in the fast reactor transients you described?

M.A. Perks

For rod ejection problems we find 3 energy groups sufficient, but for coolant voiding problems, 9 groups are required for accurate results. This was checked by one-dimensional calculations in 3, 9, and 25 groups.
G. Dubois

THE IMPORTANCE OF FLUX SHAPE CHANGES IN SPACE-TIME KINETICS CALCULATIONS

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INTRODUCTION

The primary objective of the study was to determine whether or not three-dimensional time-dependent diffusion calculations were essential for obtaining conservative estimates of the reactor behavior when rapid and localized perturbations are introduced into the core. This analysis was initiated by the works of other authors who studied the dynamic behavior of slab reactors by using point kinetics models. These reports clearly indicate the possibility of obtaining erroneous results with simplified kinetics models.

A quite important advantage of reduced kinetics models is their relatively low computational cost. If these models fail to adequately simulate the time-dependent behavior of a perturbed assembly, one may ask how useful they can be in safety studies? This is the second point this study addresses itself.

This work is not a safety analysis of a given reactor system but instead an evaluation of some hypothesis used in such studies. For this reason, the reactor model used was kept as simple as possible. The assembly is a bare, cubical, U-metal-fuelled, water-cooled and moderated reactor. Diluted boron acts as the operational controller. The uranium rods are fresh and enriched to 2.7%. The transient is assumed adiabatic and all feedback effects are neglected except the thermal expansion of the fuel pins. The perturbation is generated by the rapid insertion of a bundle of fuel rods into the core.
As a first step, a three-dimensional mathematical representation of this situation was derived. This includes the three-dimensional time-dependent diffusion equation for one energy group and six delayed neutron groups as well as a 3-D representation of the perturbation and the feedback terms. No attempt was made to numerically solve these highly non-linear relationships.

Instead, this 3-D kinetics model was used as a starting point to construct three reduced kinetics models, one in zero-dimension and two in one-dimension geometry. The construction of these simplified kinetics models was made possible by assuming:

1) that the flux shape remains constant along two spatial directions (three for the point model) during the transient;

2) that the weight function used to operate on the diffusion equations is the steady state adjoint flux.

These are the assumptions currently used to construct the classical point kinetics model.

Parametric studies were then carried on using all three kinetics models as a basis of calculations. Among the most important input parameters studied were the reactor size, the initial power level, the inserted bundle size as well as its acceleration and its position inside the core.
2 REACTOR MATHEMATICAL REPRESENTATION

The kinetics model includes one neutron group and six delayed neutron groups. The accident condition is characterized by the rapid insertion of a bundle of fuel rods into the core with a constant acceleration. It is assumed that the reactor control system fails to function properly and that all nuclear parameters remain constant during the transient except those associated with the metallic fuel whose thermal expansion is very important among the feedback mechanisms involved.

2.1 Time dependent diffusion model

In the one-energy-group approximation, the time-dependent diffusion equation for a bare cubical reactor is given by

\[
\frac{1}{v} \frac{\partial \phi}{\partial t} = \left[ \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right] - (\Sigma_a^M + \Sigma_a^S) \phi(x,y,z,t) + \ldots
\]

\[
\left[ \| \psi(1-\beta)-1 \right] \cdot \Sigma_a^F (x,y,z,t) \psi (x,y,z,t) + \sum_{i=1}^{6} \lambda_i C_i (x,y,z,t) + s(x,y,z,t)
\]

where the symbols assume their usual meaning and the superscript M, S, and F refer to the moderator, structure, and the fuel respectively. On the other hand, the precursors concentrations satisfy the following relationship:
\[
\frac{\partial C_i}{\partial t} = \beta_i \gamma_i \rho \in \Sigma_a^F(x,y,z,t) \phi(x,y,z,t) - \lambda_i C_i(x,y,z,t)
\]

for \( i = 1, 2, \ldots, 6 \). In these equations, \( v, D, \Sigma_a^M, \Sigma_a^S, \gamma, \rho, \phi, \psi, \beta_i \), and \( \lambda_i \) are all assumed constant both in space and time since the reactor is studied at the beginning of its core life with a uniform distributed fuel. The source term \( s(x,y,z,t) \) vanishes at \( t = 0 \) and models the reactor perturbation for \( t > 0 \). As for \( \Sigma_a^F(x,y,z,t) \), it is appropriate to mention that its spatial and temporal dependencies result from the feedback mechanism. Since the assembly is initially critical, the reactor edge "2a" satisfies the following relation:

\[
B^2 = 3 \left( \frac{\gamma}{2a} \right)^2 = \frac{1}{3} \left( \eta \phi - 1 \right) \Sigma_a^F(0) - \Sigma_a^M - \Sigma_a^S
\]

where \( B^2 \) is the critical buckling.

### 2.2 Perturbation Model

At time \( t = 0 \), the assembly is perturbed by the rapid insertion of a bundle of fuel rods of the same composition as those present in the core. The bundle movement is downward, parallel to the \( Z \)-axis and the insertion point in the \( X-Y \) plane is \((x_0, y_0)\). Note that the bundle moves with a constant acceleration. Assuming that the bundle size is negligible compared to the reactor size, it can be shown that the source term in (2.1a) takes the following form:

\[
s(x,y,z,t) = \eta \phi K Z_1(t) \Sigma_a^F(x,y,z,t) \delta(x-x_0)\delta(y-y_0)\phi(x,y,z,t)
\]

\[
= 0 \quad \text{for} \ z < Z_1
\]

\[
= 0 \quad \text{for} \ z > Z_1
\]
where $Z_1$ is the distance travelled inside the core at time $t$ by the bundle, $K$ is a constant proportional to the bundle size and $\delta(x-x_0)$ is the Dirac delta function.

From a mathematical view-point, $Z_1(t)$ can take any positive value which is the same as viewing the ramp insertion as unlimited. Actually, however, the maximum value of $Z_1(t)$ should be equal to $2a$, the reactor edge. In such case, the ramp insertion becomes limited.

### 2.3 Feedback Model

The source term derived in the preceding section generates a transient that changes the neutron density level by several orders of magnitude in less that 100 msec. For metallic fuels, an important feedback is the change in fuel density resulting from the substantial increase in temperature. Let $C_F$ and $T_F$ be the heat capacity and the temperature of the fuel. Then, assuming an adiabatic transient, one can write:

\[
(2.4a) \quad C_F \frac{dT_F(x,y,z,t)}{dt} = \gamma \Sigma_F(x,y,z,t) \phi(x,y,z,t)
\]

where $\gamma$ is a constant of proportionality. On the other hand, the fuel temperature coefficient $\sigma_T^F$ is assumed constant and is defined as:

\[
(2.4b) \quad \sigma_T^F = \frac{1}{\Sigma_a^F(x,y,z,t)} \frac{d\Sigma_a^F(x,y,z,t)}{dT_F}
\]
Combining these two relationships by eliminating $T_f$ yields:

\[(2.5) \quad \Sigma_a^F(x,y,z,t) = \frac{\Sigma_a^F(0)}{1 + \rho_2 \int_0^t \hat{\phi}(x,y,z,t) \, dt} \]

where $\rho_2$ is a positive constant.

2.4 Reduction of the Calculational Model

Relations (2.1) thru (2.5) can be combined such that the source term is (2.1a) as well as the precursors concentrations can be eliminated. This rearrangement therefore yields the following relationship:

\[(2.6a) \quad \frac{1}{v} \frac{\partial \phi}{\partial t} = D \cdot \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right) + B^2 \phi \]

\[- \eta \phi \sum_{i=1}^{6} \left( R(x,y,z,t) - \rho_2 \int_0^t \hat{\phi}(x,y,z,\tau) \, d\tau \right) \hat{\phi}(x,y,z,t) \]

\[- \eta \phi \sum_{i=1}^{6} \left( \delta_{1} \right) \int_0^t e^{-\lambda_i(t-\tau)} \frac{\partial \hat{\phi}}{\partial \tau} \, d\tau \]

where

\[(2.6b) \quad R(x,y,z,t) = K Z_1(t) \cdot \delta(x-x_0) \cdot \delta(y-y_0) \quad z \leq Z_1 \]

\[0 \quad z > Z_1 \]
Note that (2.6a) is an integro-differential relationship which will be used later to construct simplified kinetics models. Homogeneous boundary conditions are associated with this equation. Since the reactor is initially critical and operating at a power $P$, it follows that:

\begin{equation}
\hat{\gamma}(x,y,z,0) = \hat{t}_0 \cos \left( \frac{B}{\sqrt{3}} x \right) \cos \left( \frac{B}{\sqrt{3}} y \right) \cos \left( \frac{B}{\sqrt{3}} z \right)
\end{equation}

where $\hat{t}_0$ is a constant related to the reactor power at steady state and $B$ is given by (2.2).

In constructing the simplified kinetics models, it was necessary to approximate (2.6b) because this function is singular and furthermore, it contains a time-dependent discontinuity along the $z$-axis. For these reasons, the Dirac delta function was approximated by the following expression:

\begin{equation}
\delta(y - y_0) \approx \sigma \frac{1}{\sqrt{\pi}} e^{-\sigma^2 (y - y_0)^2}
\end{equation}

where $\sigma$ takes on a large but finite value. Note that if $\sigma \rightarrow \infty$, (2.8) is exact. For the time-dependent discontinuity along the $z$-axis, a similar approximation was used but this time, the approximating function was the error function which in the limit becomes the step function.
CONSTRUCTION OF REDUCED KINETICS MODELS

No attempt was made to solve equation (2.6a) as it stands because the numerical effort that would be required is exceedingly important in terms of computer cost. For this reason, three simplified kinetics models have been constructed using (2.6a) as a starting point. These include the classical point kinetics model and two one-dimensional kinetics representations.

In deriving these simplified kinetics models, the assumption was made that the flux shape remains constant along two spatial axis (three for the point model) during the transient and the weight function used was the steady state adjoint flux. Recall that in one-group theory, the adjoint flux is proportional to the direct flux.

3.1 The X-Time Kinetics Model

The approximation used in this model can be expressed as:

$$\psi(x,y,z,t) = \psi(x,t) \cos \left( \frac{B}{\sqrt{3}} y \right) \cos \left( \frac{B}{\sqrt{3}} z \right)$$

and relation (2.6a) was operated on by:

$$\int dy \int dz \cos \left( \frac{B}{\sqrt{3}} y \right) \cos \left( \frac{B}{\sqrt{3}} z \right)$$

which yielded a non-linear integro-differential equation in x and t for \( \psi(x,t) \).
3.2 The Z-Time Kinetics Model

In this case, the flux representation takes on the following form:

$$\Psi(x, y, z, t) = \psi(z, t) \cos \left( \frac{B}{\sqrt{3}} x \right) \cos \left( \frac{B}{\sqrt{3}} y \right)$$

and the operator on (2.6a) is:

$$\int dx \int dy \cos \left( \frac{B}{\sqrt{3}} x \right) \cos \left( \frac{B}{\sqrt{3}} y \right)$$

so that in this model, (2.6a) reduces to a non-linear integro-differential problem in z and t.

3.3 The Point-Kinetics Model

Finally, in the point model, the flux shape is fixed along all spatial directions which implies that:

$$\Psi(x, y, z, t) = \psi(t) \cos \left( \frac{B}{\sqrt{3}} x \right) \cos \left( \frac{B}{\sqrt{3}} y \right) \cos \left( \frac{B}{\sqrt{3}} z \right)$$

and the operator on (2.6a) becomes:

$$\int dx \int dy \int dz \cos \left( \frac{B}{\sqrt{3}} x \right) \cos \left( \frac{B}{\sqrt{3}} y \right) \cos \left( \frac{B}{\sqrt{3}} z \right)$$

In this case therefore, the non-linear integro-differential problem involves only one independent variable, namely "t".
NUMERICAL METHODS OF SOLUTION

This study had a two-fold purpose and one of them was the testing of a new numerical technique, namely the TCNR-methods\textsuperscript{6-8}, for solving space-time kinetics problems. These methods yielded reasonable accuracy by using few meshpoints along spatial axis. This is possible since they are high order numerical techniques requiring the explicit evaluation of several mixed derivatives.

To date, four numbers of the TCNR-methods have been developed and applied to kinetics problems. These are the O(IT)-methods for ordinary differential equations, the P(IT,IX)-methods for parabolic differential equations in one spatial dimension, the P(IT,IX,IY)-methods for two-dimensional parabolic differential problems and finally, the E(IX)-methods for elliptic differential problems in one dimension. Note that TCNR stands for Taylor-Ceschino-Newton-Raphson. For the X-time kinetics model as well as the Z-time model, the method used in this study is a P(2,2)-technique whose error behaves as:

\[ E = O(\Delta t^4) + O(\Delta x^5) \]

where \( \Delta x \) represents the space variable.

In the case of the point kinetics equations, the numerical scheme used is the optimized Taylor series method\textsuperscript{9} which has the capability of varying both the stepsize and the local order of the method to minimize the computational cost of a given problem.
This mathematical model was then used for the space-time analysis of an accident condition. The main objective of this parametric analysis was to study the reactor response dependency on the reactor size, the initial neutron density level, the inserted bundle size as well as its acceleration and point of insertion along the X-axis. Note that for all these numerical experiments, \( y_0 = 0 \). When \( x_0 = 0 \), we refer to the insertion as a symmetric one. A non-symmetric insertion in this paper is equivalent to \( x_0 = a/3 \).

For each experiment, the flux shape, the prompt critical time, the time to reach the first peak of the neutron density curve, the average and the maximum fuel temperature increase, the reactivity, and the energy released during the transient have been used as indicators of the reactor response under accidental conditions. These indicators become very helpful in comparing the three kinetics models for a given situation.

In Table 5.1, we present the design parameters of the critical reactor. Two reactor sizes, 60 cm and 240 cm, were studied. Except for a few simulations, the initial neutron density level was fixed to \( 5 \times 10^7 \) n/cc while the bundle size approximately equals 2% of the fuel present in the core at criticality.

Before analyzing the results of specific experiments, it is of interest to look at how each kinetics representation models the perturbations
TABLE 5.1
Design Parameters of the Critical Reactor

<table>
<thead>
<tr>
<th>Reactor Type</th>
<th>Metal-fuelled</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coolant</td>
<td>Water</td>
</tr>
<tr>
<td>Fuel</td>
<td>Uranium</td>
</tr>
<tr>
<td>Enrichment (atomic)</td>
<td>2.7%</td>
</tr>
<tr>
<td>Clad Material</td>
<td>SS-304</td>
</tr>
<tr>
<td>Control Material</td>
<td>Boron</td>
</tr>
<tr>
<td>Clad Thickness (inches)</td>
<td>0.0240</td>
</tr>
<tr>
<td>Fuel-Clad Gap (inches)</td>
<td>0.0075</td>
</tr>
<tr>
<td>Neutron Velocity (m/sec)</td>
<td>2200</td>
</tr>
<tr>
<td>Fuel Temp. Coefficient (1/°C)</td>
<td>-4.5 x 10⁻⁵</td>
</tr>
<tr>
<td>Fuel Heat Capacity (cal./gr.-°C)</td>
<td>0.0276</td>
</tr>
<tr>
<td>Fuel Density (gr./cc)</td>
<td>19.1</td>
</tr>
<tr>
<td>Shutdown Coefficient</td>
<td></td>
</tr>
<tr>
<td>a) Point Kinetics (cc/sec)</td>
<td>7.29 x 10⁻¹²</td>
</tr>
<tr>
<td>b) Space-time Kinetics (cm²)</td>
<td>8.81 x 10⁻¹⁷</td>
</tr>
</tbody>
</table>

function. A typical example appears in Figures 5.1 A, B, C for x₀ = 0 (i.e. symmetric insertion). For the X-time kinetics model, the perturbation is always a local phenomenon while it is just the opposite for the point-model. In the case of the Z-time kinetics model, the perturbation is always local and non-symmetric until the bundle has reached the bottom of the core; then, the perturbation becomes uniform along the Z-axis.
FIGURE 5.1A-UNLIMITED RAMP INSERTION FUNCTION FOR THE X-AXIS PROBLEM.
FIGURE 5.1 B-UNLIMITED RAMP INSERTION FUNCTION FOR THE Z-AXIS PROBLEM.
FIGURE 5.1C-UNLIMITED RAMP INSERTION FUNCTION FOR THE POINT KINETICS MODEL.
On Figures 5.2 A, B, C, D, E, F, are shown the computations for one typical simulation: this is the case of an asymmetric perturbation ($x_0 = a/3$) introduced into a large core (240 cm). On Figure 5.2 A, it is seen that the flux shape in the X-time model is strongly modified even at prompt criticality. For the Z-time model, Figure 5.2B indicates a relatively mild flux shape change. Recall that the point model assumes a non-changing flux shape. On Figure 5.2C, the normalized average neutron density curves for all kinetics models are presented. The point $t=t_L$ indicates the time at which the bundle reaches the bottom of the core. Note that for the X-time model, the neutron density level is much higher at $t_L$ than for the other two models. Note also that the Z-time model yields results that are very similar to those of the point model. On Figure 5.2D, the reactivity curve of each kinetics model is shown. The conclusions here are similar to the previous ones. Finally, Figures 5.2E and F illustrate the variation of the average temperature increase and the maximum temperature increase. One can see that the X-time model predicts a local melt down before the bundle is fully inserted while the other two kinetics models indicate a rather small maximum temperature change at $t = t_L$. Similar results were obtained for a symmetric insertion ($x_0 = 0$) into a large core.

Considering now the perturbation of a small core (60 cm), it is to be noted that in this case, the flux shape changes become much less important especially when the insertion is symmetric ($x_0 = 0$). This is the situation where the disagreement between the three kinetics models is less pronounced. The same conclusion was reached by Yasinsky and Henry.
FIGURE 5.2A - NORMALIZED X-FLUX IN THE X-TIME KINETICS MODEL FOR AN ASYMMETRIC INSERTION INTO A LARGE CORE.
Figure 5.2b - Normalized Z-flux in the Z-time kinetics model for an asymmetric insertion into a large core.
FIGURE 5.2C- NORMALIZED AVERAGE NEUTRON DENSITY FOR AN ASYMMETRIC INSERTION INTO A LARGE CORE
FIGURE 5.2D- VARIATION OF THE REACTIVITY FOR AN ASYMMETRIC INSERTION INTO A LARGE CORE.
FIGURE 5.2E-AVERAGE TEMPERATURE INCREASE FOR AN ASYMMETRIC INSERTION INTO A LARGE CORE.
FIGURE 5.2 \( T \)-MAXIMUM TEMPERATURE INCREASE FOR AN ASYMMETRIC INSERTION INTO A LARGE CORE
and by Johnson's et al. Of importance also is the fact that in small core calculations, the Z-time kinetics model and the point model give approximately the same results.

A detailed analysis of the results of these calculations has lead us to the following conclusions:

1) for both space-time kinetics models, the flux shape is generally easier to deform in a loosely-coupled core than in a tightly-coupled one;

2) The X-time kinetics model predicts substantial changes in the flux shape and this is the model that suggests a reactor accident of greater importance from the viewpoint of the consequences; this is true independently of the reactor coupling and the symmetry of the insertion;

3) the Z-time kinetics model and the point kinetics model predict essentially the same reactor response; this is due to the fact that the flux shape deformation is not appreciable enough in the Z-time kinetics model. This clearly illustrates the possibility that a one-dimensional kinetics model can be as poor as the point model in kinetics simulations of this type;

4) it is interesting to point out that in the Z-time model, a symmetric insertion \( x_0 = 0 \) yielded a shorter prompt critical time than an asymmetric perturbation \( x_0 = a/3 \): this was also noted for the point
kinetics model;

5) at the time the bundle reaches the bottom of the core, the normalized neutron density predicted by the X-time model can be several orders of magnitude larger than the value predicted by the other two kinetics models; this statement holds for both symmetric or asymmetric insertion into a small or large core; the main consequence of the result is the fact that the X-time model is the only one that predicts possible core damage;

6) the magnitude of the first peak in the neutron density curves depends primarily on the feedback model and flux shape changes;

7) the prompt critical time as computed by the three models vary appreciably (as much as 30%); as we shall see below, even the X-time estimate is not conservative because flux shape changes along the y-axis are neglected in this model; this suggests that the point model value as well as the Z-time value may be wrong by a factor as large as two; this statement holds also for the time at which the first peak of the neutron density curve occurs;

8) in kinetics studies, the instantaneous power level depends heavily on the perturbation model, the feedback model, and the control mechanism (external corrective action) model; it appears highly desirable in such analysis to extract the influence of each model on the simulation results; this is because unless these models are very sophisticated and
accurate, parametric studies even in 3-D analysis could lead to erroneous conclusions;

9) the comparative analysis of the simulations obtained for the three kinetics models indicates that none of these models yield conservative results because they all neglect flux shape changes along at least two spatial dimensions; this is particularly important for the Y-flux shape; consequently, for fast, localized perturbations, it appeared that 3-D kinetics simulations are essential for reactor safety studies assuming that the perturbation model, the feedback model and the control mechanism model are sophisticated and accurate;

10) the agreement between the three reduced kinetics models is very good for times smaller than the prompt critical time;

11) the three models yield approximately the same result for the amount of energy released up to the first peak of the neutron density curves;

In addition to the computer simulations mentioned earlier, parametric studies have been carried out for an asymmetric insertion into a large core. The aim of these additional runs was to determine the influence of the inserted bundle acceleration and its size as well as the initial neutron density level on the transients. From these numerical experiments, we arrived at the following conclusions:

12) for all three kinetics models, the bundle acceleration "G"
and the prompt critical time "tp.c." are related by:

\[ G, t_{p.c}^2 = a_1 \]

where "a_1" is a constant characterizing each model; note that this law holds even for the X-time model which shows substantial flux shape changes; such a law could be useful in safety studies; a similar law was obtained for the time at which the first peak of the neutron density curves occurs;

13) for all three kinetics models, it was found that the first-peak normalized neutron density "N(t_f.p.)" is related to the bundle acceleration "G" by the following relationship:

\[ N(t_f.p.) = N(0) a_2 G^3 \]

where a_3 approximately equals to unity for the point model and is smaller than unity for the two space-time models. Flux shape changes therefore tend to attenuate the influence of "G" on N(t_f.p.);

14) for all three kinetics models, the prompt critical time "t_p.c." is related to the bundle size S_B by the following relationship:

\[ S_B^{a_5} . t_{p.c.} = a_4 \]

where a_4 and a_5 are constant; however, a_5 strongly depends upon the kinetics model used and the analysis indicates very clearly that a_5 increases as the
surface under the normalized flux shape decreases; Table 5.2 shows the value of $a_5$ for the three models analyzed in this study;

<table>
<thead>
<tr>
<th>MODEL</th>
<th>$a_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-time</td>
<td>7.0</td>
</tr>
<tr>
<td>Z-time</td>
<td>2.25</td>
</tr>
<tr>
<td>Point</td>
<td>3.5</td>
</tr>
</tbody>
</table>

15) in view of remarks 12) and 14), it appears that for a safer design (larger $t_{p.c.}$), it is much more important to limit "G" than "S_B";

16) for all three kinetics models, the first-peak time of the neutron density curves is independent of the initial average neutron density level; this statement is also applicable to the prompt critical time;

17) for all three kinetics models, the first-peak average neutron density level slightly decreases as the initial neutron density level increases.

In view of the last six remarks, it is evident that reduced kinetics models can provide useful information about the dependency of important parameters (such as the prompt critical time) upon the reactivity insertion rate, the amount of reactivity introduced into the core, the
initial power level, and flux shape changes.
The main conclusion to draw from this study is that simplified kinetics models present serious drawbacks in the analysis of super-prompt-critical excursions. Except for a symmetric reactivity insertion into a tightly-coupled core, the three kinetics models display substantial disagreements. In addition, the analysis shows that a one-dimensional kinetics model can be as poor as the point model in describing properly this type of accident condition. In view of the important flux shape changes, it appeared that both one-dimensional kinetics models were inadequate for safety studies since they do not yield conservative estimates of the reactor dynamic behavior.

Despite serious disagreements on some points, the three kinetics models agree on others: 1) the prompt critical time is nearly independent of the initial neutron density; 2) the magnitude of the first peak of the neutron density curves decreases as the initial power level increases; 3) the amount of energy released up to the first peak of the neutron density curve is approximately the same; 4) for reactivity insertions less than one dollar, the three kinetics models essentially predicts the same power excursion. It thus appears that reduced kinetics models could be useful in carrying out sub-prompt-critical analysis as well as parametric studies even though they can be erroneous in computing the value of some important parameters such as the prompt critical time and the reactivity at any given time.
This study agrees with the recent findings of Birkhofer, Schmidt and Werner\textsuperscript{10} on the urgent need to solve three-dimensional kinetics problems for super-prompt-critical excursions. This implies the development of much faster numerical techniques, capable of reasonable accuracy. It would greatly enhance the reliability of reactor safety studies.


Session IV/1

REVIEW OF KINETICS BENCHMARK CALCULATIONS

Chairman: A.F. Henry, USA

D.E. Billington, G. Buffoni, E.H. Childs
D.K. Cooper, A. Galati, S. Gnattas,
F.M. McDonnell, R. Mosiello, A. Musco,
F. Norelli, T. Otsuka, K. Pörn, J. Sidell,
S. Tsunoyana

SURVEY OF THE RESULTS OF A ONE-DIMENSIONAL BENCHMARK PROBLEM TYPICAL FOR A THERMAL REACTOR

P.S. Christensen, F.J. Fayers, S. Langenbuch,
F.N. McDonnell, A. Schmidt, E. Vincenti,
H. Yoshikawa, W. Werner

SURVEY OF THE RESULTS OF A TWO- AND THREE-DIMENSIONAL KINETICS BENCHMARK PROBLEM TYPICAL FOR A THERMAL REACTOR

SURVEY OF THE RESULTS OF A ONE-DIMENSIONAL KINETIC BENCHMARK PROBLEM TYPICAL FOR A THERMAL REACTOR
I INTRODUCTION

There is a growing awareness of the need to improve representational details and accuracy in computing the fault and operational transient behaviour of nuclear power reactors. The problems involved, however, are significant since the solutions of kinetic equations involving all the relevant feedback phenomena in a multi-dimensional representation of a whole reactor are not readily achievable with current computer systems. In these circumstances there is a need to pursue numerical and computer techniques which offer improvements in solution time and cost. Furthermore, since this is a common basic goal of many national laboratories, the pooling of relevant experience and research is beneficial.

In order to stimulate mutual interest in this area, the Nuclear Energy Agency Committee on Reactor Physics has assembled a series of 'benchmark' kinetic problems and has invited workers in the field to attempt their solution with a view to subsequent exchange of experience and inter-comparison of performance of the computer models used.

This paper reviews the contributions submitted to a series of one-dimensional problems conceived as a starting point for subsequent multi-dimensional problems. The aim in setting the problems (which are detailed in the attached note) has been to focus attention on promising methods of solution so that no 'real' reactor problem or simulation is implied. The problems contain a simplified form of reactivity feedback in an axial core representation with reflectors and a controller. The basis of the problem is to compute an initial steady state and then to follow a transient caused either by moving the control rod or by varying cross-section.

In response to this series of problems, nine submissions were returned from various interested parties solving some or all of the cases. Section II of the paper lists the submissions received and summarises the codes and methods used.

In Section III the quantitative results of the nine submissions are given. The results and methods used are compared and discussed in Section IV.
Many of the methods used for the solution of the benchmark cases are relatively new, in the sense that either they incorporate some new feature, based on an existing method or else they contain some improved method of solving resulting sets of equations. This introduction contains a brief summary of the basic methods from which the benchmark set have been derived.

1) **Finite Difference**

This method, dating back to classical numerical analysis, attempts to approximate the time dependent diffusion equation by representing the spatial and time derivatives as a local sum of flux values, which matches the Taylor series of the variables up to some required order. In general, the smaller the spacing between the flux values and the larger the number of terms retained in the sum, the more accurate the representation will become.

The diffusion equation ultimately reduces to a set of algebraic equations, the solution of which forms the basis of the codes.

Points in favour of such methods are that the differences give a true representation of the equations in the sense that in the limit the exact solution will be obtained, and that the method will work equally well on any reactor configuration. Points against these methods are that in general many equations are required to obtain an adequate representation of the physical situation and that the solution of these equations may be costly in computer time.

2) **Adiabatic Method**

This method assumes that at every instant, during a transient, the flux shapes can be obtained by static calculations. The space-time flux can then be represented as a product of an amplitude function depending on time only and a spatial function representing the flux shapes at the particular time, produced by solving the steady state equations of current conditions.

The diffusion equation ultimately reduces to a set of ordinary differential equations in time for the amplitude functions, and a set of static equations, usually solved by finite difference methods, in the spatial co-ordinates.

This method is relatively fast in computing time but has the drawback that the static flux shapes may not in general be good approximations to the true flux shapes at any particular time, especially when feedback terms are present.

3) **Synthesis Methods**

In these methods the flux is decomposed into a sum of products of amplitude functions and spatial functions. This has the advantage over the adiabatic method in the sense that all that is required of the spatial functions is that a linear combination of them be a good approximation to the true flux shapes. The diffusion equation ultimately reduces to a set of ordinary differential equations for the amplitude functions. The trial spatial functions are chosen to satisfy reasonable estimates of reactor conditions which bracket those actually to be experienced.

The appeal of flux synthesis methods resides in their ability to partition a multi-dimensional problem into a sequence of simpler problems thus providing a means of obtaining a multidimensional solution, albeit an approximate one, in a degree of detail which is impossible or economically impracticable with a direct solution.

The question of how many trial functions to use in the approximation frequently occurs. The accuracy of the representation depends very strongly on which trial functions and how many, are chosen.
KINAX is a one-dimensional one-group reactor kinetic program. Up to six delayed neutron groups are included. Special facilities of the code include reactor tripping initiated by outlet temperatures and an elaborate heat transfer model. Transient calculations can be continued from a previous run without recomputation. The model incorporates a fixed optional time step between output points.

METHODS

The time-dependent solutions of the diffusion and heat transfer equations are computed using the Crank-Nicholson finite difference technique to produce tridiagonal matrix difference equations which are solved directly. The delayed neutron precursors are treated differently. The precursor equations are integrated by parts assuming that the gradients of the prompt neutron fluxes are constant over a time step, and the resulting expressions are substituted into the diffusion equations. The values of the precursors are updated only once for each time step after the prompt flux solution has converged.

REFERENCE

ELLIS J. The KINAX One-dimensional Reactor Kinetic Program KINAX 3. CD/NS/11, NPCC/RKMP/P286, August 1963

NAKIN is a one-dimensional code for the solution of the time dependent multi-group neutron diffusion equations. The neutronic calculation is coupled with the feedbacks due to the temperature effects on the cross-sections. The code incorporates an automatic adjustment of the time step. There are options on the number of energy groups, number of mesh points, number of material regions.
and number of delayed neutrons, but is subject to maximum dimensions on all.

METHODS

There is no English write-up of this code but the numerical methods are based on those used in the code GAKIN.

The multi-group neutron diffusion equations are centrally finite differenced in the spatial dimensions and the set of differenced equations is treated as a large set of simultaneous ordinary differential equations in time, one equation for each flux and precursor group at each mesh point. The scattering and absorption in group terms are collated with the time derivative to impose a pure exponential factor on the neutron group fluxes and presursors at each space point.

The resulting equations are integrated over a time step by assuming that the new variables behave in a purely exponential form with a decay rate equal to that of the thermal flux. This rate, at each space point, is computed from two adjacent time values of the thermal flux. The resulting form is exact in the case of constant reactivity.

The coolant temperature equations are solved by the Crank-Nicholson finite difference scheme.

REFERENCE


3 CENS

SUBMISSOR: S Grattas
Service d'Etudes des Reacteurs et de Mathematiques Appliques
CEA, Saclay
BP No 2
91190 GIF-SUR-YVETTE
France

CASES SUBMITTED: C

COMPUTER: IBM 360/91 (Equivalent to IBM 370/165 at CENS estimate)

CODE: CINTAX

CINTAX is a code to solve the one-dimensional, two-group, time-dependent neutron diffusion equation with fuel temperature feedback. At present CINTAX is still in the stage of development and is not as yet in its optimal form. The benchmark submission is by way of a test on the code.

METHODS

As no write-up exists, there is little knowledge of the methods employed in CINTAX. The only information available is that it is a discontinuous time synthesis model.
ADEP is a one- or two-dimensional code to solve the time-dependent few-group neutron diffusion equations. A special feature of the code is full variable dimensioning on the number of energy groups, number of delayed precursors, number of regions and number of mesh points.

A steady state subroutine is included and may be used to calculate the initial conditions, adjoint fluxes and point kinetics parameters for a given configuration.

The time step size may be varied but the code does not have an automatic choice.

**METHODS**

The time dependent diffusion equation is solved by the alternating direction explicit method or, as an option, the exponentially transformed alternating direction explicit method.

The alternation occurs at each time step. The finite difference equations are arranged so that at odd time steps the flux values are found at each space point one by one from the bottom of the reactor from those immediately preceding at the same time step and those immediately succeeding at the previous time step. While at even timesteps, the computation reverses and proceeds from the top of the reactor to the bottom. The prompt neutron group fluxes are centrally averaged in time and the multi-group equations are solved by Gaussian elimination for each space point.

In order to cut down on the number of equations, the delayed neutron precursors retain the values held at the previous time step and these are updated when the fluxes have been computed.

The temperature feedback equations are solved exactly assuming that the power generated is constant at its mean value, over each time step.

**REFERENCE**

CYCLOPS is a new code for the solution of the multi-group time dependent neutron diffusion equations. There is as yet no write-up of the code, its facilities or method of use.

METHODS

The method of solution is an improved quasi-static method. The flux is decomposed into an amplitude function of time and a spatial flux shape. The spatial shape is initially computed and updated, as necessary, by a source calculation. The adjoint flux is computed at the initial state and is then held for the future source calculations. The time dependent amplitude function is found from a point kinetics model.

The temperature equations are solved by a piecewise polynomial representation. The temperature equations are resolved into two separable vectors by a similarity transformation, which has a purely exponential and independent form.

TRANS is a code for the solution of the two-group time dependent neutron diffusion equation. The code has been specially designed to produce accurate solutions with a moderate calculational effort.

METHODS

At present there is no report on the numerical methods employed in TRANS. In general all the differential equations are solved by unconditionally stable implicit methods with iterative sharpening of the accuracy for each time step. All time derivative terms are retained in the solution.
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Km 1+3005 Maria di Galeria
ROME

CASES SUBMITTED: A, B, C, D

COMPUTER: IBM 360/75 (Factor 2 slower than IBM 370/165; based on
CRNL estimate of CDC 6600 and IBM Year Book 1970 estimate
of IBM 370/165 and CDC 6600)

CODE: NADYP-A

NADYP-A is a two-dimensional code to solve the time dependent few group neutron
diffusion equations. The reactor is described in r,z geometry. The thermo-
dynamic model involves an appropriate subdivision of the reactor in any number
of radial shells, any one of which is described by a single channel model.

METHODS

The steady state equations are solved by assuming that the fluxes are a sum of
trigonometric and/or Bessel functions.

The time dependent neutron diffusion equations are solved by the metastatic
method. The metastatic method is an offshoot of the adiabatic method. It
assumes that the group fluxes can be decomposed into the product of an ampli-
tude function depending only on time, and a shape function to be determined by
static calculations. The static source calculations are achieved by one of
an option of two fast converging iterative schemes, one of which always con-
verges when the other diverges. The amplitude function is found from a point
kinetics model, which differs from the adiabatic model in that the unperturbed
adjoint fluxes at the current time replace the asymmetric ones. These
approximations imply a lower limit on the size of step length.

The heat equations are solved by the method of characteristics.

REFERENCE

GALATI A. The Metastatic Method in Nuclear Reactor Core Kinetics

UK-WIN

SUBMISSOR: J Sidell
UKAEA
AEE Winfrith
DORCHESTER
Dorset

CASES SUBMITTED: A, B, C, D

COMPUTER: KDF 9 (Factor 10 slower than IBM 370/165 at UK-WIN
estimate)
EXTRA is a code for the solution of a set of initial value ordinary differential equations. The code incorporates an automatic choice of step length.

METHODS

The time dependent neutron diffusion equations are centrally finite differenced in space. The coolant temperature equation is backward differenced and the resulting set of equations is treated as a large set of ordinary differential equations. A pure exponential transformation is made on each equation of the set, which is designed to minimise the sum of squares of eigenvalues of the system. The method then uses a simple one step method to cross an interval of time, which is then repassed with halving time steps. The end interval results of these steps are extrapolated with Romberg-type extrapolations.

UK-AN

SUBMISSOR: E H Childs
UKAEA
ABB Winfrith
DORCHESTER
Dorset

CASES SUBMITTED: A, D

COMPUTER: PACE Analogue (Real time comparison with IBM 370/165)

METHODS

All neutron flux and temperature equations were centrally finite differenced in space. The resulting set of equations are then treated as a large set of ordinary differential equations. The delayed neutron precursor equations were condensed into groups. The time dependent equations were then integrated by analogue techniques.

The steady state was computed by the program SIMES which treats the resulting spacial difference equations as a set of algebraic equations and solves by the Newton-Raphson technique.

III CASE COMPARISON

In each of cases A, C and D, the tabular output from each submissor is listed. The results have been rounded to the least accurate of those quoted in order to make comparison easier.

The best solution of the cases has been taken as the average value of those submitted. Since the only available code which was capable of obtaining answers to a high degree of precision was also one of the submissions, any attempt at obtaining an exact solution must then have been biased towards the answers obtained, and would therefore have given an unfair advantage. The average value is, of course, not the true solution, so percentage deviations from the average, unless large in magnitude, should not be in any way related to the accuracy of any code or solution but merely act as a qualitative guide.

Similarly the relative timings must suffer from the same criticisms. Inter-computer comparison is a well known difficulty. The only true comparison of
times would be to run each code and case, written comparably efficiently in the
same language, through the same computer on the same machine to the same
accuracy. In many cases the relative machine comparisons were supplied by the
submissions, however, where omitted relative timings by other means were
obtained, these at times were severely inaccurate. Thus the relative timings
quoted may be a factor of two or perhaps three out either way in magnitude.

For the submissions which did not complete the transients in the cases, for
various reasons, the times have been scaled up linearly to produce the relative
timing. This, in fact, is a little harsh on these submissions because in
cases A, C and D the transients are tending towards a steady state, so that the
actual time steps used can be lengthened as the approach is made. These
timings may then be read only as an estimated upper bound of the actual time
which would have been taken to complete the transient.

The average deviation of all submissions from the mean was 4% in Case A. This
indicates that the majority of codes coped well with the slow moving control rod.

The fastest result was obtained by UK-WIN but this appears to be a case of the
quicker result producing the least accurate solution. Although the average
deviation from the mean was only 5.7% at the time of 50 seconds, when the
control rod is still moving the average deviation becomes 11.0% with a maximum
of 21.7% on the thermal flux. The cost of improving the accuracy on this case
would be great for reasons which will be deferred to the discussion of the
NAEC entry.

The CEGB one-group code shows up very favourably. However, the advantages in
finite difference solution in one group over two groups is well known.
Although the number of flux equations would only double, the tridiagonal struc-
ture of the spatial matrix would expand into a five-band, three-block structure
which is not amenable to the one-elimination-down and one-elimination-up
Gaussian method of solution. There appears, however, to be a factor of two
in the time ratio between this and the next solution time so allowing that the
small 2.9% deviation from the mean is at least some indication that fewer time
steps could have been taken. It is far from inconceivable that a multi-group
code based on these methods would be slower than the other multi-group entries.

There can be no criticism or defect in the next three fastest submissions - UK-RIS,
ABA and CSN. The results tie in very closely together with the average span
covering only 2%.

The UK-RIS result is the fastest of the three but the ABA results lie nearer
the absolute mean at only a fraction more time. As a general trend all three
results are higher than the mean for all variables, the IFA result being the
smallest in magnitude. The solution by ABA is by a fully stable implicit method.
This would tend to suggest that since the transient of this case is rising, the
fully implicit methods, if classical, tend to overestimate the time solution.
(This is born out by the mean value.) Therefore, if the steps of the ABA
method are increased in magnitude the error would increase in a positive sense
and the result tend upwards towards the UK-RIS results at some less cost.
This suggests that the two codes of UK-RIS and ABA have produced results
both in accuracy and speed which are very comparable.

The CSN time is approximately a factor of two up on the other two. There is no
indication of the relevant steady state solution time, so how much is transient
solution cannot be estimated, but by comparison with the trends of the other
codes it would not appear to be any great amount. The metastatic method
requires an eigen-solution for the adjoint flux at points in the transient as
well as the neutron flux. The UK-RIS code requires only the neutron flux.
If one can guess that the flux calculations take up the bulk of the computation time, and that both UK-RIS and CSN have computed the flux solutions approximately often, then the factor of two may be accounted for. It may well be that this case has been too much over-simplified in that the adjoint flux at the initial state could be a perfectly good enough estimate for all points of the transient and that recomputation during the transient is unnecessary.

For more complex configurations and transients the differences in accuracies and timings may well be diminished.

The analogue computer results (UK-AN) are, on average, farthest away from the mean value. This is probably due to an inadequate representation of the spatial mesh. Analogue integration is in general more efficient than digital integration but the large digital memory stores are more readily adaptable to the solution of large sets of equations.

The CRNL result was surprisingly slow. On paper it seemed that this code would produce the fastest step turn-round time of all. The methods are designed for a speedy solution so that it can only be surmised that a lot of time steps or mesh points were taken. The methods employed are purely explicit and thus should underpredict the rising true solution. This is again borne out by comparison with the mean value. The CRNL results are the most accurate of the under-predicted methods and thus the number of steps or mesh points could be reduced to produce comparable accuracies. However, a factor of nine or so is probably asking far too much.

The NAIG result was the slowest. In many ways this case was harsh on a code of this form. The method employed is exponentially dominated with the factor being chosen from successive thermal flux values. This factor is necessarily real, however, as the driving eigenvalue of Case A is complex, producing small oscillations. The exponential factor computed by the code, therefore, will not give any gain to the truncation error and in all probability will worsen the effect, so that shorter steps would have to be taken than on a similar code without exponential transformations. (This reasoning tends to suggest that the UK-WIN entry's time could well escalate when tighter accuracy is forced.) The NAIG code incorporates an automatic time step. However, since case A is strongly stable and the error after a large number of steps bears little relationship to the step by step error, ie whatever the step length chosen, and however inaccurate the steady state solution is, the result from any stable methods must reach the steady state at infinite time, simply because there is nowhere else the transient can go. Therefore, in the main, a step by step criterion will only slow down the computation rate and demand more steps than are necessary for a point to point comparison.

This case could well point out some of the dangers of exponentially based methods. An interesting point to note is that the metastatic method does not fall down over this point. Since, although there is an exponential weighting on the eigenfunction flux, the complex eigenvalue, which arises due to the feedback effect between flux and temperature, is retained through the point kinetics relationship and temperature solution without the imposed exponential factor dominating.

Case C follows the same patterns as Case A. The CEGB one-group code was again twice as fast as its nearest competitor and the same remarks apply. The results were very close to the mean value, as in Case A.

The comparability in performance between UK-RIS and ABA is even more underlined. The similarity between results and timings is very noticeable and they form almost a perfect match.
This time the CSN result was 25% slower than the UK-RIS result but the deviation from the mean is twice that of the other two, and is practically the same as that attained in Case A.

The CENS submission takes the next place in time order. As this was the only entry from CENS, comments will have to be restricted to this case. The results quoted for \( t = 200 \) are in fact at \( t = 190 \) (the limit of their integration) but as the transient at this stage is practically at its steady state the difference should be negligible. Secondly, the time quoted for CENS must be overestimated as the time step to cover the last 110 seconds could be very large. This therefore puts the CENS code at a speed comparable to CSN at a similar accuracy. Since the code is still in the development stage the results may be described as very encouraging.

The CRNL results are some way out of line compared with the others. Most noticeable are the flux values at \( t = 50 \) and 100, and the corresponding coolant outlet temperatures. This would tend to suggest, contrary to Case A, that the step lengths in space or time would have to be tightened up, but the timing suggests that much computational effort has been expended. It is difficult to believe that any step approximations made in the code could produce truncation errors of this magnitude even though the transient is rising rapidly.

The NAIG result was again slow. This seems to be for the same reasons as in Case A. The maximum value of \( T_{\text{max}} \) at the steady state is noticeably different from the other submissions. The stated value was transmitted to the other cases. However, as Case C returns to its original steady state, which NAIG states as a different result, the initial value has been taken as a mis-read/type rather than any inaccuracy.

The UK-WIN result this time was the slowest. The values produced are a little more evenly near the average value although the fluxes seem on average quite a bit high. The time taken has escalated rapidly suggesting that the exponential method found some degree of difficulty in coping with the pronounced oscillation.

Whereas in Cases A and C the mean value served some useful purpose, the same cannot be said about Case D. The flux solutions are so widely dispersed and the submissions so few that the norm need not be anywhere near the true solution. It is a pity that this case did not attract more entries as it gives such widespread results. However, since the transient was caused by varying a particular cross-section, rather than rod movement, the paucity of cases was due to lack of facility, rather than trouble with any of the methods. Consequently, not too much may be said about accuracy of solution in this case.

The most rapid solution was obtained by CSN who were also nearest to the mean, if this can be indicative, and rounds off a very reliable set of results for all cases.

The analogue real time solution produced temperature results close to the other values. The fluxes were not included in the output results because the fall through many decades produced the loss of too many figures in the solution.

The UK-WIN result was quicker this time but it is noticeable that the temperatures are at all points higher than the corresponding other entries.

The CRNL result was slow again in comparison. The results, however, seem reasonable.
The NAIG result was slowest. This time it is slightly surprising. The equations still have the complex eigenvalue but from the graphical output it appears that the solution curves lack the oscillatory form of Cases A and C. Therefore, one would suspect some gain in the NAIG result time over their previous cases, but the run time is slowest of all in Case D.
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**Mean Difference**

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| Tip Position | 249 | 247 | 246 | 258 | 250 | 245 | 247 | 217 |

| Year Difference | 6 | 5.7 | 5.7 | 2.9 |

**Approx Relative Timestep (sec)**

<table>
<thead>
<tr>
<th>Steady State</th>
<th>210</th>
<th>328</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transient</td>
<td>900</td>
<td>37</td>
</tr>
</tbody>
</table>
CASE B

Comparison of $\Theta^1, \Theta^2, T_{f,\text{max}}$ at $t = 10$ secs and times at which $\Theta^1$ reaches $10^{15}$

<table>
<thead>
<tr>
<th></th>
<th>CSN</th>
<th>NAIG</th>
<th>CRNL</th>
<th>ABA</th>
<th>UK-WIN</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{f,\text{max}} (150)$</td>
<td>2350</td>
<td>2500</td>
<td>2200</td>
<td>2400</td>
<td>2100</td>
</tr>
<tr>
<td>$\Theta^2 (150)$</td>
<td>$8.0 \times 10^{14}$</td>
<td>$1.8 \times 10^{15}$</td>
<td>$2.7 \times 10^{14}$</td>
<td>$7.8 \times 10^{14}$</td>
<td>$2.3 \times 10^{14}$</td>
</tr>
<tr>
<td>$\Theta^1 (150)$</td>
<td>$1.2 \times 10^{15}$</td>
<td>$1.8 \times 10^{15}$</td>
<td>$4.6 \times 10^{14}$</td>
<td>$1.3 \times 10^{15}$</td>
<td>$4.4 \times 10^{14}$</td>
</tr>
<tr>
<td>$T_{f,\text{max}} (250)$</td>
<td>2100</td>
<td>2000</td>
<td>1900</td>
<td>2200</td>
<td>2100</td>
</tr>
<tr>
<td>$\Theta^2 (250)$</td>
<td>$5.5 \times 10^{14}$</td>
<td>$2.8 \times 10^{14}$</td>
<td>$2.3 \times 10^{14}$</td>
<td>$6.5 \times 10^{14}$</td>
<td>$2.2 \times 10^{14}$</td>
</tr>
<tr>
<td>$\Theta^1 (250)$</td>
<td>$8.0 \times 10^{14}$</td>
<td>$5.0 \times 10^{14}$</td>
<td>$4.2 \times 10^{14}$</td>
<td>$1.1 \times 10^{15}$</td>
<td>$3.9 \times 10^{14}$</td>
</tr>
<tr>
<td>$T (150) \Theta^1 = 10^{15}$</td>
<td>9</td>
<td>9</td>
<td>17</td>
<td>9</td>
<td>32</td>
</tr>
<tr>
<td>$T (250) \Theta^1 = 10^{15}$</td>
<td>11</td>
<td>18</td>
<td>17</td>
<td>10</td>
<td>34</td>
</tr>
<tr>
<td>Rel time per 10 sec trans</td>
<td>20</td>
<td>215</td>
<td>472</td>
<td>17</td>
<td>94</td>
</tr>
</tbody>
</table>

Case B proved to be the most difficult to analyse, since the variables rose so sharply that no requested tabular points were reached before the submitters terminated their transients. To obtain some feel for this case, the above table was read from the submitted graphs, therefore there is liable to be some marked error in the results quoted. For this reason, the comments on case B have been detached from the rest of the cases.

The general trend of this case, however, is much the same as in the cases already discussed. The two most rapid codes of ABA and CSN produced results which were very close. Owing to the difficulties in reading values it is impossible to distinguish between the performances.

The UK-WIN solution produced the slowest rate of transient rise, and judging by the other submissions required more accuracy and hence more computing time.

The NAIG result was slow, this time inexplicably. The real eigenvalues of the system, should favour the exponential methods, but the timings, being a factor of ten down, do not indicate that this is the case.

The CRNL time was the slowest on this case. The results also appear to be a fraction low in magnitude, indicating that more accuracy would be required.

The differences between the explicit and implicit methods were highlighted more readily in this case. The three explicit solutions of NAIG, CRNL and UK-WIN produced the slower rates of rise of transient, while the fully implicit ABA and at least semi-implicit CSN solutions produced the sharpest rises. This tends to suggest that the true solution of case B must lie somewhere between these two sets of results.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Tem</th>
<th>Mean</th>
<th>CEN</th>
<th>CEC</th>
<th>UE-31S</th>
<th>UE-29N</th>
<th>ABA</th>
<th>NAIG</th>
<th>CENS</th>
<th>CLUB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cooler</td>
<td>0</td>
<td>600</td>
<td>800</td>
<td>800</td>
<td>800</td>
<td>800</td>
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<td>800</td>
</tr>
<tr>
<td>Outlet Temperature</td>
<td>50</td>
<td>667</td>
<td>867</td>
<td>800</td>
<td>804</td>
<td>830</td>
<td>894</td>
<td>867</td>
<td>873</td>
<td>874</td>
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<td>100</td>
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<td>816</td>
<td>760</td>
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<td>521</td>
<td>819</td>
<td>828</td>
<td>836</td>
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<tr>
<td></td>
<td>150</td>
<td>801</td>
<td>800</td>
<td>805</td>
<td>801</td>
<td>801</td>
<td>801</td>
<td>801</td>
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<td>800</td>
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<td>800</td>
<td>800</td>
<td>800</td>
<td>800</td>
<td>800</td>
<td>800</td>
</tr>
</tbody>
</table>

| $T_{r, max}$ (350) | 0    | 104.7| 1050| 1031| 1047   | 1064   | 1044| 1043 | 1040 | 1055 |
|                   | 50   | 1420 | 1456| 1104| 1146   | 1122   | 1235| 1244 | 1326 | 1359 |
|                   | 100  | 1227 | 1236| 1054| 1134   | 1110   | 1129| 1120 | 1177 | 1199 |
|                   | 150  | 1052 | 1052| 1018| 1050   | 1067   | 1058| 1056 | 1044 | 1055 |
|                   | 200  | 1051 | 1051| 1015| 1047   | 1064   | 1044| 1043 | 1042 | 1055 |

| $T_d$ (350) | 0    | 884  | 844 | 844 | 844    | 843    | 844 | 844  | 844  | 844  |
|             | 50   | 955  | 976 | 976 | 978    | 933    | 869 | 867  | 865  | 868  |
|             | 100  | 863  | 871 | 864 | 872    | 870    | 869 | 867  | 865  | 868  |
|             | 150  | 866  | 815 | 815 | 815    | 814    | 814 | 814  | 814  | 814  |
|             | 200  | 845  | 844 | 844 | 844    | 843    | 843 | 843  | 843  | 843  |
|             | 250  | 845  | 844 | 844 | 844    | 843    | 843 | 843  | 843  | 843  |

| $\beta^1$ (350) | 0    | 7.5 10^13 | 7.2 10^13 | 7.2 10^13 | 7.6 10^13 | 8.0 10^13 | 7.5 10^13 | 7.5 10^13 | 7.1 10^13 | 1.2 10^14 |
|                 | 50   | 6.8 10^13  | 6.4 10^13  | 3.4 10^13  | 7.0 10^13  | 8.8 10^13  | 7.0 10^13  | 7.0 10^13  | 6.9 10^13  | 1.2 10^14  |
|                 | 100  | 8.1 10^13  | 7.0 10^13  | 1.0 10^14  | 7.5 10^13  | 8.5 10^13  | 7.4 10^13  | 7.4 10^13  | 9.2 10^13  | 1.2 10^14  |
|                 | 150  | 7.5 10^13  | 7.2 10^13  | 7.0 10^13  | 7.6 10^13  | 7.9 10^13  | 7.5 10^13  | 7.5 10^13  | 7.1 10^13  | 1.2 10^14  |
|                 | 200  | 7.5 10^13  | 7.2 10^13  | 7.0 10^13  | 8.0 10^13  | 8.0 10^13  | 7.5 10^13  | 7.5 10^13  | 7.1 10^13  | 1.2 10^14  |

| $\beta^2$ (350) | 0    | 3.8 10^13  | 3.9 10^13  | 3.5 10^13  | 3.8 10^13  | 4.0 10^13  | 3.7 10^13  | 3.7 10^13  | 3.5 10^13  | 1.2 10^14  |
|                 | 50   | 3.6 10^13  | 3.5 10^13  | 1.8 10^13  | 3.5 10^13  | 4.6 10^13  | 3.5 10^13  | 3.5 10^13  | 3.5 10^13  | 1.2 10^14  |
|                 | 100  | 4.1 10^13  | 3.8 10^13  | 5.2 10^13  | 3.7 10^13  | 4.3 10^13  | 3.7 10^13  | 3.7 10^13  | 4.8 10^13  | 1.2 10^14  |
|                 | 150  | 3.8 10^13  | 3.9 10^13  | 3.4 10^13  | 3.2 10^13  | 4.1 10^13  | 3.7 10^13  | 3.7 10^13  | 3.5 10^13  | 1.2 10^14  |
|                 | 200  | 3.8 10^13  | 3.9 10^13  | 3.4 10^13  | 4.0 10^13  | 3.7 10^13  | 3.7 10^13  | 3.7 10^13  | 3.7 10^13  | 1.2 10^14  |

| Position of $T_{r, max}$ | 0    | 152  | 110 | 110 | 110    | 110    | 110 | 110  | 110  | 110  |
|                           | 50   | 177  | 130 | 130 | 130    | 130    | 130 | 130  | 130  | 130  |
|                           | 100  | 154  | 120 | 120 | 120    | 120    | 120 | 120  | 120  | 120  |
|                           | 150  | 154  | 120 | 120 | 120    | 120    | 120 | 120  | 120  | 120  |
|                           | 200  | 154  | 120 | 120 | 120    | 120    | 120 | 120  | 120  | 120  |

| Cool Tip Position | 248  | 247  | 246 | -    | 256    | 250   | 247 | 246  | 247  | 247  |
|                   |      |      |     |      |        |       |     |      |      |      |
| Relative Error %   | 4.5  | 9.9  | 2.3 | 5.8  | 2.0    | 3.4   | 4.7 | 2.7  | 4.7  | 2.7  |

| Steady State       | 1    | 4    | 65  | 1    | 6     | 3    | 25  |      |      |      |
|                    | 500  | 156  | 1299| 157  | 1250  | 204  | 61  |      |      |      |

<table>
<thead>
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<th>Approx Relative Timings (sec)</th>
<th>Steady State</th>
<th>Transient</th>
</tr>
</thead>
<tbody>
<tr>
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<td>156</td>
</tr>
<tr>
<td></td>
<td>1299</td>
<td>157</td>
</tr>
<tr>
<td></td>
<td>1250</td>
<td>204</td>
</tr>
<tr>
<td></td>
<td>61</td>
<td></td>
</tr>
<tr>
<td>PARAMETER</td>
<td>TIME</td>
<td>MEAN</td>
</tr>
<tr>
<td>-----------</td>
<td>------</td>
<td>------</td>
</tr>
<tr>
<td>Coolant Outlet Temperature</td>
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<td>800</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>556</td>
</tr>
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<td></td>
<td>100</td>
<td>392</td>
</tr>
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<td></td>
<td>200</td>
<td>311</td>
</tr>
<tr>
<td>T_{max} (350)</td>
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<td>1036</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>814</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>524</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>328</td>
</tr>
<tr>
<td>T_s (350)</td>
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</tr>
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<td>50</td>
<td>588</td>
</tr>
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<td>100</td>
<td>406</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>312</td>
</tr>
<tr>
<td>( \beta^1 ) (350)</td>
<td>0</td>
<td>7.5E+13</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>3.5E+12</td>
</tr>
<tr>
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<tr>
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<td>200</td>
<td>3.0E+10</td>
</tr>
<tr>
<td>( \beta^2 ) (350)</td>
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<td>3.8\times10^{13}</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>1.4\times10^{12}</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>8.0\times10^{10}</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>3.3\times10^{8}</td>
</tr>
<tr>
<td>Position of</td>
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<td>164</td>
</tr>
<tr>
<td>max T_{max}</td>
<td>50</td>
<td>193</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>352</td>
</tr>
<tr>
<td></td>
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<td>481</td>
</tr>
<tr>
<td>Maximum Value of T_{max}</td>
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<td>2132</td>
</tr>
<tr>
<td></td>
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<td>1096</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>542</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>338</td>
</tr>
<tr>
<td>Rod Tip Position</td>
<td>249</td>
<td>247</td>
</tr>
<tr>
<td>Mean % Difference from Mean</td>
<td>14.3</td>
<td>22.1</td>
</tr>
<tr>
<td>Approx Relative Steady State Timings (sec)</td>
<td>160</td>
<td>72</td>
</tr>
<tr>
<td>Transient</td>
<td>1000</td>
<td>453</td>
</tr>
</tbody>
</table>
IV SUMMARY AND CONCLUSIONS

On the basis of the benchmark test, the two fastest and most reliable codes were the UK-RIS (CYCLOPS) and the ABA (TRANS). There does not appear to be much between the performance of these codes. Both codes are new in the sense that no write-ups exist for the methods used. The UK-RIS code, with modifications to permit interpolation of fluxes rather than full source solutions, could have permitted a faster solution of the benchmark problems. There are few details of the ABA code. The method appears to be some form of finite difference method. There does not appear to be any physical approximation in the solutions and since all time derivative terms are retained one assumes that some very fast solution of the implicit equations must take place.

Since no material is available, it is difficult to assess what makes these two codes perform so very well in comparison with the other submissions or whether the same degree of success can be obtained on two- or three-dimensional problems. This would probably form the basis of another benchmark test.

The CEGB one-group code (KINAX) performed very successfully on the benchmark cases. There is a factor of two in the time ratio between this code and its nearest multi-group neighbour. Many of the non-desirable properties of one-group solution would disappear if the code were converted to multi-group solution. Moreover, on the basis of the times and results produced, such a conversion could prove to be valuable.

The success of the quasi-static and metastatic type solutions was most apparent. There must be some doubt about whether this series of benchmark problems provided a real test of their efficiency; certainly from the submitted graphs only minor distortions of flux shape occurred during the transients. For this reason, the difficulties between the CSN code (NAIDP-A) and the UK-RIS code may not have been highlighted. Whereas the CSN code performed superficially at least; more slowly, the effort of computing adjoint fluxes at each spacial solution may well have been wasted in these problems. It may well be that the CSN code has certain advantages over the UK-RIS code which, although not immediately obvious, may become so under more complex situations.

The CENS code (CINTAX) on Case C performed favourably compared with the CSN code. The only details available are that it is a discontinuous time-synthesis method and that it is still in the development stage. The results produced are very encouraging.

The most puzzling point of this benchmark test was the slow computing speeds of the CRNL code (ADEP). The implicit codes of ABA and CEGB produced very fast solution times whereas the explicit and hence simpler algorithm of CRNL produced a much slower turnaround. One cannot see that the truncation errors between the methods would necessitate many more mesh points or time steps. In Case A, CRNL have, as far as can be told, an accurate result, but in Case C the results vary from other submissions in a similar amount of computing time as in Case A. Therefore, it cannot be said that the solutions have been made to a degree of over-precision. Perhaps something more fundamental may have been overlooked.

The exponential methods performed the worst. It is true that the benchmark cases A, C and D were not the ideal for methods of this type; but they performed equally badly on Case B where some sort of gain might be expected. Both the NAIG code (GAKIN) and the UK-WIN code (EXTRA) are similar in concept and so it is not surprising that the solution times and performance should be equally as good or bad. These were also the only codes which had an automatic time step and it would be interesting to compare these with another non-exponential code to see whether the automatic time step was a significant factor in the slow running times.
The analogue computer, UK-AN, provided an alternative slant to the methods of solution. However, with the increase in size and complexity of reactor modelling it is unlikely that this size of the analogue computer would be able to cope on its own. The answer to this problem could lie in hybrid computation.

The benchmark submissions did not give any clear cut sign of which of the various classes of method is to be preferred. Of the two most favoured, one was quasi-static and the other finite difference (assumed). On average the flux shape methods performed better than the finite difference techniques, which may be some indication that the more analytic type of methods are advantageous.

30 May 1974
ONE-DIMENSIONAL KINETICS BENCHMARK PROBLEMS

1 This note describes a series of 1-dimensional kinetic problems aimed at providing suitable testbed calculations for the various numerical and computational techniques currently in use for this type of problem. It has become usual to refer to this type of test calculation as a 'benchmark' calculation although the actual detail of the problem may be very simplified. We will continue to use the word 'benchmark' although recognising that the problems here are indeed much simplified. No relation with real reactors or problems is implied; the problems are chosen in order to explore numerical techniques using parameters which are regarded as plausible.

2 The following principal assumptions have been made in setting up the calculations:
   a Only 2 prompt neutron groups and 6 delayed neutron groups.
   b Temperature feedback in first group only.
   c Absorber effect in second group only.
   d Data constant within each material region in axial direction apart from movable control absorber and temperature-dependent data.
   e Radial leakage is ignored.

3 The model chosen is based on a system consisting of a fuel region with axial reflectors at both ends. Control absorber is inserted from one end only in a direction opposite to the coolant flow. At the beginning of each problem the absorber is assumed to be set at such a penetration that $k_{eff} = 1.0$ and the power level is defined by the inlet/outlet coolant temperatures and the heat transfer equations. Xenon variations are ignored. Equations defining the problem are given in Appendix 1 and the problem illustrated schematically in Fig 1. Definitions, notations and case independent values of parameters are given in Appendix 2.

4 It will be noted that the direct coupling between the first and second neutron groups is in 2 parts. Firstly we have the conventional fission source term appearing only in group 1 but arising from fission events in both groups. Secondly there is coupling from first to second group through a first group removal (slowing down) cross-section. Control absorber is in the second group only.

5 The simplified form of time-dependent feedback in the solution is introduced by having the first group absorption cross-section coupled to fuel temperature through the parameter $\alpha$. The sign of $\alpha$ determines the nature of the feedback. Depending on whether $\alpha$ is negative or positive, the eigenvalues of the system will be all real or may have imaginary parts.

6 Heat is generated by fission in the fuel in the active core; there is no heat source in either top or bottom reflectors. Heat is transferred from fuel surface to a perfect coolant and then transported out of the reactor. We have allowed the heat transfer data to be constant at all heights in the core and reflector. In principle this means that in the reflectors there is a small interchange of heat between the coolant and the 'fuel' material.
The following problems are proposed for this study. All start from a just critical state with absorber positioned at approx half insertion (see Appendix 3). As an alternative to searching for the just critical absorber position, the absorber may be positioned at these values of z and a standard eigenvalue search undertaken to define the steady state starting conditions.

CASE A: Rod withdrawal at fixed rate of 1 cm/sec (corresponding to a reactivity release of about 20 mN/sec). The feedback parameter α is positive so that cross-section increases with temperature. The problem run time is 300 sec.

CASE B: As Case A above except that the feedback parameter α is negative making the cross-section decrease with temperature and producing a 'run away' situation. Rod withdrawn for 100 sec and then held. The problem run time is 200 sec.

CASE C: As Case A above except that the rod withdrawal rate is 20 cm/sec for 10 sec and the rod is then returned to its initial position linearly in 1 sec. Feedback parameter α is positive. The problem run time is 300 sec.

CASE D: As Case A except that the rod remains fixed at its initial position. Transient is caused by a linear decrease in the first to second group transfer cross-section $\Sigma_{l\rightarrow 2}$ with time over a period of 200 sec. The problem run time is 200 sec.

The cases are defined more fully in Appendix 3.

CALCULATION AND PRESENTATION OF RESULTS

6 The aim of the current exercise is of course to compare the performance, in terms of results, costs, etc, of a number of alternative ways of solving these benchmark problems. In order to facilitate intercomparisons of results, they must be submitted in the fixed forms described in Appendix 4. Additionally, participants are asked to summarise the characteristics of codes used in a standard NEA CPL Abstract form and to provide run details in the format given in Appendix 5.

9 In the preparation of replies it is suggested that participants restrict the number to not more than 3 different sets corresponding to 3 different numerical techniques. Several sets generated by simply varying the solution tolerances should not be sent, although a view as to how the accuracy of the solution is affected by such changes would be useful. The results in which we are interested are those which the participants regard as the most satisfactory from a computing cost and solution accuracy point of view.

10 All results and figures and communications about data and results should be sent to:

Dr H Küsters
Kernforschungszentrum Karlsruhe
Institut für Neutronenphysik und Reaktortechnik
75 KARLSRUHE 1
Postfach 3640
West Germany

Results and figures should arrive before 1 May 1973.
APPENDIX I

THE EQUATIONS

1 NEUTRONICS

\[ \frac{1}{v} \frac{d\phi'}{dt} = D \frac{d^2 \phi'}{dz^2} - \Sigma' \phi' + (1 - \rho) \left[ v' \Sigma_f \phi' + v^2 \Sigma_f \phi^2 \right] + \sum_{i=1}^{6} \lambda_i c_i \]

\[ \frac{1}{v^2} \frac{d\phi^2}{dt} = D^2 \frac{d^2 \phi^2}{dz^2} - \Sigma^2 \phi^2 + \Sigma_{1+2} \phi' \]

\[ \frac{dC}{dt} = \rho_1 \left[ (v' \Sigma_f \phi' + v^2 \Sigma_f \phi^2) - \lambda_i c_i \right] \quad i = 1, \ldots, 6 \]

where \( \Sigma' = \Sigma_a' + \Sigma_{1+2} \); \( \Sigma_a' = \Sigma_{ao} (1 + a_{ao}) \); \( \Sigma^2 = \Sigma_a + \Sigma_c \)

2 HEAT REMOVAL

\[ K_f (T_f - T_s) = \nu_f \cdot (HFF) \cdot \left[ \Sigma_f \phi' + \Sigma_f \phi^2 \right] - C_f \cdot \frac{\partial T_f}{\partial t} \]

\[ T_f,_{\text{max}} = 2T_f - T_s \]

\[ K_f (T_f - T_s) = h(T_s - T_c) \]

\[ C_c \left[ \frac{\partial T}{\partial t} + \frac{\partial T}{\partial z} \right] = h(T_s - T_c) \]

NOTES:

1 For end reflector material \( vE_f = 0 \), \( c_i = 0 \) and \( \Sigma_{ao}' = 0 \)

2 \( z \) is measured in the direction of the core coolant flow.

3 The neutronics data are allowed to vary between the core and reflector regions. The heat transfer data do not vary.

4 All data are constant between the various cases posed except for the fast absorption cross section \( \Sigma_{ao}' \) and the feedback term \( \alpha \).
## APPENDIX 2

### NOTATION AND CASE INDEPENDENT PARAMETER VALUES

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi'$</td>
<td>First group neutron flux</td>
<td>cm$^{-2}$sec$^{-1}$</td>
<td>See Appendix 3</td>
</tr>
<tr>
<td>$\phi'^2$</td>
<td>Second group neutron flux</td>
<td>cm$^{-2}$sec$^{-1}$</td>
<td>-do-</td>
</tr>
<tr>
<td>$C_i$</td>
<td>Delayed neutron precursor concentration in group $i$</td>
<td>cm$^{-3}$</td>
<td>-do-</td>
</tr>
<tr>
<td>$\beta_i$</td>
<td>Delayed neutron yields in group $i$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\beta$</td>
<td>Decay constants for delayed neutron group $i$</td>
<td>sec$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$\lambda_i$</td>
<td>Delayed neutron yields in group $i$</td>
<td>sec$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$v'$</td>
<td>Mean neutron velocity in first group</td>
<td>cm/sec</td>
<td>2.10$^7$</td>
</tr>
<tr>
<td>$v^2$</td>
<td>Mean neutron velocity in second group</td>
<td>cm/sec</td>
<td>3.10$^5$</td>
</tr>
<tr>
<td>$D'$</td>
<td>Diffusion coefficient for neutrons in first group</td>
<td>cm</td>
<td>1.1</td>
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<tr>
<td>$D^2$</td>
<td>Diffusion coefficient for neutrons in second group</td>
<td>cm</td>
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<tr>
<td>$\Sigma_{10}$</td>
<td>Macroscopic absorption cross-section in first group (at 0°C)</td>
<td>cm$^{-1}$</td>
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<tr>
<td>$\alpha$</td>
<td>Feedback parameter</td>
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<td>$\Sigma_{1\rightarrow2}$</td>
<td>First group slowing down cross-section</td>
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### HEAT TRANSFER DATA

<table>
<thead>
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<th>Unit</th>
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<tr>
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<td>cm$^{-1}$</td>
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<tr>
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<td>Macroscopic absorption cross-section due to absorber</td>
<td>cm$^{-1}$</td>
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<tr>
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<td>Number of neutrons per fission in first neutron group</td>
<td></td>
<td>2.5</td>
</tr>
<tr>
<td>$\nu^2$</td>
<td>Number of neutrons per fission in second neutron group</td>
<td></td>
<td>2.4</td>
</tr>
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<td>$T_f(z,t)$</td>
<td>Mean fuel temperature</td>
<td>°C</td>
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<tr>
<td>$T_{f,max}(z,t)$</td>
<td>Maximum fuel temperature in radial plane</td>
<td>°C</td>
<td></td>
</tr>
<tr>
<td>$T_s(z,t)$</td>
<td>Fuel surface temperature</td>
<td>°C</td>
<td></td>
</tr>
<tr>
<td>$T_c(z,t)$</td>
<td>Coolant temperature</td>
<td>°C</td>
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<table>
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<tr>
<th>(HPF)</th>
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<th>10$^{-9}$</th>
<th>10$^{-9}$</th>
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<td>cal/cm°C sec</td>
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<td>0.5</td>
<td>0.5</td>
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<td>$C_f$</td>
<td>Thermal capacity of unit length of fuel</td>
<td>cal/cm°C</td>
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<td>$h$</td>
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<td>Thermal capacity of unit length of coolant</td>
<td>cal/cm°C</td>
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<td>$A$</td>
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<td>3000</td>
<td>3000</td>
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Length of top reflector = length of bottom reflector = 40 cm
Length of active core = 420 cm
STEADY STATE AND KINETIC BOUNDARY CONDITIONS

1 STEADY STATE AND BOUNDARY CONDITIONS

All transients are started from the steady state position (i.e., all time derivatives are set to zero).

Boundary conditions for the steady state calculations are:

a. The fluxes are zero at the edges of the reactor, i.e.,
\[ \phi'(0,0) = \phi'(500,0) = \phi^2(0,0) = \phi^2(500,0) = 0 \]
b. The coolant inlet and outlet temperatures are specified
\[ T_c(0,0) = 300^\circ \text{C} \quad T_c(500,0) = 800^\circ \text{C} \]
c. The initial rod insertion and initial values of fluxes, delayed neutron precursors, and temperatures are obtained from the steady state.

Boundary conditions for the transient calculations are:

d. The neutron fluxes are assumed zero at the ends of the reactor, i.e,
\[ \phi'(0,t) = \phi'(500,t) = \phi^2(0,t) = \phi^2(500,t) = 0 \]
e. The coolant inlet temperature is specified
\[ T_c(0,t) = 300^\circ \text{C} \]

2 TRANSIENT CASES

CASE A: Rod withdrawal: negative temperature feedback on reactivity
\[ \alpha = 0.0002 \degree \text{C}^{-1}; \quad \Sigma' = 0.00086 \quad \text{(Initial absorber tip position} \ z = 246.735 \text{ cm)} \]
From the steady state position the rod is withdrawn at a rate of 1 cm/sec until the rod tip reaches the core/reflecter boundary and is then held fixed. Transient time is 300 sec.

CASE B*: Rod withdrawal: positive temperature feedback on reactivity
\[ \alpha = -0.00002 \degree \text{C}^{-1}; \quad \Sigma'_{Ao} = 0.0012 \quad \text{(Initial absorber tip position} \ z = 293.39 \text{ cm)} \]
From the steady state position the rod is withdrawn at a rate of 1 cm/sec for 100 sec and is then held fixed. Transient time is 200 sec.

CASE C: Rod blowout: negative temperature feedback
\[ \alpha = 0.0002 \degree \text{C}^{-1}; \quad \Sigma'_{Ao} = 0.00036 \quad \text{(Initial absorber tip position} \ z = 246.735 \text{ cm)} \]
The rod is blown out at a rate of 20 cm/sec for 10 sec and is then returned to its initial position linearly in 1 sec where it is held fixed. Transient time is 300 sec.

*Absolute value of \( \alpha \) differs by a factor of 10.
CASE D: Loss of moderator: negative temperature feedback

\[ \alpha = 0.0002 \, ^\circ\text{C}^{-1}; \quad \Sigma_{ao} = 0.00086 \, \text{cm}^{-1} \]  
(Initial absorber tip position \( z = 246.735 \, \text{cm} \))

The rod is held stationary at its initial value: the removal cross-section \( \Sigma_{l\rightarrow 2} \) is reduced linearly over 200 sec

\[ \Sigma_{l\rightarrow 2}(z,t) = \Sigma_{l\rightarrow 2}(z,0) \left[ 1 - \frac{t}{200} \right] \, \text{cm}^{-1} \]  
for \( t \leq 200 \, \text{sec} \) for all \( z \)

Transient time is 200 sec.
APPENDIX 4

RESULTS TO BE PRESENTED

1 DIGITAL RESULTS for all the specified cases to provide a summary of the transient:

<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>Coolant Outlet Temperature (°C)</th>
<th>At z = 350 cm</th>
<th>Maximum Value and Position of $T_{f, \text{max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 Initial Value</td>
<td></td>
<td>$T_{f, \text{max}}$</td>
<td>$T_s$</td>
</tr>
<tr>
<td>50</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100</td>
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<td></td>
<td></td>
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<tr>
<td>300*</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Cases A and C

Absorber tip position at $t = 0$ is $z = \ldots$ Cases A, C and D

Absorber tip position at $t = 0$ is $z = \ldots$ Case B

2 GRAPHICAL RESULTS to be presented on translucent graph paper, log 5 cycles x mm for all graphs.

Five graphs should be presented for each case:

- Graph 1 should plot $T_{f, \text{max}}$, $\phi'$, $\phi^2$ as a function of $z$ at $t = 0$
- Graph 2 should plot $T_{f, \text{max}}$, $\phi'$, $\phi^2$ as a function of $z$ at $t = 50$ sec
- Graph 3 should plot $T_{f, \text{max}}$, $\phi'$, $\phi^2$ as a function of $z$ at termination of the transient, i.e., $t = 300$ sec for Case A
  - 200 sec for Case B
  - 300 sec for Case C
  - 200 sec for Case D
- Graph 4 should plot $T_{f, \text{max}}$, $\phi'$, $\phi^2$ vs time for $z = 150$ cm
- Graph 5 should plot $T_{f, \text{max}}$, $\phi'$, $\phi^2$ vs time for $z = 250$ cm
The scales to be used in these graphs are as follows:

Abscissa - Time and space dimension

Time 10 mm = 20 sec
Space 30 mm = 100 cm

Ordinate - Flux and Temperature

Flux $10^{11}$ to $10^{16}$ over 5 cycles
Temperature 1 to $10^5$°C over 5 cycles

NOTE: The accompanying figures are not meant to represent actual runs - they are for illustrative purposes only.
APPENDIX 5

RUN DETAILS

Participants are asked to supply the following information concerning details of the individual computer runs which form the basis of their submitted results:

1 DATA SPECIFICATION

Give details of any respects in which the data used are necessarily different from those specified. Hopefully zero return under this item.

2 STEADY STATE

a Give initial steady state eigenvalues for Cases A and B in terms of critical absorber penetration or eigenvalue (on \( v \)) for an absorber tip position of

\[
\begin{align*}
z &= 246.735 \text{ (Case A)} \\
z &= 298.39 \text{ (Case B)}
\end{align*}
\]

NB: Because the temperature feedback term in Case A is positive (0.0002) and in Case B is negative (-0.00002), the steady state condition will be different. This is reflected in the different absorption terms used and the different rod positions.

b State computer used and give computer time for initial steady state computation in terms of

\[
\begin{align*}
\text{CPU (sec)} \\
\text{I/O (sec)}
\end{align*}
\]

3 TRANSIENTS

For each case provide the following details:

CPU time taken (sec)
I/O time taken (sec)
Core storage used (Kb, words etc)

4 COMPUTER PERFORMANCE

Provide an estimate of the performance of your computer relative to an IBM 370/165 computer.
FIGURE 1

SCHEMATIC DIAGRAM OF CORE LAYOUT

- 500 cm -

- 460 cm -

Absorber tip position

- 40 cm -

- 0 cm -

COOLANT FLOW

TOP REFLECTOR AND ABSORBER

FUEL AND ABSORBER

Graphical Output

FUEL

BOTTOM REFLECTOR

z = 350 cm

z = 250 cm

z (cm)
CYCLOPS - A Program for the solution of the
few group one dimensional neutron kinetics equations
with temperature feedback

By

D. E. Billington
UKAEA Risley, England

December 1974
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<tr>
<td>2.</td>
<td>Method of Calculation</td>
<td>1</td>
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<tr>
<td>3.</td>
<td>Results</td>
<td>2</td>
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<tr>
<td>4.</td>
<td>Discussion</td>
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## Figures

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<td>Solution of the Amplitude Function Equations.</td>
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<td>4</td>
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<td>38</td>
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<td>5</td>
<td>Notation</td>
<td>41</td>
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</table>
1. Introduction

There has been a considerable effort at a number of national centres to produce efficient computer methods for the solution of kinetics problems in nuclear power reactors where flux distortions in space and energy have a significant effect on the course of a transient.

The Nuclear Energy Agency Committee on Reactor Physics has assembled a series of 'benchmark' problems and has invited workers in the field to attempt a solution. A review of the solutions to a series of one-dimensional problems has been provided by Sidell (Reference 3).

One such solution was obtained by use of the UK code CYCLOPS, which was originally conceived for use with thermal reactors although the method of solution used is not so limited. This paper details the procedures used in the code and demonstrates the effect on results and computing time of variations in the time steps used in the solution.

2. Method of Calculation

The method used is the improved quasi-static. The space, energy and time dependent flux is decomposed into a spatial function in one dimension and an amplitude function. The spatial function contains all the space and energy dependence but only depends on time through spatial distortions, whilst the amplitude function contains most of the temporal dependence and is independent of space and energy. The obvious advantage is that the gross time behaviour is calculated on a point basis and the space and energy distortions, which occur on a longer time-scale, can be calculated less frequently.

The derivation of the equations governing the behaviour of these two functions is given in Appendix 1. The spatial function is the solution of an eigenvalue problem which includes a spatial function independent source term deriving from the time history of the delayed neutron precursors and also from a backward-difference representation of the time derivative of the spatial function. The solution of this problem is performed in a specially written module described in Appendix 3.

The amplitude function is the solution of the familiar point kinetics equations. These equations are solved by the piecewise polynomials method with collocation weighting. The method has been modified to improve the conditioning, particularly in the case of small time-steps and is described in Appendix 2.

The steady-state calculation proceeds by iteration between evaluation of the steady-state spatial function (Appendix 3) and the steady-state temperature distribution (Appendix 4) in order to obtain the specified coolant temperature rise and to allow for temperature feedback onto the spatial function. This procedure is taken to convergence and the steady-state adjoint spatial function calculation (Appendix 3) completes the initialisation of the problem.

Over one amplitude function time-step the procedure is as follows. An estimate of the amplitude function over the time-step is obtained by linear extrapolation from the previous time-step. This estimate is combined with the current spatial function in the calculation of the local linear heat rating over the spatial mesh and the temperatures at the end of the time-step are calculated (Appendix 4). The effect on cross-sections of the change in mean
fuel temperature and rod position is obtained and the coefficients of the amplitude function equations derived by the inner product procedures of Appendix 1. These are stored for use in the recalculation of the amplitude function described below. The equations are solved over the time-step for the amplitude function and integrated precursor densities (Appendix 2) and the distributed precursor densities are updated as in Appendix 3.

There is no iteration in the present version of the code between the amplitude function calculation and the temperature calculation. Such an iteration may lead to a lengthening of the time-step at the expense of an increase in computation per time-step. In the benchmark study it is plausible that recalculation of the temperatures (possibly without subsequent re-calculation of the amplitude function) may lead to advantages in running times in view of the simple heat transfer model.

Consider a spatial function recalculation yielding $\Psi_{k-1}$ at time $t_{k-1}$. After a number of amplitude function time-steps it is necessary to recompute the spatial function (Appendix 3) to account for the distortions in space and energy which may have occurred. As a result of this computation of $\Psi_k$ at time $t_k$ there is a step change in the coefficients of the amplitude function equations. Allowance is made for this effect by recalculating the amplitude function over the time interval $t_k - t_{k-1}$. The modified coefficients of the amplitude function equations over this interval are assessed by first calculating the change in the coefficients at $t_k$ when $\Psi_k$ is used rather than $\Psi_{k-1}$. The change in the coefficients when $\Psi_{k-1}$ is replaced by $\Psi_k$ at an amplitude function calculation step $t_i$ inside the interval is approximated by linear interpolation between the changes at $t_{k-1}$ and $t_k$. Of course the spatial function appropriate to $t_i$ is neither $\Psi_{k-1}$ nor $\Psi_k$ and this is allowed for in a linear fashion. Taking $\rho(t_j)$ as an example,

$$
\rho(t_j) = \rho_{k-1}(t_j) + \alpha \left\{ \Delta \rho(t_{k-1}) + \alpha \left[ \Delta \rho(t_k) - \Delta \rho(t_{k-1}) \right] \right\}
$$

in obvious notation,

and $\alpha = t_j - t_{k-1} / (t_k - t_{k-1})$.

During this phase of the calculation the temperatures from the first sweep are retained. It is possible that recalculations of the temperatures could lead to a reduction in the frequency of spatial function recalculation. Again, particularly for a more realistic heat transfer model than that specified for the benchmark calculation, this advantage would need to be balanced against the computation time required to recalculate the temperatures.

Finally the code allows for iteration on the amplitude function recalculation, although this feature was not used in the benchmark submission.

3. Results

A specification of the one-dimensional benchmark problems is included in Reference 3 and is not repeated here. Solutions obtained using CYCLOPS to cases A and C of these problems constituted the benchmark submission; the digital results and running times relative to an IBM 370/165 computer are compared with those for other submissions in Reference 3. Tables 6.2 and 6.4 of this paper include the above information and Figures 1 to 8 present the graphical information prepared for the CYCLOPS submission.
The time available for preparation of the benchmark submission was limited and the accent was necessarily on obtaining reliable solutions to the problems. In particular no advantage was taken of time-step relaxation as the final steady-state was approached. The effect of variations in time-step selection on running times and results is a matter of obvious interest, especially when the variations in results can be viewed in the light of corresponding variations between results obtained using different methods of solution as discussed in Reference 3.

It has been found that significant improvements in running times can be obtained without undue effect on the results. This is illustrated in tables 6.2 and 6.4, which show improvements in running times of factors of two and three for cases A and C respectively. Detailed time-step information is given in tables 6.1 and 6.3 together with corresponding details of the benchmark submission.

Results were obtained for case B but not included in the submission as the problem was not felt to be realistic over the time-scale on which the results were requested. Reference 3 includes a limited amount of information from a number of submissions over a short time-scale. Table 6.5 of this paper presents the same information extracted from a number of CYCLOPS runs. The results underline the agreement between CYCLOPS and the ABA code TRANS noted in Reference 3 for cases A and C.

4. Discussion

The code appears to have performed satisfactorily when judged on the solutions obtained to the benchmark problems and on the running times achieved. Furthermore there remains the possibility (as mentioned in section 2) of further improvements in running times by means of a modified temperature re-calculation strategy.

A desirable feature in this type of code is an automatic procedure for time-step selection. Such a procedure leads generally to an increase in computation per accepted time-step, but this should be more than outweighed in practice by a relaxation of time-steps whenever this is acceptable. Of course the time-step selection criteria must be chosen on the basis of experience and with the global accuracy in mind, but there should follow an increased confidence in the accuracy of the results obtained.

Due to the efficiency of the spatial function recalculation procedure discussed in Appendix 3, the computation times for the present cases were roughly equally divided between evaluation of the spatial function behaviour and the amplitude function behaviour. Thus there may be some interest in comparing the present piecewise polynomials scheme used in solving for the amplitude function with one using spline functions, although the amplitude function time-steps may well be limited by the requirement to adequately represent the temporal behaviour of reactivity rather than by the accuracy of the piecewise polynomials method used.

The quasi-static approach employed in this work clearly extends to two or three dimensions and the amplitude function solution would be unchanged. The computation of the spatial function would in these cases consume relatively more calculation time and a critical issue would be the development of an efficient spatial function calculation method.
It seems that the methods of Appendix 3 could be applied iteratively in more dimensions by treating the problem as a series of one-dimensional problems and allowing for leakage between 'channels' by modification of the source terms. However any advantage over alternative methods would need to be demonstrated.

5. References

1. Tyror, J G

2. Fuller, E L
   Weighted-residual methods in space-dependent reactor dynamics. 1969. ANL-7565

3. Sidell, J
   The analysis of one-dimensional reactor kinetic benchmark computations. 1974.
   Paper to be presented at the Nuclear Energy Agency meeting on spatial kinetics at Munich, January 1975.

6. Tables

   Table 6.1 Time-steps used in calculation, case A

<table>
<thead>
<tr>
<th>End of time interval (sec.)</th>
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<table>
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<tr>
<th>Benchmark submission (Quadratic piecewise polynomials)</th>
<th>Variation (Cubic piecewise polynomials)</th>
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<tr>
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</tr>
<tr>
<td>Spatial function time-step (sec.)</td>
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</table>
Table 6.2  Results and calculation times, case A

Spatial mesh interval 20 cms.
Figures in brackets denote height in cms. above core inlet

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Time (sec.)</th>
<th>Benchmark submission</th>
<th>Variation</th>
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<td>7.6 10$^{1.3}$</td>
<td>7.6 10$^{1.3}$</td>
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<td>1.8 10$^{1.4}$</td>
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<td>$\varrho_{1}(350)$ (cm$^{-2}$ sec$^{-1}$)</td>
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<td>Steady-state</td>
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<tr>
<td>Transient</td>
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<td>110</td>
<td>51</td>
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Table 6.3  Time-steps used in calculation, case C

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<tr>
<th>End of time interval (sec.)</th>
<th>Benchmark submission (Quadratic piecewise polynomials)</th>
<th>Variation (Cubic piecewise polynomials)</th>
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<td>Amplitude function time-step (sec.)</td>
<td>Spatial function time-step (sec.)</td>
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<td>10</td>
<td>0.025</td>
<td>0.125</td>
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<tr>
<td>11</td>
<td>0.0125</td>
<td>0.0625</td>
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Table 6.4  Results and calculation times, case C
Spatial mesh interval 20 cms.
Figures in brackets denote height in cms. above core inlet

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Time (sec.)</th>
<th>Benchmark submission</th>
<th>Variation</th>
</tr>
</thead>
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<td>Coolant outlet temperature ($^\circ$C)</td>
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<td>0</td>
<td>800</td>
<td>800</td>
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</tr>
<tr>
<td>300</td>
<td>800</td>
<td>800</td>
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</tr>
<tr>
<td>$T_f$ (350) ($^\circ$C)</td>
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</tr>
<tr>
<td>300</td>
<td>1047</td>
<td>1047</td>
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</tr>
<tr>
<td>$T_b$ (350) ($^\circ$C)</td>
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</tr>
<tr>
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<td>844</td>
<td>844</td>
<td></td>
</tr>
<tr>
<td>$\varphi^1$ (350) (cm$^{-2}$ sec$^{-1}$)</td>
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<td>$7.6 \times 10^{13}$</td>
<td>$7.6 \times 10^{13}$</td>
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<tr>
<td>50</td>
<td>$7.0 \times 10^{13}$</td>
<td>$7.1 \times 10^{13}$</td>
<td></td>
</tr>
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<td>$7.5 \times 10^{13}$</td>
<td>$7.5 \times 10^{13}$</td>
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</tr>
<tr>
<td>200</td>
<td>$7.6 \times 10^{13}$</td>
<td>$7.6 \times 10^{13}$</td>
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</tr>
<tr>
<td>300</td>
<td>$7.6 \times 10^{13}$</td>
<td>$7.6 \times 10^{13}$</td>
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<tr>
<td>$\varphi^2$ (350) (cm$^{-2}$ sec$^{-1}$)</td>
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<td>$3.8 \times 10^{13}$</td>
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<td>$3.5 \times 10^{13}$</td>
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</tr>
<tr>
<td>100</td>
<td>$3.7 \times 10^{13}$</td>
<td>$3.7 \times 10^{13}$</td>
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</tr>
<tr>
<td>200</td>
<td>$3.8 \times 10^{13}$</td>
<td>$3.8 \times 10^{13}$</td>
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</tr>
<tr>
<td>300</td>
<td>$3.8 \times 10^{13}$</td>
<td>$3.8 \times 10^{13}$</td>
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</tr>
<tr>
<td>Position of max $T_f$,max (cms.)</td>
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<td>150</td>
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<tr>
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</tr>
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</tr>
<tr>
<td>300</td>
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</tr>
<tr>
<td>Maximum value of $T_f$,max ($^\circ$C)</td>
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<tr>
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</tr>
<tr>
<td>Approx. timings (sec.) on IBM 370/165 computer</td>
<td>Steady-state</td>
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<td>4</td>
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<tr>
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<td>Transient</td>
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<td>56</td>
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Table 6.5  
Comparison of $\phi^1$ $\phi^2$ $T_{f,\text{max}}$ at $t = 10$ secs and time at which $\phi^1$ reaches $10^{15}$, case B

Spatial mesh interval 20 cms.
Figures in brackets denote height in cms. above core inlet

<table>
<thead>
<tr>
<th></th>
<th>Case B1</th>
<th>Case B2</th>
<th>Case B3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{f,\text{max}}$ (150) ($^\circ$C)</td>
<td>2373</td>
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<td>2352</td>
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<tr>
<td>$\phi^1$ (150) ($\text{cm}^{-2} \text{sec}^{-1}$)</td>
<td>$1.3 \times 10^{15}$</td>
<td>$1.3 \times 10^{15}$</td>
<td>$1.3 \times 10^{15}$</td>
</tr>
<tr>
<td>$\phi^2$ (150) ($\text{cm}^{-2} \text{sec}^{-1}$)</td>
<td>$7.6 \times 10^{14}$</td>
<td>$7.6 \times 10^{14}$</td>
<td>$7.3 \times 10^{14}$</td>
</tr>
<tr>
<td>$T_{f,\text{max}}$ (250) ($^\circ$C)</td>
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<tr>
<td>$\phi^1$ (250) ($\text{cm}^{-2} \text{sec}^{-1}$)</td>
<td>$1.1 \times 10^{15}$</td>
<td>$1.1 \times 10^{15}$</td>
<td>$1.1 \times 10^{15}$</td>
</tr>
<tr>
<td>$\phi^2$ (250) ($\text{cm}^{-2} \text{sec}^{-1}$)</td>
<td>$6.4 \times 10^{14}$</td>
<td>$6.4 \times 10^{14}$</td>
<td>$6.2 \times 10^{14}$</td>
</tr>
<tr>
<td>$t(150)\phi^1 = 10^{15}$ (sec)</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>$t(250)\phi^1 = 10^{15}$ (sec)</td>
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<td>10</td>
<td>10</td>
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<tr>
<td>Time per 10 sec. transient (sec.)</td>
<td>8</td>
<td>4</td>
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Case B1:  
Amplitude function time-step 0.25 sec.
Spatial function recalculation 1 sec.
Quadratic piecewise polynomials.

Case B2:  
Amplitude function time-step 0.5 sec.
Spatial function recalculation 2 secs.
Cubic piecewise polynomials.

Case B3:  
Amplitude function time-step 1.0 sec.
Spatial function recalculation 2 secs.
Cubic piecewise polynomials.
Fig. 1
Fig. 3
CASE A PLOT AT \( z = 150 \text{ cm/s} \).

FLUX AND TEMPERATURE AGAINST TIME.

FLUX

\((\text{cm}^{-2} \text{sec}^{-1})\)

FIG. 4
CASE A PLOT AT Z = 250 cm:
FLUX AND TEMPERATURE AGAINST TIME.

FLUX
(cm\(^{-2}\) Sec\(^{-1}\))

TIME (Secs)

CICLOPS(UWAEA)

FIG. 5
CASE C PLOT AT TIME T = 50 SEC.

FLUX AND TEMPERATURE AGAINST SPACE.

FLUX
(cm$^{-2}$ sec$^{-1}$)

$T_{e,max}$

$Z$ (cm)$^\text{fig. 6}$
CASE C PLOT AT 23:150 CMS

FLUX AND TEMPERATURE AGAINST TIME

FLUX
(cm² Sec⁻¹)

TIME (SECS.)

FIG. 7
FIG. 8

CASE C PLOT AT Z=350 CMS.

FLOW AND TEMPERATURE AGAINST TIME

FLUX
(cm⁻² Sec⁻¹)

$T_{i,\text{max}}$

$\phi_1$

$\phi_2$

TIME (SECS)

CYCLOPS (IKKA EA)
Appendix 1

Derivation of Improved Quasi-Static Equations

The three group source free time dependent neutron diffusion equations may be written as:

$$\nabla \cdot D \nabla \phi_a - (\Sigma_{a_3} + \Sigma_{r_3 \rightarrow 2}) \phi_a + X(E) \left[ \frac{3}{g_{g=1}} \nu_{g} \phi_g \right] (1 - \beta)$$

$$+ \sum_{i=1}^{3} X_{di}(E) \lambda_{1i} e_i = \frac{1}{v_3} \frac{\partial}{\partial t} \phi_3$$

$$\nabla \cdot D \nabla \phi_2 - (\Sigma_{a_2} + \Sigma_{r_2 \rightarrow 1}) \phi_2 + X(E) \left[ \frac{3}{g_{g=1}} \nu_{g} \phi_g \right] (1 - \beta)$$

$$+ \Sigma_{r_3 \rightarrow 2} \phi_3 + \sum_{i=1}^{3} X_{di}(E) \lambda_{1i} e_i = \frac{1}{v_2} \frac{\partial}{\partial t} \phi_2$$

$$\nabla \cdot D \nabla \phi_1 - \Sigma_{a_1} \phi_1 + X(E) \left[ \frac{3}{g_{g=1}} \nu_{g} \phi_g \right] (1 - \beta)$$

$$+ \Sigma_{r_2 \rightarrow 1} \phi_2 + \sum_{i=1}^{3} X_{di}(E) \lambda_{1i} e_i = \frac{1}{v_1} \frac{\partial}{\partial t} \phi_1$$

$$\frac{\partial}{\partial t} e_i = \beta_{1i} \sum_{g=1}^{3} \nu_{g} \phi_g \phi_1 - \lambda_{1i} e_i, i=1, ..., I$$

Here 1 indicates the thermal group, 2 the resonance group 3 the fast group as in Reference 1. Only downscatter from a group to the next lower has been considered.

These equations are written concisely as:

$$\nabla \cdot D \nabla - A + (1 - \beta) X_p . \phi' \quad \cdot g + X_d \cdot \lambda \cdot \xi \quad \ldots(1.1)$$

$$\frac{\partial}{\partial t} \xi = \beta \cdot \phi' \cdot \phi - \lambda \cdot \xi \quad \ldots(1.2)$$

where $\phi = \begin{bmatrix} \phi_3 \\ \phi_2 \\ \phi_1 \end{bmatrix}$ and $\xi = \begin{bmatrix} \xi_1 \\ \xi_2 \\ \ldots \xi_I \end{bmatrix}$
Factorize \( g(z,t) \) as follows:

\[
g(z,t) = \varphi(t) \tilde{g}(z,t); \varphi(0) = 1.0
\]  

...(1.3)

where \( \varphi(t) \) is a scalar function of time.

An additional constraint is required to render the splitting unique. This is taken as:

\[
\int_z w'(z).V^{-1}.\tilde{g}(z,t)dz = \text{constant}
\]  

...(1.4)

where \( w(z) \) is a time independent weighting function. This constraint is chosen to ensure that most of the temporal variation is included in \( \varphi(t) \).
1.1 **Equations for ϕ(t) - the amplitude function**

Substitute (1.3) into (1.1), multiply on the left by y'(z) and integrate over the reactor.

\[ \phi(t) \int_z \psi'(z) \cdot V^{-1} \frac{\partial}{\partial t} \psi(z,t) \, dz + \int_z \psi'(z) \cdot V^{-1} \psi(z,t) \, dz \frac{d}{dt} \phi(t) \]

\[ = \int_z \psi'(z) \cdot \left[ \nabla \cdot \nabla - A + (1-\beta) X_p \cdot \xi' \right] \cdot \psi(z,t) \, dz \phi(t) \]

\[ + \int_z \psi'(z) \cdot X_d \cdot \lambda \cdot \xi(z,t) \, dz \]

The first of the integrals on the L.H.S. of this equation is zero by (1.4).

Multiply (1.2) on the left by \( \text{diag} \left( \psi'(z) \cdot X_d \right) \) and integrate over the reactor.

\[ \frac{\partial}{\partial t} \int_z \text{diag} \left( \psi'(z) \cdot X_d \right) \cdot \xi(z,t) \, dz \]

\[ = \int_z \text{diag} \left( \psi'(z) \cdot X_d \right) \cdot \beta \cdot \xi' \cdot \psi(z,t) \, dz \phi(t) \]

\[ - \int_z \text{diag} \left( \psi'(z) \cdot X_d \right) \cdot \lambda \cdot \xi(z,t) \, dz \]

Put \( \eta(t) = \frac{1}{\eta} \int_z \text{diag} \left( \psi'(z) \cdot X_d \right) \cdot \xi(z,t) \, dz \)

\[ \eta \text{ will be used later to obtain the usual definition of reactivity in the point kinetics equations.} \]

Then \[ \frac{d}{dt} \eta(t) = \frac{1}{\eta} \int_z \text{diag} \left( \psi'(z) \cdot X_d \right) \cdot \beta \cdot \xi' \cdot \psi(z,t) \, dz \phi(t) - \lambda \cdot \eta(t) \]

since we may reverse the order of multiplication for diagonal matrices.

Define the following scalars:

\[ L(t) = \frac{1}{\eta} \int_z \psi'(z) \cdot V^{-1} \psi(z,t) \, dz \]

\[ \rho(t) = \frac{1}{\eta} \int_z \psi'(z) \cdot \left[ \nabla \cdot \nabla - A + (1-\beta) X_p \cdot \xi' + X_d \cdot \beta \cdot \xi' \right] \cdot \psi'(z,t) \, dz \]

\[ \bar{\rho}(t) = \frac{1}{\eta} \int_z \psi'(z) \cdot X_d \cdot \beta \cdot \xi' \cdot \psi(z,t) \, dz \]

and the vector

\[ \bar{\rho}(t) = \frac{1}{\eta} \int_z \text{diag} \left( \psi'(z) \cdot X_d \right) \cdot \beta \cdot \xi' \cdot \psi(z,t) \, dz \]
Equations (1.5) and (1.7) become:

\[
L(t) \frac{d}{dt} \phi(t) = \left[ \rho(t) - \tilde{\beta}(t) \right] \phi(t) + \frac{1}{\eta} \int_z \psi'(z) \cdot X_d \cdot \lambda \cdot \xi(z,t) dz
\]

\[
\frac{d}{dt} \zeta(t) = \tilde{\beta}(t) \phi(t) - \lambda \cdot \zeta(t)
\]

Now \( \frac{1}{\eta} \int_z \psi'(z) \cdot X_d \cdot \lambda \cdot \xi(z,t) dz \)

\[
= \frac{1}{\eta} \int_z (1,1, \ldots, 1) \cdot \text{diag} (\psi'(z) \cdot X_d) \cdot \lambda \cdot \xi(z,t) dz
\]

\[
= \frac{1}{\eta} (1,1 \ldots, 1) \cdot \lambda \int_z \text{diag} (\psi'(z) \cdot X_d) \cdot \xi(z,t) dz
\]

reversing the order of multiplication of diagonal matrices as before.

\[
\cdot \cdot \cdot \frac{1}{\eta} \int_z \psi'(z) \cdot X_d \cdot \lambda \cdot \xi(z,t) dz = \lambda' \zeta(t)
\]

Finally equations (1.6) and (1.8) become:

\[
L(t) \frac{d}{dt} \phi(t) = \left[ \rho(t) - \tilde{\beta}(t) \right] \phi(t) + \lambda' \cdot \zeta(t)
\]  \hspace{2cm} (1.12)

\[
\frac{d}{dt} \zeta(t) = \tilde{\beta}(t) \phi(t) - \lambda \cdot \zeta(t)
\]  \hspace{2cm} (1.13)

which are the well known point kinetics equations.

It is conventional to take \( \psi(x) \) to be the steady state adjoint flux and \( \eta \) to be defined by:

\[
\eta = \int_z \psi'(z) \cdot \left[ \left( 1 - \beta \right) X_p \cdot \xi' + X_d \cdot \beta \cdot \xi' \right] \cdot \psi(z,t) dz
\]

The coefficients of the point kinetics equations are then:

\[
L(t) = \frac{\langle \psi^*'(z) \cdot \psi^{-1} \cdot \psi(z,t) \rangle}{\langle \psi^*'(z) \cdot \xi' \cdot \psi(z,t) \rangle \cdot \left[ \left( 1 - \beta \right) X_p + X_d \cdot \beta \right]}  \hspace{2cm} (1.8.1)
\]

\[
\rho(t) = \frac{\langle \psi^*'(z) \cdot \left[ \nabla \cdot \nabla - A + \left( 1 - \beta \right) X_p + X_d \cdot \beta \right] \cdot \xi' \rangle \cdot \psi(z,t) \rangle}{\langle \psi^*'(z) \cdot \psi(z,t) \rangle \cdot \left[ \left( 1 - \beta \right) X_p + X_d \cdot \beta \right]}  \hspace{2cm} (1.9.1)
\]

\[
\tilde{\beta}(t) = \frac{\langle \psi^*'(z) \cdot \xi' \cdot \psi(z,t) \rangle \cdot X_d}{\langle \psi^*'(z) \cdot \psi(z,t) \rangle \cdot \left[ \left( 1 - \beta \right) X_p + X_d \cdot \beta \right]}  \hspace{2cm} (1.10.1)
\]
diagonal (I*, z, X_d) • \psi(z, t) > \left( (1 - \beta) \sum_{p} X_p \phi_p - X_d \phi_d \right) 
since \psi'(z, t) is a scalar.

The appearance of the total production operator in the denominator of (1.10.1) and the net production operator in the numerator leads to a meaningful definition of reactivity.

If the delayed neutron spectrum of each delayed group is the same as the prompt spectrum,

\[ X_d = \left[ \sum_{p} X_p, \ldots, X_p \right] = X_p (1, \ldots, 1) \]

Then \[ X_d \cdot \phi = X_p (1, \ldots, 1) \cdot \phi = \phi_p \]

\[ (1 - \beta) X_p + X_d \cdot \phi = X_p \]

and \[ \text{diag} (\psi'(z, t) X_d) = \text{diag} (\psi'(z) X_p (1, \ldots, 1)) \]

\[ = \psi'(z). X_p \phi \]

Hence in this case the effective delayed neutron fractions reduce to the actual delayed neutron fractions, which is a desirable result. Furthermore,

\[ (1, \ldots, 1) \cdot \bar{\phi}(t) = \bar{\phi}(t) \] by inspection of (1.10.1) and (1.11.1)

Thus the effective delayed neutron fractions sum to the total effective delayed neutron fraction.

1.2 Equations for \( \psi(z, t) \) - the spatial function

Substitute (1.3) into (1.1)

\[ V^{-1} \left[ \frac{\partial}{\partial t} \psi(z, t) + \frac{1}{\phi(t)} \frac{d}{dt} \phi(t) \psi(z, t) \right] = \left[ \nabla \cdot \nabla - \lambda + (1 - \beta) \sum_{p} X_p \phi' \right] \psi(z, t) \]

\[ + \frac{1}{\phi(t)} X_d \cdot \lambda \cdot \xi(z, t) \]

Since \( \psi(z, t) \) is slowly varying with time (through spatial distortions only) the time derivative is approximated by a simple backwards-difference scheme.

If \( t_k \) is the time of the current spatial calculation and \( t_{k-1} \) the time of the previous one,

\[ \frac{\partial}{\partial t} \psi(z, t_k) \approx \frac{1}{t_k - t_{k-1}} \left[ \psi(z, t_k) - \psi(z, t_{k-1}) \right] \]

Then

\[ - \nabla \cdot \nabla \psi(z, t_k) + \left[ A + V^{-1} \left( \frac{1}{\phi(t_k)} \frac{d}{dt} \phi(t_k) + \frac{1}{t_k - t_{k-1}} \right) \right] \psi(z, t_k) \]
\[
(1 - \beta) X_p \cdot \xi' \cdot \bar{\psi}(z, t_k) + \left[ \frac{1}{t_k - t_{k-1}} \psi^{-1} \cdot \bar{\psi}(z, t_{k-1}) + \frac{1}{\phi(t_k)} X_d \cdot \lambda \cdot \xi(z, t_k) \right] \quad (1.14')
\]

From equation (1.2),
\[
\frac{\partial}{\partial t} \xi(z, t) + \lambda \cdot \xi(z, t) = B \cdot 
\frac{\partial}{\partial t} \bar{\psi}(z, t) \cdot \phi(t) \quad t_{k-1} \leq t \leq t_k
\]

Then
\[
\xi(z, t_k) = e^{-\lambda(t_k - t_{k-1})} \cdot \xi(z, t_{k-1}) + \int_{t_{k-1}}^{t_k} e^{-\lambda(t_k - t)} \cdot B \cdot \xi' \cdot \bar{\psi}(z, t) \cdot \phi(t) \, dt \quad (1.15)
\]
Appendix 2

Solution of the amplitude function equations

The method used is piecewise polynomials with collocation weighting, (see for example Reference 2). A modification has been included to improve the conditioning of the method, particularly for small time-steps.

The amplitude function is the solution of the point kinetics equations, derived as equations (1.12) and (1.13) and reproduced below.

\[ \frac{d}{dt} \phi(t) = (\rho - \beta) \phi(t) + \lambda' \varphi(t) \]  \hspace{1cm} \ldots (2.1)

\[ \frac{d}{dt} \varphi(t) = \beta \phi(t) - \lambda \varphi(t) \]  \hspace{1cm} \ldots (2.2)

2.1 The Weighted residual method

Assuming that the integration is to be performed from known conditions at time \( t_{j-1} \), the formal solution to equations (2.2) is:

\[ \varphi(t) = e^{-\lambda (t-t_{j-1})} \varphi(t_{j-1}) + \int_{t_{j-1}}^{t} e^{-\lambda (t-t_{j-1})} \beta \phi(t_{j-1}) dt_{j-1} \]  \hspace{1cm} \ldots (2.3)

Substitute (2.3) into (2.1)

\[ \frac{d}{dt} \phi(t) = (\rho - \beta) \phi(t) + \lambda' \left[ e^{-\lambda (t-t_{j-1})} \varphi(t_{j-1}) \right. \]
\[ + \int_{t_{j-1}}^{t} e^{-\lambda (t-t_{j-1})} \beta \phi(t_{j-1}) dt_{j-1} \]  \hspace{1cm} \ldots (2.4)

Approximate \( \phi(t) \) over the interval as a linear combination of known functions of time:

\[ \phi(t) = \sum a_i \varphi_i(t) \]  \hspace{1cm} \ldots (2.5)

where \( a = \begin{bmatrix} a_0 \\ \vdots \\ a_p \end{bmatrix} \) is a set of constant amplitudes, to be determined.

\[ \varphi_i(t) = \begin{bmatrix} T_0(t) \\ \vdots \\ T_p(t) \end{bmatrix} \]  \hspace{1cm} is the set of trial functions to be fitted.

It is convenient to choose \( a_0 \) to be \( \varphi(t_{j-1}) \) so that \( T_0(t) = 1 \) and \( T_i(t_{j-1}) = 0, \ i \neq 0. \)
This ensures continuity of the piecewise solutions at \( t_{j-1} \).

We write

\[
\begin{bmatrix}
\varphi(t_{j-1}) \\
\varphi
\end{bmatrix}
\begin{bmatrix}
1 \\
\varphi(t)
\end{bmatrix}
\]

where

\( \varphi(t_{j-1}) = 0 \) \hspace{1cm} \ldots (2.6)

If we substitute \( \varphi_f(t) \) for \( \varphi(t) \) in equation (2.4) the equations are no longer satisfied and we form the residual

\[
R(t) = \frac{d}{dt} \varphi_f(t) - (p-\beta) \varphi_f(t) - \lambda ' e^{-\lambda(t-t_{j-1})}
\]

\[
+ \int_{t_{j-1}}^{t} e^{-\lambda(t-t')} \varphi_f(t')dt
\]

\[
\ldots (2.7)
\]

Using the weighting functions

\[
\varphi_1(t) = \begin{bmatrix}
\varphi_1(t) \\
\vdots \\
\varphi_p(t)
\end{bmatrix}
\]

the unknown elements of \( \varphi \) (i.e. the elements of \( \varphi \)) are determined from:

\[
\int_{t_{j-1}}^{t} \varphi(t) R(t) \, dt = 0 \hspace{1cm} \ldots (2.8)
\]

It is in this weighted residual sense that \( \varphi_f(t) \) will satisfy equations (2.4) and there is some freedom in the choice of a suitable set of weighting functions.

2.2 Piecewise polynomials with collocation weighting

In the present case, the fitted function is taken as a polynomial in time and \( R(t) \) is forced to zero at \( p \) points within the interval.

i.e.

\[
\varphi(t) = \begin{bmatrix}
W(t-t_{j-1}) \\
W^2(t-t_{j-1})^2 \\
\vdots \\
W^p(t-t_{j-1})^p
\end{bmatrix}
\]

and

\[
\begin{bmatrix}
\delta(t-t_{j-1}) \\
\delta(t-t_{j-2}) \\
\vdots \\
\delta(t-t_p)
\end{bmatrix}
\]

where \( \delta \) is the Dirac delta function.

Note that conditions (2.6) are satisfied.

\( W \) is a coefficient which does not appear in the standard piecewise polynomials method. It has been introduced to improve the conditioning of the method and is discussed later.
Use of collocation weighting leads to the following set of equations for $g$:

$$R(t_{jj}) = 0, \quad jj = 1, \ldots, p.$$ 

i.e. the requirement on $g(t)$ is that the equations shall be satisfied exactly at $p$ points within the time interval $t_j - t_{j-1}$.

$$[L \frac{d}{dt} \lambda'(t_{jj}) - (\rho - \bar{\beta}) \lambda'(t_{jj}) - \lambda'] \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} \bar{\beta} \cdot \lambda'(t) dt] \cdot g$$

$$= \lambda' \cdot e^{-\lambda(t_{jj} - t_{j-1})} \cdot g(t_{j-1}) + \left[ (\rho - \bar{\beta}) + \lambda' \right] \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} \bar{\beta} \cdot \lambda'(t) dt \cdot g$$

Now

$$\int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} dt = \lambda_{j-1} \cdot [1 - e^{-\lambda(t_{jj} - t_{j-1})}]$$

$$\therefore \lambda' \cdot \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} dt \cdot \bar{\beta} = \bar{\beta} - (1, \ldots, 1) e^{-\lambda(t_{jj} - t_{j-1})} \cdot \bar{\beta}$$

since $(1, \ldots, 1) \cdot \bar{\beta} = \bar{\beta}$

$$\therefore \lambda' \cdot \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} dt \cdot \bar{\beta} = \bar{\beta} - E(t_{j-1})$$

where $E(t) = (1, \ldots, 1) \cdot e^{-\lambda(t - t_{j-1})}$

$$\therefore [L \frac{d}{dt} \lambda'(t_{jj}) - (\rho - \bar{\beta}) \lambda'(t_{jj}) - \lambda'] \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} \bar{\beta} \cdot \lambda'(t) dt] \cdot g$$

$$= \lambda' \cdot e^{-\lambda(t_{jj} - t_{j-1})} \cdot g(t_{j-1}) + \left[ \rho - E(t_{j-1}) \right] g(t_{j-1}) \quad \ldots(2.9)$$

This equation is seen to be correct for $t_{jj} = t_{j-1}$.

Consider $P(t_{jj}) = \lambda' \cdot \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} \bar{\beta} \cdot \lambda'(t) dt \cdot g$

Integrate by parts:

$$P(t_{jj}) = \lambda' \cdot \left[ \lambda^{-1} \cdot e^{-\lambda(t_{jj} - t)} \bar{\beta} \cdot \lambda'(t) \right]_{t_{j-1}}^{t_{jj}} + \lambda' \cdot \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} \bar{\beta} \cdot \frac{d}{dt} \lambda'(t) dt \cdot g$$
\[ P(t_{jj}) = \left[ \tilde{Q} (t_{jj}) - E(t_{j-1}) \right] \left[ (t_{jj}) \int_{t_{j-1}}^{t_{jj}} E(t) \frac{d}{dt} \gamma'(t) dt \right]. \]  

But \( \gamma'(t_{j-1}) = 0 \)

\[ P(t_{jj}) = \left[ \tilde{Q} (t_{jj}) - E(t_{j-1}) \right] \left[ \int_{t_{j-1}}^{t_{jj}} E(t) \frac{d}{dt} \gamma'(t) dt \right]. \]  

Substituting equation (2.10) into equation (2.9) yields:

\[ \left[ L \frac{d}{dt} \gamma'(t_{jj}) - \rho \gamma'(t_{jj}) + \int_{t_{j-1}}^{t_{jj}} E(t) \frac{d}{dt} \gamma'(t) dt \right] \tilde{Q} = 0 \]

Consider \( \gamma'(t_{jj}) = \int_{t_{j-1}}^{t_{jj}} E(t) \frac{d}{dt} \gamma'(t) dt \)

Each element of \( \gamma'(t_{jj}) \) takes the form:

\[ \zeta_r(t_{jj}) = \int_{t_{j-1}}^{t_{jj}} (r+1)E(t) \tilde{X}_r(t_{jj} - t_{j-1}) dt \text{ where } 0 \leq r \leq p-1 \]

\[ = (r+1)(1, \ldots, 1) \cdot \int_{t_{j-1}}^{t_{jj}} \tilde{X}_r(t_{jj} - t) e^{-\lambda(t_{jj} - t)} \tilde{E}(t-t_{j-1})^r dt \]

\[ \therefore \zeta_r(t_{jj}) = (r+1)(1, \ldots, 1) \cdot Q_r(t_{jj}) \]

where \( Q_r(t_{jj}) = \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} \tilde{E}(t-t_{j-1})^r dt. \)

Integrate by parts

\[ Q_r(t_{jj}) = \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} \tilde{E}(t-t_{j-1})^r dt \]

\[ = \left[ e^{-\lambda(t_{jj} - t)} \tilde{E}(t-t_{j-1})^r \right]_{t_{j-1}}^{t_{jj}} - \int_{t_{j-1}}^{t_{jj}} r e^{-\lambda(t_{jj} - t)} \tilde{E}(t-t_{j-1})^r-1 dt \]

\[ \therefore Q_r(t_{jj}) = W^{r+1} \lambda^{-1} \left[ e^{-\lambda(t_{jj} - t)} \tilde{E}(t-t_{j-1})^r - r Q_{r-1}(t_{jj}) \right] \]

But \( Q_0(t_{jj}) = \int_{t_{j-1}}^{t_{jj}} e^{-\lambda(t_{jj} - t)} dt \cdot \tilde{E} \)

\[ \therefore Q_0(t_{jj}) = W \lambda^{-1} \left[ 1 - e^{-\lambda(t_{jj} - t_{j-1})} \right] \cdot \tilde{E} \]

\[ \therefore Q_0(t_{jj}) = W \lambda^{-1} \left[ 1 - e^{-\lambda(t_{jj} - t_{j-1})} \right] \cdot \tilde{E} \]
Equations (2.12) and (2.13) yield \( Q_1(t_j) \) to \( Q_{p-1}(t_{jj}) \)

Define matrix \( Q = [Q_0, Q_1, \ldots, Q_{p-1}] \)

Then \( \xi'(t_{jj}) = (1, \ldots, 1) \cdot Q \cdot \begin{bmatrix} 1 \\ 2 \\ 0 \\ 0 \end{bmatrix} \) ... (2.14)

Rewrite equation (2.11) as follows:

\[ h'(t_{jj}) \cdot \xi = \xi_j \] ... (2.15)

where \( h'(t_{jj}) = L \frac{d}{dt} \xi'(t_{jj}) - \rho \xi'(t_{jj}) + \xi'(t_{jj}) \) ... (2.16)

and \( \gamma_{jj} = [\rho - E(t_{j-1})] \xi(t_{j-1}) + \lambda \cdot e^{-\lambda(t_{jj}-t_{j-1})} \cdot \xi(t_{j-1}) \) ... (2.17)

Equation (2.15) represents one equation in the \( p \) unknowns \( \xi \). A full set of equations is obtained by using \( p \) points.

\( t_{jj}, jj=1, \ldots, p \)

Then \( H \cdot \xi = \gamma \) ... (2.18)

where \( H = \begin{bmatrix} h'(t_1) \\ \vdots \\ h'(t_p) \end{bmatrix} \) and \( \gamma = \begin{bmatrix} \gamma_1 \\ \vdots \\ \gamma_p \end{bmatrix} \)

Solution of equations (2.18) gives \( \xi \)

\( \xi = H^{-1} \cdot \gamma \) ... (2.19)

Note that the method requires a matrix inversion of order \( p \), the degree of polynomial fitted.

Then \( \xi(t_j) = \xi(t_{j-1}) + \xi \cdot \xi'(t_j) \) ... (2.20)

From equation (2.3)

\[ \xi(t_j) = e^{-\lambda(t_{j-1})} \cdot \xi(t_{j-1}) + \int_{t_{j-1}}^{t_j} e^{-\lambda(t-t)} \cdot \xi(t) dt \]

\[ \xi(t_j) = e^{-\lambda(t_{j-1})} \cdot \xi(t_{j-1}) + \int_{t_{j-1}}^{t_j} e^{-\lambda(t_{j-1})} \cdot \xi(t) dt \]
Replacing \( \varphi(t) \) by \( \varphi_f(t) \) inside the integral,

\[
C(t_j) = e^{-\lambda(t_j-t_{j-1})} \cdot C(t_{j-1}) + \int_{t_{j-1}}^{t_j} e^{-\lambda(t_j-t')} \cdot \bar{E} \cdot \varphi(t_{j-1}) \cdot \mathcal{G}
\]

Then

\[
C(t_j) = e^{-\lambda(t_j-t_{j-1})} \cdot C(t_{j-1}) + \frac{1}{W} \left\{ \varphi(t_j) \varphi(t_{j-1}) + \left[ \varphi(t_j), \varphi(t_j), \ldots, \varphi(t_j) \right] \mathcal{G} \right\}
\]

In the conventional formulation of the piecewise polynomials method with collocation weighting the scaling factor \( W \) introduced in this paper does not appear and the \( \varphi_r, r=0, \ldots, p \) are derived from

\[
\varphi_0(t_j) = \lambda^{-1} \left[ I - e^{-\lambda(t_j-t_{j-1})} \right] \cdot \bar{E}
\]

and the recurrence relationship

\[
\varphi_r(t_j) = \lambda^{-1} \cdot \left[ \bar{E}(t_j-t_{j-1})^r - r \varphi_{r-1}(t_j) \right]
\]

(Equations (2.12) and (2.13) with \( W = 1 \))

There is the possibility of rounding errors in this process, especially in the case of small time-steps. The factor \( W \) is introduced to remove this difficulty.

With \( \delta t = t_j - t_{j-1} \) and \( \theta \delta t = t_j - t_{j-1} \), the modified equations (2.12) and (2.13) for \( \varphi_r \) and \( \varphi_0 \) may be written:

\[
\varphi_r = W \lambda^{-1} \cdot \left[ W^r \bar{E} \theta^r \delta t^r - r \varphi_{r-1} \right]
\]

\[
\varphi_0 = W \lambda^{-1} \cdot \left[ I - e^{-\lambda \theta \delta t} \right] \cdot \bar{E}
\]

2.3 Derivation of the \( \varphi \)-functions

The requirement on \( W \) implied by the analysis is that it should be independent of time over the time-step. That is not to say that it should be independent of the time-step.

Put \( W = \frac{1}{\delta t} \)

Then

\[
\varphi_r(\delta t, \theta) = \left[ \frac{\theta^r}{r} \bar{E} - \varphi_{r-1}(\delta t, \theta) \right]
\]
Expanding the exponentials:

\[ Q_0 (8t, \theta) = \frac{1}{8t} \lambda^{-1} \left[ I - e^{-\lambda 8t} \right] \cdot \bar{\rho} \]

\[ Q_0 (8t, \theta) = \left[ \theta - \frac{\theta^2}{2!} (\lambda 8t)^2 - \frac{\theta^3}{3!} (\lambda 8t)^3 + \ldots \right] \cdot \bar{\rho} \]

\[ Q_1 (8t, \theta) = \left[ \frac{\theta^2}{2!} - \frac{\theta^3}{3!} (\lambda 8t)^2 - \frac{\theta^4}{4!} (\lambda 8t)^3 + \ldots \right] \cdot \bar{\rho} \]

\[ Q_2 (8t, \theta) = \left[ \frac{\theta^3}{3!} - \frac{\theta^4}{4!} (\lambda 8t)^2 - \frac{\theta^5}{5!} (\lambda 8t)^3 + \ldots \right] \cdot \bar{\rho} \]

\[ Q_r (8t, \theta) = \left[ \frac{\theta^{r+1}}{(r+1)!} - \frac{\theta^{r+2}}{(r+2)!} (\lambda 8t)^2 + \frac{\theta^{r+3}}{(r+3)!} (\lambda 8t)^3 + \ldots \right] \cdot \bar{\rho} \]

\[ Q_r (8t, \theta) = \left[ \frac{\theta^{r+1}}{r+1} \left[ I + \sum_{i=1}^{\infty} \left( \frac{1}{r+1} \right)^i (\lambda 8t)^i \right] \right] \cdot \bar{\rho} \]

\[ Q_r (8t, \theta) = \frac{\theta^{r+1}}{r+1} \left[ I + \frac{1}{r+1} (\lambda 8t)^{r+1} \right] \cdot \bar{\rho} \]

The series expansions for the Q-functions involved in equations (2.22) are rapidly convergent since they involve the relatively slow time constants associated with the delayed neutron groups. Further, powers of \( \lambda \) involve only scalar operations since \( \lambda \) is diagonal.

Writing equation (2.21) in the new notation,

\[ \varphi(t_j) = e^{-\lambda 8t} \cdot \varphi(t_{j-1}) + \left\{ Q_0 (8t, 1) \varphi(t_{j-1}) + \ldots + Q_p (8t, 1) \right\} \cdot \hat{8} \]

2.4 Behaviour of the Q-functions for small time-steps

Since \( \lim_{\delta t \to 0} Q_r (8t, \theta) = \frac{\theta^{r+1}}{r+1} \cdot \bar{\rho} \)

the Q-functions are well-behaved for small time-steps and from equations (2.23)

\[ \lim_{\delta t \to 0} \left[ \varphi(t_j) \right] = \left[ \varphi(t_{j-1}) + \delta t \left\{ \varphi(t_{j-1}) + \frac{\varphi(t_{j-1})}{2} + \frac{\varphi(t_{j-1})}{3} + \ldots + \frac{\varphi(t_{j-1})}{p+1} \right\} \right] \cdot \bar{\rho} \]

\[ \varphi(t_{j-1}) + \int_{t_{j-1}}^{t_j} \bar{\rho} \varphi(t) dt \]

which corresponds with the limiting behaviour of equations (2.3) with \( \varphi(t) \) replaced by \( \varphi_f(t) \). (Bearing in mind the slow time constants associated with delayed neutrons).

The method does not require that the coefficients of the point kinetics equations should be constant over the time-step. Rather the vectors used in the calculation of \( \eta \) in Appendix I are taken as constant over the time-step, thus \( L \) is constant. The assumption is then made that \( \rho \) and \( \bar{\rho} \) vary linearly over the time-step.
2.5 **Numerical example**

The procedures are best illustrated by means of a simple example such as the fitting of a quadratic in the case of one delayed group.

\[ L = 5 \times 10^{-7} \text{ secs.} \]
\[ \bar{\beta} = 3 \times 10^{-3}. \]
\[ \lambda = 0.3 \text{ sec}^{-1}. \]
\[ \varphi(t) = 100 \]
\[ C(t) = 0.5 \]

The first two examples assume a constant reactivity over the time-step \( \varphi(t > 0) = 95 \) cents. In this case the solution for the amplitude function can be obtained by evaluation of the eigenvalues and eigenvectors of the kinetics matrix as:

\[ \varphi(\delta t) = 964.424 e^{5.59015 \delta t} - 864.424 e^{-306.108 \delta t} \tag{2.24} \]

Evaluating the series to order 3, we have:

\[ \varphi(\delta t) = 100 + 26.99998 \times 10^4 \delta t - 0.404841 \times 10^2 \delta t^2 + 0.00413254 \times 10^1 \delta t^3 \tag{2.25} \]

Hence for \( \delta t = 10^{-4} \) sec. the solution should be well represented by a quadratic and this is the first example

**Example 1. \( \delta t = 10^{-4} \) sec., constant reactivity**

Using equations (2.22),

\[ Q_0(10^{-4}, \frac{1}{2}) = 0.499996 \bar{\beta} \quad Q_1(10^{-4}, \frac{1}{2}) = 0.124999 \bar{\beta} \]
\[ Q_0(10^{-4}, 1) = 0.999985 \bar{\beta} \quad Q_1(10^{-4}, 1) = 0.499995 \bar{\beta} \]

It is interesting to check these values with the limiting behaviour of the \( Q \)-functions for small time-steps.

Using equations (2.14),

\[ \xi'(5 \times 10^{-5}) = (0.499996, 0.249998) \bar{\beta} \]
\[ \xi'(10^{-4}) = (0.999985, 0.999990) \bar{\beta} \]

Naturally the unit vector in equations (2.14) becomes scalar unity for one delayed group.

Using equations (2.16),

\[ h'(5 \times 10^{-5}) = 5 \times 10^{-7} (10^4, 10^4) - 2.85 \times 10^{-3} (0.5, 0.25) + (0.499996, 0.249998) 3 \times 10^{-3} \]

\[ \therefore h'(5 \times 10^{-5}) = (5.07499 \times 10^{-3}, 5.03749 \times 10^{-3}) \]
Using equations (2.17),
\[
\gamma = \begin{bmatrix} 0.135002 \\ 0.135005 \end{bmatrix}
\]
\[
\therefore \begin{bmatrix} 5.07499 \times 10^{-3} & 5.03749 \times 10^{-3} \\ 5.14966 \times 10^{-3} & 1.01500 \times 10^{-2} \end{bmatrix} \cdot \alpha = \begin{bmatrix} 0.135002 \\ 0.135005 \end{bmatrix}
\]
(see equations (2.18))

Then \[
\phi_f(\delta t) = 100 + 26.9937 \times 10^4 \delta t - 0.395230 \times 10^8 \delta t^2
\]
C.f. equation (2.25)

Now \[
\phi_f(10^{-4}) = 126.599, \text{ in exact agreement with (2.24)}.\]

In this example the time-step was chosen to be such that the series expansion (2.25) of (2.24) was well represented by the quadratic. The example confirms that the fitted polynomial is a good representation of (2.25) and that the solution agrees well with (2.24). It is easy to see that for a time-step of \(10^{-2}\) sec. equation (2.25) is badly represented by the quadratic and the next example illustrates the behaviour of the method in this situation.

Example 2. \(\delta t = 10^{-2}\) sec., constant reactivity

\[Q_0(10^{-2},\frac{1}{2}) = 0.499963 \bar{p} \quad Q_1(10^{-2},\frac{1}{2}) = 0.124938 \bar{p}\]

\[Q_0(10^{-2},1) = 0.998502 \bar{p} \quad Q_1(10^{-2},1) = 0.499500 \bar{p}\]

\[g'(5 \times 10^{-3}) = (0.499963, 0.249876) \bar{p}\]

\[g'(10^{-2}) = (0.998502, 0.999000) \bar{p}\]

\[h'(5 \times 10^{-3}) = 5 \times 10^{-7} (10^2, 10^2) - 2.85 \times 10^{-3} (0.5, 0.25) + (0.499963, 0.249876) 3 \times 10^{-3}\]
\[
\therefore h'(5 \times 10^{-3}) = (1.24889 \times 10^{-4}, 8.7128 \times 10^{-5})
\]

\[h'(10^{-2}) = 5 \times 10^{-7} (10^2, 2 \times 10^2) - 2.85 \times 10^{-3} (1, 1) + (0.998502, 0.999000) 3 \times 10^{-3}\]
\[
\therefore h'(10^{-2}) = (1.95506 \times 10^{-4}, 2.47000 \times 10^{-4})
\]
\[
\begin{bmatrix}
0.135225 \\
0.135449
\end{bmatrix}
\]

\[
\begin{bmatrix}
1563.62 \\
-689.264
\end{bmatrix}
\]

\[
\gamma = \begin{bmatrix} 0.135225 \\ 0.135449 \end{bmatrix}
\]

\[
\alpha = \begin{bmatrix} 1563.62 \\ -689.264 \end{bmatrix}
\]

\[
\varphi_f(8t) = 100 + 1563.62 \times 10^8 t - 689.264 \times 10^8 t^2
\]

This quadratic bears little resemblance to the corresponding terms in (2.25). However,

\[
\varphi_f(10^{-2}) = 974.356
\]

This compares with \( \varphi(10^{-2}) = 979.385 \) from equation (2.24) and the agreement between the two solutions at the end of the time-step is striking for an example of this nature.

The present method is able to account for the variation of the coefficients of the kinetics matrix over the time-step insofar as the coefficients may be different at each of the collocation points. This facility contrasts with most other methods where the coefficients must necessarily be assumed to be stepwise constant. The final example illustrates the effect of representing the reactivity as a ramp from zero to average 95 cents over the time-step.

**Example 3.** \( 8t = 10^{-4} \) sec., reactivity ramp

\[
\begin{align*}
\rho(5 \times 10^{-5}) &= 95 \text{ cents} \\
\rho(10^{-4}) &= 190 \text{ cents}
\end{align*}
\]

\[
\begin{align*}
\zeta'(5 \times 10^{-5}), \xi'(5 \times 10^{-5}) \text{ and } \zeta'(10^{-4}) \text{ as in example 1} \\
\zeta'(10^{-4}) &= 5 \times 10^{-7} (10^4, 2 \times 10^4) - 5.7 \times 10^{-3} (1, 1) + (0.999985, 0.999990) 3 \times 10^{-3}
\end{align*}
\]

\[
\begin{align*}
\zeta'(10^{-4}) &= (2.29996 \times 10^{-3}, 7.29997 \times 10^{-3})
\end{align*}
\]

\[
\begin{bmatrix}
0.135002 \\
0.420005
\end{bmatrix}
\]

\[
\begin{bmatrix}
-44.3915 \\
71.5213
\end{bmatrix}
\]

\[
\begin{align*}
\varphi_f(8t) &= 100 - 44.3915 \times 10^8 t + 71.5213 \times 10^8 t^2 \\
\text{and } \varphi_f(10^{-4}) &= 127.130
\end{align*}
\]

The functional fit is quite different from (2.25). In particular

\[
\left( \frac{d\varphi_f}{dt} \right)_j = -4.44 \times 10^5 \text{ sec}^{-1} \text{ compared with } \left( \frac{d\varphi}{dt} \right)_j = 2.7 \times 10^5 \text{ sec}^{-1}
\]

from equation (2.25). Of course an initial reactivity of 95 cents was implied in deriving equations (2.24) and (2.25) whereas the reactivity ramp used in deriving equation (2.26) implies an initial reactivity of zero. In this case

\[
\left( \frac{d\varphi}{dt} \right)_j = \frac{1}{L} \left( -\beta R_0 + \lambda C_0 \right) = -3.0 \times 10^5 \text{ sec}^{-1}
\]
Hence the behaviour of (2.26) is plausible for the reactivity variation imposed on the solution, although the numerical value of the time derivative of the amplitude function at time $t_{j-1}$ is not numerically exact. This feature is readily understood as the $j-1$ start of the time-step is not a collocation point and so the corresponding reactivity is not imposed on the solution. This may be an argument in favour of the use of spline functions.
Appendix 3

Solution of the spatial function equations

Equations (1.14) of Appendix 1 may be written:

\[- \nabla \cdot \nabla \psi + \left[ A + V^{-1} \left( \frac{1}{\rho} \frac{d}{dt} \varphi + \frac{1}{\Delta t} \right) \right] \psi = k(1-\beta) \chi_{p} \cdot \xi' \cdot \psi + \xi \ldots (3.1)\]

where \( \xi = \frac{1}{\Delta t} V^{-1} \cdot \psi_{k-1} + \frac{1}{\rho} \chi_{d} \cdot \lambda \cdot \xi \) is a spatial function independent source. \( k \) is an eigenvalue (multiplier on prompt source) introduced in order to satisfy the requirement \( \langle \psi^{*}, V^{-1} \psi \rangle = 1 \) (arbitrary constant) which is used in the derivation of the amplitude function equations and \( \psi_{k-1} \) refers to the spatial function calculated at the previous spacial function recalculation.

The spatial function is the solution of equations (3.1), which are at the same time a source problem and an eigenvalue problem.

3.1 Finite difference approximation

The space is divided into a number \( m \) of finite intervals, the general mesh interval is denoted \( \delta z_{i} \) and the corresponding spatial function vector \( \psi_{i} \). This spatial function vector is taken as relating to the average over the mesh interval and the subscript \( i \) identifies the diffusion constants inside that interval.

Integrate equations (3.1) over mesh interval \( i \).

\[ \int_{z_{i-1},i}^{z_{i+1},i} \nabla \cdot \nabla \psi_{i} \, dz = \left[ D \cdot \nabla \psi_{i} \cdot \eta \right]^{z_{i+1},i} \left[ \psi_{i} \right]_{z_{i-1},i} \ldots (3.2) \]

where \( D_{j} \) represents the diffusion coefficient between mesh intervals \( j \) and \( j+1 \).

Expression (3.2) is approximated by

\[ \int_{z_{i-1},i}^{z_{i+1},i} \nabla \cdot \nabla \psi_{i} \, dz = D_{i+1} \cdot \frac{\psi_{i+1} - \psi_{i}}{\delta z_{i+1}} - D_{i-1} \cdot \frac{\psi_{i} - \psi_{i-1}}{\delta z_{i-1}} + \Delta_{i-1,i} \cdot \psi_{i-1} - \left[ \Delta_{i+1,i} + \Delta_{i-1,i} \right] \cdot \psi_{i} \]

where \( \Delta_{j+1,i} = \frac{D_{j+1,i}}{\delta z_{j+1} + \delta z_{i+1}} \), and \( D_{j,j+1} \) is calculated from

\[-\nabla \cdot \nabla \psi + \left[ A + V^{-1} \left( \frac{1}{\rho} \frac{d}{dt} \varphi + \frac{1}{\Delta t} \right) \right] \psi = k(1-\beta) \chi_{p} \cdot \xi' \cdot \psi + \xi \ldots (3.1)\]
\[
\frac{\delta z_j + \delta z_{j+1}}{D_j \cdot j+1} = \frac{\delta z_j}{D_j} + \frac{\delta z_{j+1}}{D_{j+1}}
\]

Equations (3.1) become

\[
- \Delta_{i,i+1} \psi_{i+1} - \Delta_{i-1,i} \psi_{i-1} + \left[ \Delta_{i,i+1} + \Delta_{i-1,i} \right] \psi_i
\]

\[
+ \delta z_i \left[ A_i + \nu^{-1} \left( \frac{1}{\partial} \frac{d}{dt} \varphi + \frac{1}{\Delta t} \right) \right] \psi_i = k \delta z_i (1-\beta) \psi_{i-1} - \psi_i + \delta z_i S_i
\]

and \( \psi_i \) represents the average spatial function vector in mesh interval \( j \).

i.e. \( \Delta_{i-1,i} \psi_{i-1} + \Delta_{i,i+1} \psi_{i+1} = k \delta z_i (1-\beta) \psi_{i-1} + \delta z_i S_i \) \( \ldots \) (3.3)

where \( \Omega_i = \Delta_{i-1,i} \psi_{i-1} + \Delta_{i,i+1} \psi_{i+1} \) and \( \Delta_{i-1,i} \psi_{i-1} + \Delta_{i,i+1} \psi_{i+1} = k \delta z_i (1-\beta) \psi_{i-1} + \delta z_i S_i \)

Expand the spatial function to first order, about the outer boundaries.

When the space is divided into \( m \) mesh intervals, equations (3.3) hold for mesh intervals 2, \ldots, \( m-1 \). For the end mesh intervals a boundary condition is required which will be applied at the outer boundaries of the system.

This is taken as

\[ D \cdot \nabla \psi = -\lambda_{\text{ex}} \psi \] where \( \lambda_{\text{ex}} \) is an inverse extrapolation length.

In obvious notation:

\[
\psi_m = \psi_{m+} - \frac{1}{2} \delta z_m \frac{\partial}{\partial z} \psi_{m+}
\]

\[
\psi_1 = \psi_{1-} + \frac{1}{2} \delta z_1 \frac{\partial}{\partial z} \psi_{1-}
\]

Here \( \psi_m \) and \( \psi_1 \) are taken as referring to the centroids of the mesh intervals.
Using these expressions in (3.2) leads to the following equations for mesh intervals \( m \) and 1.

\[
-\Delta \psi_{m-1}^{\text{m}} + \Omega \psi_{m}^{\text{m}} = k F_{m} \psi_{m}^{\text{m}} + 5z_{m} S_{m}
\]

\[
\Omega \psi_{1}^{1} - \Delta \psi_{2}^{2} = k F_{1} \psi_{1}^{1} + 5z_{1} S_{1}
\]

where \( \Omega = \Delta_{m-1}^{m} + 5z_{m} \left[ A_{m} + V^{-1} \left( \frac{1}{\partial} \frac{d}{dt} \partial + \frac{1}{\Delta t} \right) \right] + D_{m} \left[ \frac{1}{2} 5z_{m} I - \lambda_{\text{ex}} \right]^{-1} \]

The set of equations for \( \psi_{i}^{i}, i=1,m \) can now be written.

\[
\begin{bmatrix}
\Omega_{1} & -\Delta_{1,2} & & & & \\
-\Delta_{1,2} & \Omega_{2} & -\Delta_{2,3} & & & \\
& & \ddots & \ddots & & \\
& & & \ddots & \ddots & \ddots \\
& & & & \ddots & \ddots & \ddots \\
\end{bmatrix}
\begin{bmatrix}
\psi_{1}^{1} \\
\psi_{2}^{2} \\
\vdots \\
\psi_{m}^{m} \\
\end{bmatrix}
= k
\begin{bmatrix}
F_{1} \\
F_{2} \\
\vdots \\
F_{m} \\
\end{bmatrix}
\begin{bmatrix}
\psi_{1}^{1} \\
\psi_{2}^{2} \\
\vdots \\
\psi_{m}^{m} \\
\end{bmatrix}
+ \begin{bmatrix}
5z_{1} S_{1} \\
5z_{2} S_{2} \\
\vdots \\
5z_{m} S_{m} \\
\end{bmatrix}
\]

\[
(3.4)
\]

### 3.2 Solution of the difference equations

These equations must be solved for the eigenvalue \( k \) and fluxes \( \psi_{1}, \ldots, \psi_{m} \). The equations are first subjected to a form of matrix powering, modified by the inclusion of the source term. Let the estimate of \( k \) at the \( N \)th iteration be \( k^{(N)} \), the input estimate of the spatial function be \( \psi_{i}^{(N-1)} \), \( i=1,m \) and the output estimate \( \psi_{i}^{(N)} \), \( i=1,m \).
The improved estimate of the spatial function is derived from the set of linear inhomogeneous equations

\[
\begin{bmatrix}
\Omega_1 & -\Delta_{1,2} & & & \\
-\Delta_{1,2} & \Omega_2 & -\Delta_{2,3} & & \\
& -\Delta_{m-2,m-1} & \Omega_{m-1} & -\Delta_{m-1,m} & \\
& & -\Delta_{m-1,m} & \Omega_m & \\
& & & & \Omega_m
\end{bmatrix}
\begin{bmatrix}
\psi_1(N) \\
\psi_2(N) \\
\psi_3(N) \\
\vdots \\
\psi_m(N)
\end{bmatrix}
= \begin{bmatrix}
\xi_1(N) \\
\xi_2(N) \\
\xi_3(N) \\
\vdots \\
\xi_m(N)
\end{bmatrix}
\]

... (3.5)

where \( \xi(N) = k(N) \)

Equations (3.5) are solved using the Choleski method modified to use matrix elements, i.e., the following transformation is performed.

\[
\begin{bmatrix}
I - S_2 \\
I - S_3 \\
\vdots \\
I - S_m \\
I
\end{bmatrix}
\begin{bmatrix}
\psi_1(N) \\
\psi_2(N) \\
\psi_3(N) \\
\vdots \\
\psi_m(N)
\end{bmatrix}
= \begin{bmatrix}
R_1(N) \\
R_2(N) \\
\vdots \\
R_m(N)
\end{bmatrix}
\]

where \( S_n^{-1} = \Omega^{-1} \cdot \Delta_{1,2} \)

\[
S_i = \left[ \Omega_{i-1} - \Delta_{1,2,1-1} \cdot S_{i-1} \right]^{-1} \cdot \Delta_{i-1,i}, \quad i = 3, m
\]

\[
R^{(N-1)}_i = \Omega^{-1}_i \cdot \xi^{(N-1)}_i = S_2 \cdot \Delta^{-1}_1 \cdot \xi^{(N-1)}_i
\]

\[
R^{(N-1)}_i = \left[ \Omega_i - \Delta_{1,2,1-1} \cdot S_i \right]^{-1} \cdot \left[ \xi^{(N-1)}_i + \Delta_{i-1,i} \cdot R^{(N-1)}_{i-1} \right], \quad i = 2, m
\]

\[
\psi^{(N)}_m \text{ is obtained directly and the remaining } \psi^{(N)}_i \text{ by back substitution.}
\]

In this phase of the calculation use is made of the lower triangular form of the matrices to be inverted. Furthermore the inversions need be performed only once as the matrices are independent of the iterations.

The revised estimate of the eigenvalue is derived as follows.

\( \psi^{(N)}_i \) is the solution of the equations

\[
\begin{bmatrix}
A_i + V^{-1} \left( \frac{1}{\varrho} \frac{d}{dt} \varrho + \frac{1}{\Delta t} \right) - \nabla \cdot D_i \nabla
\end{bmatrix} \cdot \psi^{(N)}_i = \frac{k^{(N)}}{\rho^{(N-1)}} \cdot (1-\beta) \xi^{(N-1)} \cdot \psi^{(N-1)}_i + S_i \quad \ldots (3.6)
\]

where the inner product \( P^{(N-1)}_i = \langle \psi^{(N-1)}_i, V^{-1} \psi^{(N-1)}_i \rangle \) and is a scalar divided into the output spatial function estimate from each iteration to ensure the required property \( \langle \psi^{(N)}_i, V^{-1} \psi^{(N)}_i \rangle = 1 \).

It is convenient to define

\[
E_i = A_i + V^{-1} \left( \frac{1}{\varrho} \frac{d}{dt} \varrho + \frac{1}{\Delta t} \right) - \nabla \cdot D_i \nabla
\]

\[
F_i = (1-\beta) \xi^{(N-1)}_i
\]

In this notation, equations (3.6) become

\[
E_i \cdot \psi^{(N)}_i = \frac{k^{(N)}}{\rho^{(N-1)}} \cdot F_i \cdot \psi^{(N-1)}_i + S_i \quad \ldots (3.8)
\]

The estimate of \( \psi^{(N)}_i \) for input to the next iteration is

\[
\psi^{(N)}_i = \frac{1}{\rho^{(N)}} \cdot \psi^{(N)}_i
\]

Then

\[
E_i \cdot \psi^{(N+1)}_i = \frac{k^{(N+1)}}{\rho^{(N)}} \cdot F_i \cdot \psi^{(N)}_i + S_i \quad \ldots (3.9)
\]
Now if \( \psi_1^{(N+1)} \) is the required solution,

\[
\psi_1^{(N+1)} = \frac{1}{p_1^{(N)}} \psi_1^{(N)}
\]  

...(3.11)

Substitute (3.11) into (3.8)

\[
E_1 \cdot \psi_1^{(N+1)} = -\frac{k^{(N)}}{p_1^{(N-1)}} F_1 \cdot \psi_1^{(N-1)} + \frac{1}{p_1^{(N)}} S_1
\]

\[
\therefore \langle \psi_1^{(N+1)} \rangle = k^{(N)} \frac{1}{p_1^{(N-1)}} \langle \psi_1^{(N-1)} \rangle + \left(1 - \frac{1}{p_1^{(N)}} \right) \frac{1}{p_1^{(N)}} \langle \psi_1^{(N)} \rangle
\]  

...(3.12)

Inspection of equations (3.10) and (3.12) yields:

\[
k^{(N+1)} = k^{(N)} \frac{\langle \psi_1^{(N-1)} \rangle}{\langle \psi_1^{(N)} \rangle} + (1 - \frac{1}{p_1^{(N)}}) \frac{1}{p_1^{(N)}} \langle \psi_1^{(N)} \rangle
\]  

...(3.13)

where \( \psi_1^{(N-1)} = \frac{1}{p_1^{(N-1)}} \psi_1^{(N-1)} \) is the normalised spatial function output from iteration (N-1).

3.3 Extrapolation procedure

The iterative procedure outlined above could be continued until the spatial function was determined to within the required accuracy. This might imply some hundreds of iterations and various extrapolation techniques have been developed to improve the rate of convergence in calculations of this nature. The approach adopted in the present work was suggested by the presence of the spatial function independent source and the fact that convergence of the eigenvalue (being an integral parameter) is much faster than convergence of the spatial function itself.

When the eigenvalue has converged to within a prescribed accuracy, the current estimate is used in (3.4) to form the set of inhomogeneous equations
These equations are solved using the same Choleski algorithm as before, except that the matrix inversions are performed on full matrices and not lower triangular.

The objection to this procedure is, of course, that the error in the estimate of the eigenvalue used in (3.15) will lead to a spatial function which, although a solution of (3.14), does not have the required property

\[ \langle \bar{\varphi}' \cdot V^{-1} \bar{\varphi} \rangle = 1 \]

Furthermore the actual value of this inner product will be highly sensitive to the eigenvalue, particularly when the \( S_i \) in equations (3.14) are small compared with the prompt spatial function multiplied source, as may occur when the amplitude function is rising rapidly.

This sensitivity can be put to good use, however, by devising an iterative scheme which uses the value of the inner product to produce an improved estimate of the eigenvalue.

In the notation of equations (3.7), \( \bar{\varphi}_i^{(N)} \) is the solution of the set of equations

\[ E_i \bar{\varphi}_i^{(N)} = k^{(N)} F_i \bar{\varphi}_i^{(N)} + S_i \]

In general,

\[ \langle \bar{\varphi}' \cdot V^{-1} \bar{\varphi} \rangle \neq 1. \]

At this stage the best estimate of the spatial function would be

\[ \bar{\varphi}_i^{(N+1)} = \frac{1}{p_i^{(N)}} \bar{\varphi}_i^{(N)} \]

\[ \text{(3.17)} \]
Substituting in (3.16),
\[ E_{i} \psi_{i}^{(N+1)} = k(N) F_{i} \psi_{i}^{(N+1)} + \frac{1}{p_{i}} S_{i} \]

Then
\[ \langle \psi \cdot E \cdot \psi \rangle^{(N+1)} = k(N) \langle \psi \cdot F \cdot \psi \rangle^{(N+1)} + \left\{ \frac{1}{p_{i}} - 1 \right\} \langle \psi \cdot S \rangle + \langle \psi \cdot S \rangle \quad \ldots (3.18) \]

Similarly
\[ \langle \psi \cdot E \cdot \psi \rangle^{(N+2)} = k(N+1) \langle \psi \cdot F \cdot \psi \rangle^{(N+2)} + \left\{ \frac{1}{p_{i}} - 1 \right\} \langle \psi \cdot S \rangle + \langle \psi \cdot S \rangle \quad \ldots (3.19) \]

If the \((N+1)\)th iteration produces the required solution,
\[ p_{i}^{(N+1)} = 1 \quad \text{and} \quad \psi_{i}^{(N+2)} = \psi_{i}^{(N+1)} \]

From (3.19),
\[ \langle \psi \cdot E \cdot \psi \rangle^{(N+1)} = k(N+1) \langle \psi \cdot F \cdot \psi \rangle^{(N+1)} + \langle \psi \cdot S \rangle \quad \ldots (3.20) \]

Comparing equations (3.18) and (3.20):
\[ \frac{k(N+1)}{k(N)} = \left\{ \frac{1}{p_{i}} - 1 \right\} \frac{\langle \psi \cdot S \rangle}{\langle \psi \cdot F \cdot \psi \rangle^{(N+1)}} \]
\[ \text{ie} \quad k(N+1) = k(N) \left\{ 1 - \frac{1}{p_{i}} \right\} \frac{\langle \psi \cdot S \rangle}{\langle \psi \cdot F \cdot \psi \rangle^{(N)}} \quad \ldots (3.21) \]

using (3.17).

As would be expected, (3.21) is the special case of (3.13) with the input estimate of the spatial function equal to the output estimate.

The above procedure (which we will call "direct iteration") is treated as an extrapolation procedure as a precaution against ill-conditioning. The eigenvalue and spatial function estimates from the direct iteration scheme are submitted to the power iteration scheme, which is taken to convergence. This procedure guards against a situation which could occur in a rapidly rising transient where the precursor derived source term would become small. It was thought that in this event it might have been necessary to switch the direct iteration scheme to the modified version used in extrapolating the steady state and adjoint calculations and described below.

In practice the direct iteration scheme has been well-conditioned in all cases attempted, despite rises in the amplitude function of many orders of magnitude. (Super prompt critical excursions in fast reactor situations without temperature feedback). This may be due to use of the improved quasi-static method, which contributes a source term which does not decay to zero with increase in amplitude function.
One or two power iterations provide an adequate estimate of the eigenvalue for submission to the direct iteration scheme and three direct iterations are generally sufficient for convergence. The estimate of the spatial function provided by the direct iteration scheme has always been accepted by the power iteration scheme and numerical checks have shown the spatial function to be converged to the accuracy of the computer.

In fact the preliminary estimation of the eigenvalue as described above is a precaution suggested by the sensitivity of the direct iteration scheme to errors in the eigenvalue estimate. It has not been demonstrated to be strictly necessary in any particular case.

3.4 Calculation of distributed precursors

The distributed precursors are updated from one spatial function recalculation to the next by integrating equations (1.15) over each amplitude function time-step, subject to the assumptions that $\psi(z,t) = \psi(z,t_{k-1})$ and that $f$ is constant over one amplitude function time step.

The following procedure was suggested by the similarity between equations (1.15) and (2.3)

$$
\xi(z,t_j) = e^{-\lambda(t_j-t_{j-1})} \cdot \xi(z,t_{j-1}) + f' \cdot \psi(z,t_{k-1})
$$

since $f' \cdot \psi(z,t_{k-1})$ is a scalar.

Replace $\varphi(t)$ by $\varphi_{j-1}(t)$ including $\xi(t)$ over the amplitude function time-step. (See Appendix 2).

Then

$$
\xi(z,t_j) = e^{-\lambda(t_j-t_{j-1})} \cdot \xi(z,t_{j-1}) + f' \cdot \psi(z,t_{k-1}) \left\{ e^{-\lambda(t_j-t_{j-1})} \int_{t_{j-1}}^{t_j} \varphi_{j-1}(t) dt + \sum_{n=1}^{p} Q_n(\delta t, 1) \right\}
$$

in the notation of equations (2.23) except that the actual delayed fractions replace the effective delayed fractions in the $Q$-functions.

Note that by multiplying equations (3.22) on the left by $(1/\eta) \text{diag}(\varphi'(z), \lambda_d)$, integrating over the system and using (1.6) and (1.11) we retrieve equations (2.23). This ensures consistency between the distributed and integrated precursor densities.
3.5 Steady-state spatial function calculation

Set $\frac{\partial}{\partial t} \xi = \frac{\partial}{\partial t} \xi = 0$ in equations (1.1) and (1.2) and $\xi = \psi$ since the amplitude function assumes the value unity in steady state (definition).

$$\nabla \cdot D \nabla \psi + (1-\beta) X_p \cdot \mathbf{f}' \cdot \psi + X_d \cdot \lambda \cdot \psi = 0 \quad \cdots (3.23)$$

$$\lambda \cdot \psi = \mathbf{f}' \cdot \psi \quad \cdots (3.24)$$

Substitute (3.24) into (3.23)

$$\nabla \cdot D \nabla \psi + A \cdot \psi = k \left[ (1-\beta) X_p + X_d \cdot \mathbf{f}' \right] \cdot \mathbf{f}' \cdot \psi \quad \cdots (3.25)$$

where $k$ is an eigenvalue introduced to make the system just critical.

Equations (3.25) have the same form as equations (3.1) with the source term $S = 0$. The source iterations can proceed as before to produce an estimate of the eigenvalue. This estimate is used in equations (3.14) to obtain a set of linear equations for $\psi_i$. This set of equations is, of course, homogeneous in the $\psi_i$ and the Choleski transformations are valid only as far as

$$\left[ U_m - \Delta_{m-1,m} \cdot S_m \right] \cdot \psi_m = 0 \quad \cdots (3.26)$$

If the estimate of the eigenvalue used in forming the matrices $U_i$, $i = 1, m$ had been exact, then $\left[ U_m - \Delta_{m-1,m} \cdot S_m \right]$ would be singular and the required solution for $\psi_m$ would be the eigenvector of $\left[ U_m - \Delta_{m-1,m} \cdot S_m \right]$ corresponding to the zero eigenvalue. In general the estimate of the eigenvalue will not be exact and equations (3.26) are therefore replaced by

$$\left[ U_m - \Delta_{m-1,m} \cdot S_m \right] \cdot \psi_m = \omega_m \psi_m \quad \cdots (3.27)$$

and $\omega_m \to 0$ as the error in the estimate of eigenvalue $k$ approaches zero.

The required eigenvector of (3.27) is determined by inverse iteration, ie we calculate the eigenvector corresponding to the dominant eigenvalue of matrix $\left[ U_m - \Delta_{m-1,m} \cdot S_m \right]^{-1}$ by matrix multiplication. Since $\left[ U_m - \Delta_{m-1,m} \cdot S_m \right]$ is almost singular for a good estimate of eigenvalue $k$, the inverse matrix has a strongly dominant eigenvalue and the process is rapidly convergent. Furthermore the original eigenvalue problem is reduced to an eigenvalue problem on a full matrix of size $G \times G$, where $G$ is the number of energy groups in the spatial function.

The remaining $\psi_i$ are determined from $\psi_m$ by back substitution and finally the output estimate of the spatial function is normalised so that

$$<\psi^* \cdot \mathbf{V}^{-1} \cdot \psi> = 1.$$ 

It has been found that when this estimate of the spatial function is input to the source iteration, convergence is achieved in about ten iterations.

Finally the steady state distributed precursor population is derived from equations (3.24).
3.6 Steady-state adjoint function calculation

Transposition of the matrix operators in equations (3.25) destroys the lower triangular nature of the matrices inverted in the Choleski procedure of the source iterations. The elements of the adjoint function at each spatial position are therefore symmetrically re-ordered in energy. The adjoint matrix operators are then formed by transposing about the non-leading diagonal, thus retaining the lower triangular form where appropriate.

Since the eigenvalue is the same as in the direct spatial function problem, the extrapolation technique of the preceding section is used without previous resource to source iteration. When the output estimate of the adjoint function is submitted to source iteration it is immediately accepted. Finally the elements of the adjoint function solution are re-ordered.
Appendix 4

Temperature calculation and reactivity feedback

This section of the code was written specifically for the 1-D benchmark calculation and follows the notation used in the specification as far as possible. This explains any inconsistency in notation between this appendix and other parts of the paper.

Local linear heat rating $Q_i = V_f (\text{HPP}) \left( \Sigma_{f_1}^1 \phi_i^1 + \Sigma_{f_2}^2 \phi_i^2 \right)$ where $i$ refers to the $i$th axial slice.

The steady state calculation iterates between the temperature calculation and the spatial function calculation to allow for temperature feedback and the imposed coolant temperature rise.

\[ ie \sum_{a_1}^1 = \sum_{a_0}^1 (1 + \alpha T_{fi}) \]
\[ m \sum_{i=1}^n Q_{0,1} \delta z_i = AC \delta T_c \]

The equations governing heat removal in axial slice $i$ at time $t$ are given as:

\[ K_f (\bar{T}_{fi} - T_{si}) = Q_i - \frac{\partial}{\partial t} T_{fi} \]  \hspace{1cm} (4.1)
\[ K_f (\bar{T}_{fi} - T_{si}) = h (T_{si} - T_{ci}) \]  \hspace{1cm} (4.2)
\[ C_f \left( \frac{\partial}{\partial t} T_{ci} + A \frac{\partial}{\partial z} T_{ci} \right) = h(T_{si} - T_{ci}) \]  \hspace{1cm} (4.3)
\[ T_{fi, max} = 2 \bar{T}_{fi} - T_{si} \]  \hspace{1cm} (4.4)

From (4.2),
\[ T_{si} = \frac{1}{h+K_f} (K_f \bar{T}_{fi} + hT_{ci}) \]  \hspace{1cm} (4.5)

Eliminating $T_{si}$ from (4.1) and (4.2):
\[ \frac{\partial}{\partial t} \bar{T}_{fi} = \frac{-hK_f}{C_f (h+K_f)} \bar{T}_{fi} + \frac{hK_f}{C_f (h+K_f)} T_{ci} + \frac{Q_i}{C_f} \]  \hspace{1cm} (4.6)
\[ \frac{\partial}{\partial t} T_{ci} = \frac{hK_f}{C_f (h+K_f)} \bar{T}_{fi} - \frac{hK_f}{C_f (h+K_f)} T_{ci} - A \frac{\partial}{\partial z} T_{ci} \]  \hspace{1cm} (4.7)

Now \[ \frac{\partial}{\partial z} T_{ci} = \frac{1}{\delta z_i} (T_{ci}^+ - T_{ci}^-) \]
\[ 1 \] and \[ T_{ci} = \frac{1}{2} (T_{ci}^+ + T_{ci}^-) \]

in obvious notation.
\[
\frac{\partial}{\partial t} T_i = B \cdot T_i + \mathcal{S}_i \tag{4.8}
\]

and \( T_i = -B^{-1} \cdot \mathcal{S}_i \) in steady state. \( \tag{4.9} \)

where \( B = \begin{bmatrix}
  -hK_f \\
  \frac{hK_f}{C_f(h+K_f)}
\end{bmatrix}
\]

and \( \mathcal{S}_i = \begin{bmatrix}
  0 \\
  \frac{hK_f}{2C_f(h+K_f)}
\end{bmatrix}
\)

\[
\frac{\partial}{\partial t} T_{ci} \text{ is obtained from the solution for the preceding axial segment.}
\]

\[
\frac{\partial}{\partial t} T_{ci} \equiv 0 \text{ for constant coolant inlet temperature.}
\]

The formal solution of equations (4.8) over a time-step is given by

\[
T(t+\delta t) = e^{B\delta t} \cdot T(t) + B^{-1} \cdot \left[ e^{B\delta t} - I \right] \cdot \mathcal{S}_i \tag{4.10}
\]

The usual procedure would be to approximate the exponential matrix by one of the first order Padé approximants. The time-step size for the temperature calculation would then be limited by the requirement for an adequate representation of the source term in (4.10). Further by the requirement that the Padé approximant should adequately represent the exponential of the largest eigenvalue in absolute magnitude of matrix \( B \) whose eigenvector makes a significant contribution to the solution of equations (4.8). This latter requirement is complicated by the dependence of the dominant eigenvalue of matrix \( B \) on the spatial mesh. The smaller the spatial mesh, the smaller the time-step necessary to adequately represent the exponential matrix.

Finally the relationship between the time-steps required for the amplitude function calculation and those for the temperature calculation would derive from the relative magnitudes of the eigenvalues of the kinetics matrix and the temperature system matrix and on the relative efficiencies of the piecewise polynomials method and the Padé method used.

In view of the relatively short time-scale for production of the benchmark results it was decided to avoid the numerical experiments which would be needed if such an approach was adopted by transforming the temperature calculation to the normal coordinates, employing scalar exponentiation on the eigenvalues of the temperature system matrix \( B \) and performing the inverse similarity transformation to enable the calculation of feedbacks. The two
eigenvalues and the modal matrix were calculated by direct and inverse matrix multiplication, which is efficient for widely separated eigenvalues as is the case in the benchmark problems.

With the use of this approach it was felt to be adequate to calculate the temperatures on the same time mesh as the amplitude function. This time-mesh is now dictated by the efficiency of the piecewise polynomials method, the need for an adequate representation of sources into the temperature equations and the requirement for recalculation of reactivity feedbacks.
### Appendix 5

#### Notation

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_g$</td>
<td>Neutron flux, group g</td>
<td>$L^{-2} T^{-1}$</td>
</tr>
<tr>
<td>$v_g$</td>
<td>Mean neutron velocity in group g</td>
<td>$LT^{-1}$</td>
</tr>
<tr>
<td>$D_g$</td>
<td>Diffusion coefficient for neutrons in group g</td>
<td>L</td>
</tr>
<tr>
<td>$n_g$</td>
<td>Number of neutrons per fission in group g</td>
<td></td>
</tr>
<tr>
<td>$\Sigma_{fg}$</td>
<td>Macroscopic fission cross-section in group g</td>
<td>$L^{-1}$</td>
</tr>
<tr>
<td>$\Sigma_{ag}$</td>
<td>Macroscopic absorption cross-section in group g</td>
<td>$L^{-1}$</td>
</tr>
<tr>
<td>$\Sigma_{rg'}-g$</td>
<td>Macroscopic removal cross-section from group g' to group g</td>
<td>$L^{-1}$</td>
</tr>
<tr>
<td>$X_p(E_g)$</td>
<td>Fraction of prompt fission neutrons born into group g</td>
<td></td>
</tr>
<tr>
<td>$\epsilon_i$</td>
<td>Delayed neutron precursor density, delayed group i.</td>
<td>$L^{-3}$</td>
</tr>
<tr>
<td>$\lambda_i$</td>
<td>Inverse time constant for decay of delayed group i</td>
<td>$T^{-1}$</td>
</tr>
<tr>
<td>$X_{di}(E_g)$</td>
<td>Fraction of neutrons from delayed group i born into group g</td>
<td></td>
</tr>
<tr>
<td>$\beta_i$</td>
<td>Delayed neutron fraction, group i</td>
<td></td>
</tr>
<tr>
<td>$\beta$</td>
<td>Total delayed neutron fraction</td>
<td></td>
</tr>
</tbody>
</table>

The matrix-vector equivalents of the above group dependent parameters are defined in Appendix 1.

$\phi(t)$ Amplitude function

$C(t)$ Integrated (or effective) delayed neutron precursor densities

$L(t)$ Effective prompt neutron lifetime

$\rho(t)$ Reactivity

$\tilde{\phi}(t)$ Effective delayed neutron fractions

$\tilde{\beta}$ Total effective delayed neutron fraction
\( \psi(z,t) \)  
\text{Spatial function}  
\text{\( L^{-2} T^{-1} \)}

\( \psi^*(z) \)  
\text{Steady state adjoint spatial function}  
\text{\( L^{-2} T^{-1} \)}

The notation for the temperature calculation conforms to the one-dimensional benchmark specification.
DISCUSSION

J. Devooght

The reason, why the time needed for codes using automatic time step selection is so great, can maybe simply be found in the fact that it is necessary. There are two distinct problems for time step selection. The first one is the evaluation of the final global accuracy and the choice of the strategy, i.e. the variation of the time step to achieve such accuracy. The first problem is tractable, the second one is unsolved to my knowledge. May I ask Mr. Fayers if the submitted benchmarks did contain information about the influence of the time step? At least, we should have results for the step halved and even if the result is unchanged, I should not be completely convinced that convergence has been obtained.

F.J. Fayers

Contributors were asked to submit solutions which in their experience would represent a reasonable compromise between speed and accuracy. Detailed information underlying their choice was not provided. Individual contributors may now be able to supply background results in this area.

A.F. Henry

How are the group fluxes calculated in ADEP?
F.N. McDonnell

The group fluxes at each mesh point at a given time step are calculated simultaneously using a Gauss reduction method. Dr. Ferguson has suggested that it might be better to calculate the group fluxes separately since this apparently reduces the error.

A.F. Henry

Possible problems with 1-D benchmarks?

F.N. McDonnell

When these 1-D cases were carried out, the exponential transformation option was not available in ADEP. The cases should probably use the exponential transformation. This is especially so in case B which behaves essentially exponentially. Another point with ADEP is that a coarser effective mesh is used for the feedback equation; this affects the temperature calculation.

A.F. Henry

What are the reasons for discrepancies between the results for case B?

D.A. Meneley

The exact approximation (such as mesh spacing and means of representation of the moving control rod) used in each code can strongly influence the results. Each contributor should define exactly what approximations are used.
A.F. Henry

The implications of discrepancies between results of case B could be quite broad. What can be done to resolve these discrepancies?

D.A. Meneley

The ANS Benchmark Committee is moving in the direction of defining benchmark problems as standards, following the precedent set by the US regulatory authorities' insistence that two reference thermal-hydraulics problems must be solved by each applicant. If the participants find that the results can be published, it is my impression that the ANS Benchmark Committee would be happy to publish the verified results in their standard format.

E. Infuehr

Automatic Time-Step Control: Adapting the method as used for O-D kinetics (DYN - Ein Dynamikprogramm für Kugelhaufenreaktoren, EURATOM 80) to the more-dimensional case by using any discrepancy encountered (e.g. violation of boundary conditions) as a criterion for accuracy; furthermore distinguishing between neutronic and feedback time step with different criteria (e.g. energy balance as to temperature).

D.A. Meneley

See my answer to A.F. Henry titled "further comments on automatic time step selection".

I agree that separation between neutronic and feedback time steps is a valuable procedure. Care must be taken in the de-
sign of the overall control to recognize the interval over which all of the components must reach a common point in time.

A.F. Henry

What are comments concerning automatic time step selection?

D.A. Meneley

QX1 has an automatic time step selector with reasonably tight convergence criteria built in as default values. The user may modify these values based on his own experience. This has been quite successful except for the low-accuracy end of the range, for the shape function time step. The effort involved in developing "intelligent" time step control was quite large.

A.F. Henry

Further comments regarding time step selection?

D.A. Meneley

The 2-dimensional code FX2 uses essentially the same automatic time step selector as QX1. The code decouples the time step required by neutronic und feedback algorithms, so that each subset of the equation system uses its own required time step. The step controller chooses the minimum step length on the basis of rates of change of system parameters. Details are given in ANL-1169.
A. Siebertz

Everybody recognizes the importance but also the difficulty of the time step automatic adaptation. I should appreciate very much the various contributors giving leading ideas concerning the automatic time step adaptation algorithms or giving pertinent references related to this problem.

A.F. Henry

I believe that is an excellent suggestion, and I hope the participants will comply with it.

A.F. Henry

The differences between codes for case B could be due to mesh differences and the way in which the rod effect is changed. Have we any information on this?

M.J. Bridge

Since his original submission, Cooper has run case B. His results appear to be in reasonable agreement with the CYCLOPS results just mentioned by Billington and the ABA results. These KINAX group calculations used 43 mesh points and rod changes were "phased out" from each mesh in turn, using a quadratic function.
O. Norinder

I should like to make some comments on TRANSPROGRAM. TRANS is made for BWRs and PWRs. TRANS has a neutronic, full temperature and hydraulic part. In the neutronic part, the time derivative terms are added to the diffusion equation. This can be solved directly in the standard way for 1-D diffusion except for the delayed neutrons. That causes some iterations to arrive at an accurate solution. This method cannot be extended to multi-D cases. - Time step is in general automatically selected, halved if number of iterations goes over a (small) number and time step doubled if one (or 2?) iterations are used. Time step is also kept within values set in input.
P.S. Christensen, F.J. Fayers, S. Langenbuch,
F.N. McDonnell, A. Schmidt, E. Vincenti, H. Yoshikawa,
W. Werner

SURVEY OF THE RESULTS OF A TWO- AND THREE-DIMENSIONAL
KINETICS BENCHMARK PROBLEM TYPICAL FOR A THERMAL REACTOR
I. Introduction

In 1973, NEACRP and CSNI posed a number of kinetic benchmark problems intended to be solved by different groups. Comparison of the submitted results should lead to estimates on the accuracy and efficiency of the employed codes. This was felt to be of great value since the codes involved become more and more important in the field of reactor safety.

In this paper the results of the 2d and 3d benchmark problem for a BWR are presented. The specification of the problem is included in the appendix of this survey. For the 2d benchmark problem, 5 contributions have been obtained, for the 3d benchmark problem 2 contributions have been obtained.

Section II contains the list of participants and summaries of the methods employed in their codes.

In section III, some of the essential results of the 2d-contributions are presented.

Section IV contains graphs of characteristic quantities of the 2d-solutions.

Section V contains the discussion of 2d-results.

Section VI contains graphs of characteristic quantities of the 3d-solution.
II. List of Contributions

1. Submissor: E. Vincenti
   Cases submitted:
   Computer: EURATOM, Nuclear Studies Division
   Code: 21020 ISPRA (Varese)
   Method: 2d
   IBM 370/165
   COSTANZA
   FD implicit, with line relaxation

2. Submissor: F.N. McDonnell
   Cases submitted:
   Computer: Atomic Energy of Canada Ltd.
   Code: Advance Projects and Reactor Physics Division
   Method: Chalk River, Ontario, Canada
   CDC 6600
   ADEP
   FD, Alternating direction explicit

3. Submissor: F.J. Fayers
   Cases submitted:
   Computer: United Kingdom Atomic Energy Authority
   Code: Atomic Energy Establishment
   Method: Winfrith, Dorchester, Dorset
   ICL4-70
   TUTANK
   FD, Alternating direction implicit
4. Submissor: H. Yoshikawa
   Cases submitted:
   Computer: Institute of Atomic Energy
   Code: Kyoto University
   Method: Uji, Kyoto, Japan
   2d
   2DK
   FD

5. Submissor:
   a) A. Schmidt
   b) S. Langenbuch
   Cases submitted:
   Computer: Laboratorium für Reaktorregelung
   Code: und Anlagensicherung
   Method: 8046 Garching/Munich
   a) 2d
   b) 3d
   a) Siemens 4004/55
   b) IBM 360/91
   a) PIMFUX
   b) QUABOX/CUBBOX
   a) FD, explicit (DuFort Frankel)
   b) Coarse mesh, Matrix Decomposition implicit

6. Submissor: P.S. Christensen
   Cases submitted:
   Computer: Danish Atomic Energy Commission
   Code: Research Establishment Risø
   Method: DK-4000 Roskilde - Denmark
   3d
   Burroughs B 6700
   DANO
   Nodal, one energy group representation
III. Results (2d)

For a quick comparison some characteristic quantities are listed in the following table:

<table>
<thead>
<tr>
<th>Submitter</th>
<th>k\text{eff} rod in</th>
<th>k\text{eff} rod out (without feedback)</th>
<th>Mean power density at time of peak</th>
<th>Power density at monitor P1 at time to peak (P1)</th>
<th>time to peak</th>
<th>Mean power density at second peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.996122</td>
<td>1.01446</td>
<td>$2.2 \cdot 10^3$</td>
<td>$1.7 \cdot 10^4$</td>
<td>1,575</td>
<td>$1.6 \cdot 10^2$</td>
</tr>
<tr>
<td>2</td>
<td>1.0000</td>
<td>1.0192</td>
<td>$2.4 \cdot 10^2$</td>
<td>$3.25 \cdot 10^3$</td>
<td>1,52</td>
<td>$1.7 \cdot 10^2$</td>
</tr>
<tr>
<td>3</td>
<td>1.0040</td>
<td>1.0296</td>
<td>$2.6 \cdot 10^3$</td>
<td>$1.05 \cdot 10^4$</td>
<td>1,3</td>
<td>$3.9 \cdot 10^2$</td>
</tr>
<tr>
<td>4</td>
<td>0.99312</td>
<td>1.01210</td>
<td>$2.27 \cdot 10^3$</td>
<td></td>
<td>1,79</td>
<td></td>
</tr>
<tr>
<td>5a</td>
<td>0.99794</td>
<td>1.01898</td>
<td>$2.5 \cdot 10^3$</td>
<td>$2.3 \cdot 10^4$</td>
<td>1,38</td>
<td>$3.4 \cdot 10^2$</td>
</tr>
</tbody>
</table>

Continuation

<table>
<thead>
<tr>
<th>time to second peak</th>
<th>Mean power density at 2.8 sec</th>
<th>Temperature °K at Monitor 1 at 2.8 seconds</th>
<th>Mean temperature °K at 2.8 seconds</th>
<th>number of space points</th>
<th>computing time (sec)</th>
<th>CDC 6600 equivalent</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>2.0</td>
<td>$2.0 \cdot 10^1$</td>
<td>1960</td>
<td>510</td>
<td>256</td>
<td>333</td>
</tr>
<tr>
<td>(2)</td>
<td>2.0</td>
<td>$2.6 \cdot 10^1$</td>
<td>2500</td>
<td>550</td>
<td>729</td>
<td>4000</td>
</tr>
<tr>
<td>(3)</td>
<td>2.0</td>
<td>$4.8 \cdot 10^1$</td>
<td>3360</td>
<td>650</td>
<td>256</td>
<td>3240</td>
</tr>
<tr>
<td>(4)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(5a)</td>
<td>1.93</td>
<td>$4.4 \cdot 10^1$</td>
<td>2530</td>
<td>560</td>
<td>2025</td>
<td>12000</td>
</tr>
</tbody>
</table>

*) estimated

**) improvement quoted later on
IV. Graphic Representation of Characteristic Quantities (2d)
MEAN POWER DENSITY vs TIME
2-D THERMAL REACTOR
MEAN POWER DENSITY
VS TIME
LAST 4 DECADES
Power Density
Monitor Point 1
First Three Decades
POWER DENSITY

TIME (SEC)

MONITOR POINT R
\[ P = 1.88 \text{ MW} \]

Normalized power density profile at \( t = 1.4 \text{ sec} \)
\[ \overline{P} = 974 \text{ MW} \]

**Normalized Power Density Profile**

\[ t = 1.6 \text{ sec} \]
\[ P = 510 \text{ MW} \]

Normalized Power Density Profile \( t = 2.9 \text{ sec} \)
UKAEA

$t=0\text{ sec}$ $P=2.106 \times 10^{15}\text{ MW}$

Diagram showing a graph with axes labeled $P/P^*$ and $Z_{line}^2$. The graph includes labeled sections A9 to I1.
LRA

$t = 0$ sec \[ P = 2.106 \cdot 10^{-5} \text{MW} \]
V. Discussion of Results (2d)

Comparison of the submitted solutions reveals significant discrepancies. There is strong evidence that a major portion of these discrepancies can be traced to spatial discretisation errors resulting from too large mesh-sizes. In order to substantiate this conjecture, a series of calculations using successively refined mesh-sizes has been performed at the LRA with the code CITATION. The following table shows the gain $\Delta k = k_{\text{rod out}} - k_{\text{rod in}}$ of reactivity without feedback, obtained by the various submitters, and by CITATION with various mesh-sizes.

Dependence of $\Delta k$ on mesh-size $h$

<table>
<thead>
<tr>
<th>Code</th>
<th>$h$(cm)</th>
<th>$\Delta k$ %</th>
</tr>
</thead>
<tbody>
<tr>
<td>EURATOM</td>
<td>15</td>
<td>1.84</td>
</tr>
<tr>
<td>AEC</td>
<td>~10</td>
<td>1.92</td>
</tr>
<tr>
<td>UKAEA</td>
<td>15</td>
<td>2.55</td>
</tr>
<tr>
<td>LRA FD</td>
<td>7.5</td>
<td>2.10</td>
</tr>
<tr>
<td>CITATION</td>
<td>15</td>
<td>2.55</td>
</tr>
<tr>
<td></td>
<td>7.5</td>
<td>1.98</td>
</tr>
<tr>
<td></td>
<td>7.5/3.75</td>
<td>1.81 *)</td>
</tr>
<tr>
<td></td>
<td>3.75</td>
<td>1.81</td>
</tr>
<tr>
<td></td>
<td>3.75/1.875</td>
<td>1.81 *)</td>
</tr>
</tbody>
</table>

*) finer mesh near power peak

The following graph shows the power profile along the core diagonal at $t = 0$, obtained by the submitters, and by CITATION with $h = 3.75$ cm.
--- EURATOM
--- UKAEA
--- LRA FD
--- CITATION, \( h = 3.75 / 1.875 \)

Fig. 1 Power Profile along core diagonal at \( t = 0 \)
From these results it is obvious that the mesh sizes used by the submittors have been too large. For this benchmark problem, FD-codes require a mesh size of \( h < 4 \text{ cm} \), at least in some vicinity of the power maximum, in order to produce results of acceptable accuracy.

Analysing the submitted transient solutions, one finds that their discrepancies are roughly speaking, consistent with the errors in \( \Delta k \). Since this effect presumably is much larger than other causes of error, such as time integration method or representation of feedback, it is at present impossible to make a reasonable comparison of results. The conclusion reached during the discussion at the meeting was, that the contributors should rerun the problem, employing finer mesh spacing.
VI. GRAPHIC REPRESENTATION OF CHARACTERISTIC QUANTITIES (3d)
3D-BENCHMARK PROBLEM FOR A LIGHT WATER REACTOR

S. Langenbuch

\[
\begin{align*}
\text{static multiplication factor:} & \\
\text{k}_{\text{eff}} \text{ with rod} & = 0.99530 \\
\text{k}_{\text{eff}} \text{ without rod} & = 1.01344 \\
\Delta k & = 1.814 \times 10^{-2}
\end{align*}
\]

Mesh division:

XY-plane \hspace{1cm} \text{in core 30 cm, at core boundary 15 cm and 7.5 cm, in reflector 10 cm}

Z-direction \hspace{1cm} \text{in core 33 \(\frac{1}{3}\) cm, in reflector 10 cm}

Total number of points: \(19 \times 19 \times 16 = 5776\)
Reciprocal Period
Fig. 6

Rel. Axial Power Density

Monitorpoint 1

\[ \text{\textbf{\textit{P}}/\text{\textit{P}}_{\text{ref}}} \]

\[ \text{\textbf{\textit{P}}_{\text{ref}}} = 1 \times 10^{-6} \text{ W/cm}^3 \]

\[ \text{\textbf{\textit{P}}} = 31.44 \]

\[ \text{\textbf{\textit{P}}} = 30.46 \]

\[ \text{\textbf{\textit{P}}} = 9.17 \]
Fig. 9

Ret Power Density along Diagonal

Pipe 1

Pipe 2

Zunahme in %

Abnahme in %

3.0 sec

1.0 sec

0.0 sec
3D-BENCHMARK PROBLEM
FOR A
LIGHT WATER REACTOR

by

P. Skjerk Christensen

RESEARCH ESTABLISHMENT RISÖ
DENMARK
1. INTRODUCTION

A benchmark problem concerning an example of a fast transient in a three dimensional reactor has been distributed by EACRP and the results from some calculations are reported here.

The transient may be described as the time behaviour of the reactor when a control rod near the core-reflector boundary is withdrawn from the initial delayed critical reactor. The transient is regarded so fast that the reactor is assumed adiabatic and the power controlled by the Doppler effect solely.

In this report the original version of the benchmark problem is not duplicated which means that equations and constants are not repeated.

The problem has been solved with a nodal code DANO which is a special version of a BWR-simulator. As this code could not take into account all features of the benchmark problem, the approach to the problem is given here.

In this report the methods used are very shortly described along with the necessary changes of the original geometry and nuclear constants. Next the results are presented in tables and figures. At last some data concerning the computer are given.

2. GEOMETRY

In the appendix is shown the core lay-out as given by the benchmark distributors. The core consists of various types of fuel elements and in an unsymmetric position a movable control rod is situated.

As the core has no symmetric properties it was necessary to represent each fuel element explicit, that means 312 total, and it was decided to divide the height in 18 sections making a total of 5616 mesh points.
At the points 1 and 2 detectors are placed and certain quantities are to be followed here: local power density, temperature, and reciprocal period.

As the code used contains a nodal model of the reactor the reflector is taken into account by albedo values, and thus the boundary of the problem is the interface between core and reflector.

3. NUCLEAR PARAMETERS

The code used here is based on a one energy group representation. The neutron cross sections, however, may be given in two groups but are condensed to one group according to

\[ \Sigma_f = \Sigma_{f1} \times R + \Sigma_{f2} \]

and

\[ \Sigma_a = \Sigma_{a1} \times R + \Sigma_{a2} \]

where

\[ R = \frac{\Sigma_{a2}}{\Sigma_{a1}} \]

The one group picture will also neglect the speed of the fast neutron group which is assumed in equilibrium (infinite speed), while the thermal neutrons have a finite speed.

The benchmark problem has a reflector with given nuclear constants. In the code, however, the reflector is described by an albedo concept, and the albedo values have been found by fitting the power distribution of this nodal model to the power given by a code based on ordinary difference technique. The fitting has been done with the movable rod full in and the accuracy obtained is about 5% in the power distribution.
The movable control rod has to be represented by a poison cross section and thus the equivalent poison cross section given in the problem has been used.

The nodal representation of a moving control rod gives rise to a ripple on the reactivity - and reciprocal period vs. time - functions which may be seen both on fig. 1 and 5. Although the program contains a smoothing parameter, it has not been possible to remove the ripples fully.

4. NUMERICAL METHODS AND ASSUMPTIONS

The steady state power distribution and effective multiplication factor are found by an iterative method.

The temperature is assumed constant over the core.

In the transient calculation the code assumes that the flux distribution may be separated in an amplitude and a space-dependent (the last one slowly time dependent) part. Both are integrated by a predictor-corrector method in which the time step is determined by the difference between predictor and corrector values and by the number of iterations necessary in the flux distribution corrector.

The code includes the delayed neutrons by the full equation

\[ \dot{C}_i = \beta_i \gamma E_i - \lambda_i C_i. \]

The temperature is integrated by a simple Euler method in which the truncation error is computed and compared with a given limit.

5. RESULTS

The results are given in the following tables and figures. As these are self-explanatory only a few remarks are given.
Generally it is seen that the local quantities in point 2
differ very little between the two heights, thus only one curve
has been shown in several cases.

In table 2 the static multiplication factor is given with
and without control rod.

6. COMPUTER

The calculations are performed on a Bourroughs B-6700 with
a core size of 48 K words of which the software system occupies
the half. There is a number of disks on which program and data
are stored. The program is segmented automatically and so are
some of the common blocks, in a way not governed by the programmer.
Thus, as the program plus data exceed the available core, a heavy
amount of disk transfer is necessary, and this makes the cost in
computer time high.

In table 3 the total amount of computer time is given along
with the equivalent CDC-6600 computer time. The conversion of
B-6700 central processor (CP) time to CDC-6600 CP-time is made by
a conversion factor of 10 found experimentally. The conversion of
input/output (I/O) time is based on experience and a guess, as the
program if it should be run economically on a CDC-6600, would have
to be fitted with an overlay structure and furthermore, a lot of
file storage could be replaced by arrays thus reducing the I/O time
significantly.
7. COMMENTS

Two features of the nodal model used in DANO are rather different from those normally used in models based on the diffusion theory approach whether in fine or coarse mesh approximation.

One is the use of the albedo concept in order to represent the reflector, the other the one energy group picture.

The albedo concept means that a certain fraction of the neutrons which are streaming against the core-reflector boundary, is reflected instantly back into the same node from which they came. The albedo values are found by a fitting procedure in which the overall power distribution is adjusted to one obtained by a finite difference model which includes the reflector in the usual way. However, as DANO represents the core by rather big nodes ($\Delta x \sim \Delta y \sim 15$ cm) details of the power distribution near the boundary are not taken into account.

Thus the albedo concept introduces two non-physical effects: namely the prompt reflexion of neutrons and the non-existence of transmission of neutrons from one part of the core to another through the reflector.

The one-group picture of the neutron spectrum where all neutrons are considered thermal, will enhance the absorptions near the source whereas fast neutrons normally are transmitted to greater distances before absorption. Furthermore, moderation in the reflector is disregarded.

One may therefore conclude that both mechanisms introduced in the nodal model will tend to decrease the leakage from a certain volume and thus increase the local multiplication, especially if the volume is situated at the boundary near a corner. This may be the reason for the early rise of the power found by calculations with DANO, compared with the results of other models which include reflector and two energy groups.
Figures:

1A  Total power versus time, 0. -0.8 seconds
1B  Total power versus time, 0.8-3.0 seconds
2A  Local power versus time, 0. -0.8 seconds
2B  Local power versus time, 0.8-3.0 seconds
2C  Local power versus time, 0.8-3.0 seconds
3   Average temperature versus time
4   Local temperature versus time
5   Reciprocal period, average
6   Reciprocal period, local
7A  Diagonal power trace, 1 m height
7B  Diagonal power trace, 2 m height
8A  Axial power trace, point 1
8B  Axial power trace, point 2

Appendix 3  Core description.
### Table 1
**Dimensions and Constants**

<table>
<thead>
<tr>
<th>Mesh size horizontal</th>
<th>15 cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>vertical</td>
<td>16 2/3 cm</td>
</tr>
<tr>
<td>Total Power, start</td>
<td>21.06 W</td>
</tr>
</tbody>
</table>

### Table 2
**Multiplication Factor**

<table>
<thead>
<tr>
<th>With Rod</th>
<th>0.99935</th>
</tr>
</thead>
<tbody>
<tr>
<td>Without Rod</td>
<td>1.02058</td>
</tr>
</tbody>
</table>

### Table 3
**Computer Characteristics**

<table>
<thead>
<tr>
<th>Type</th>
<th>Bourroughs B 6700</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage</td>
<td>48K words (48 bits), about 25K for the user</td>
</tr>
<tr>
<td>CP time</td>
<td>B 6700 33883 s</td>
</tr>
<tr>
<td></td>
<td>CDC-6600 3400 s</td>
</tr>
<tr>
<td>I/O time</td>
<td>B 6700 12435 s</td>
</tr>
<tr>
<td></td>
<td>CDC-6600 3600 s</td>
</tr>
</tbody>
</table>
FIG. 1B

TOTAL POWER

Power

$10^{10}$ W

$10^8$

$10^6$

Time

1 2 3 s
FIG. 2A

LOCAL POWER

POWER

\[ \frac{\text{W}}{\text{cm}^2} \]

- $10^{-3}$ - $10^{-4}$ - $10^{-5}$

TIME

0.5 s  1.0 s

POINT

1

2

HEIGHT

1 M

2 -

1 -

2 -
FIG. 2B
LOCAL POWER

POINT 1

POWER

TIME

$10^4$ W/cm$^2$

$10^3$

$10^2$

1 m height

2 m
Fig. 2c

Local Power

Point 2
Fig. 3

Average Temperature

Temperature

1000
K

0

Time

1

2

3.5
Fig. 4

Local Temperatures

Temperature

Point  Height
1  1n
2  2n
4  4n
2  2n
FIG. 5

RECIPECAL PERIOD
FIG. 6

RECIPEAL PERIOD
LOCAL VALUES

POINT HEIGHT

1
1
2
2
1 M
2 M
1 H
2 H
RELATIVE POWER DENSITY

FIG. 7A

DIAGONAL POWER TRACE
1 M HEIGHT

TIME POWER
0 s .211E2 o
14 s .260 E10 o
46 s .269 E10 x
30 s .500 E9 ▼

DIAGONAL

P2

P1
Fig. 78

Diagonal power trace
2 m height

Time  Power
0 s  241.82 5
14 s  260.640
16 s  269.610
30 s  503.697
Fig. 8B

Axial Power Trace

Point 2

Time | Power
--- | ---
0 s  | 2.11 E2 W
1.4 s | 2.60 E10 W
1.6 s | 2.69 E10 W
3.0 s | 5.03 E9 W

Relative Power Density

Height
A super prompt critical excursion in a light water reactor should be investigated. In order to emphasize space-time effects an asymmetric control rod initially fully inserted is to be withdrawn at constant velocity. The only feedback considered is the prompt Doppler effect affecting the fast absorption cross-sections.

\[
\frac{4}{v_n} \frac{\partial}{\partial t} \Phi_n(\vec{r}, t) = \nabla D_n(\vec{r}, t) \cdot \nabla \Phi_n(\vec{r}, t) + S(\vec{r}, t) - \left[ \Sigma_{a,n}(\vec{r}) + \Sigma_{n,n}(\vec{r}, t) \right] \cdot \Phi_n(\vec{r}, t)
\]

where

\[
S(\vec{r}, t) = (1 - \beta) \sum_{\nu=1}^{2} \nu \Sigma_{\nu,2}(\vec{r}) \cdot \Phi_\nu(\vec{r}, t) + \sum_{i=1}^{2} \lambda_i \cdot C_i(\vec{r}, t)
\]

and

\[
\Sigma_{a,n}(\vec{r}, t) = \Sigma_{a,n}(\vec{r}) \cdot \left[ 1 + \nu \cdot \sqrt{T_f(\vec{r}, t) - T_0} \right]
\]

\[
\frac{4}{v_2} \frac{\partial}{\partial t} \Phi_2(\vec{r}, t) = \nabla D_2(\vec{r}) \cdot \nabla \Phi_2(\vec{r}, t) + \Sigma_{a,2}(\vec{r}) \cdot \Phi_a(\vec{r}, t) - \Sigma_{a,2}(\vec{r}) \cdot \Phi_2(\vec{r}, t)
\]

\[
\frac{2}{v_f} T_f(\vec{r}, t) = \alpha \cdot \sum_{\nu=1}^{2} \Sigma_{\nu,2}(\vec{r}) \cdot \Phi_\nu(\vec{r}, t)
\]

\[
\frac{2}{v_f} C_i(\vec{r}, t) = \beta_i \sum_{\nu=1}^{2} \nu \Sigma_{\nu,2}(\vec{r}) \cdot \Phi_\nu(\vec{r}, t)
\]

\( i = 1, 2 \)
The notation is standard and is given in appendix 1. The boundary condition for the fluxes at the reactor surface are \( \phi_0 = 0 \). The initial distribution should be performed by adjusting a \( \nu \)-critical. In this case \( T_f (\vec{r},0) \) is equal to \( T_0 \) (no feedback). The initial fluxes are normalized to a mean power density and the precursor concentrations are in equilibrium with the initial flux distribution. For the transient solution the constants \( \alpha \) and \( \nu \) in the equations for the adiabatic feedback model are constant throughout the reactor. There is no feedback in the reflector. Cross-sections, kinetic parameters and other necessary constants are given in appendix 2.

Core Description

The cross-sectional area of the core is given in appendix 3. The core itself contains 312 fuel elements with a width of 15 cm. It is surrounded by a rectangular reflector. For the 2D-calculation an axial buckling constant for the entire reactor and energy groups is used. For the 3D-calculation a top and bottom reflector of 30 cm, respectively, is assumed. The width of the control rod lattice is 30 cm so that each control rod is associated to four adjacent fuel elements. There are two kinds of fuel assemblies which differ in their reactivity. In the inner quadratic region of the core the fuel assemblies with the lower reactivity are loaded, adjacent to them are two rows of fuel elements and one fuel element at each corner, with the higher reactivity. In the inner region nine control rods are withdrawn from the following positions: B2, B5, B8, E2, E5, E8, H2, H5, H8.

The transient is started by withdrawing the control rod in position I2 with constant velocity. For the 2D case, this should be accomplished by changing the composition data for the fuel elements with rod in I2 to the data without rod at
a constant velocity or a poison cross-section should be deducted from the thermal absorption cross-section to represent rod movement.

For the 3D case, the rod is moved only in the fuel zone; it does not penetrate into top or bottom reflector. For representation of the rod again a poison cross-section should be deducted from the thermal absorption cross-section.

**Evaluation of Results**

First, the static multiplication factors with and without rod (but without feedback) should be given.

The transient should be followed for about 3 seconds. For better comparison of the results it is suggested to explicitly represent the first three decades of the reactor power separately on logarithmic paper as well as the upper four decades where the maximum power will occur. For graphical display of temperatures 5 cm per 1000 K is proposed.

For the 2D and 3D case mean values of power, temperature and reciprocal periods should be given. Local values of the same quantities in the monitoring points 1 and 2 (see appendix 3) should be given. The monitoring points for the 3D case are 100 cm and 200 cm from top of the reactor fuel zone.

Of further interest are power profiles at different times along the diameter specified in appendix 3. The power profiles should be evaluated at $t_1=0$, $t_2=1.4$, $t_3=1.6$ and $t_4=3.0$ seconds. The power profiles for the 3D case should be specified at the same heights as the local monitoring points. Furthermore for the 3D case the axial power shape in the monitoring points 1 and 2 should be given at the same times.
The power shapes should be normalized to the instantaneous total power. Also these total powers should be specified.

Additional information of type of computer, storage, CPU and I/O-times (sec.) are of interest. Computing times should be estimated relative to a CDC 6600 computer.
Appendix 1

\( \alpha \) = conversion factor in adiabatic feedback model
\( B^2 \) = axial buckling
\( \beta_i \) = delayed neutron yield in group \( i \)
\( \beta \) = total yield of delayed neutrons
\( C_i \) = delayed neutron precursor concentration in group \( i \)
\( d \) = mean power density for static solution
\( D_g \) = diffusion constant
\( e \) = energy conversion factor
\( g \) = index for neutron energy group (1=epithermal, 2=thermal)

\( f' \) = feedback constant
\( H \) = active core height
\( i \) = group index for delayed neutrons (i=1,2)
\( \lambda_i \) = decay constant for delayed neutrons
\( \nu \) = mean number of neutrons per fission
\( \phi_g \) = neutron flux
\( \vec{r} \) = space vector
\( \Sigma_{\alpha,g} \) = absorption cross-section
\( \Sigma_{f,g} \) = fission cross-section
\( \Sigma_p \) = equivalent thermal poison cross-section
\( \Sigma_{1,2} \) = group transfer cross-section
\( t \) = time
\( T_f \) = fuel temperature in adiabatic feedback model
\( T_o \) = initial temperature throughout core
\( v \) = rod velocity
\( v_g \) = mean neutron velocity
Appendix 2

Composition Data

<table>
<thead>
<tr>
<th>group index</th>
<th>fuel type 1 with rod</th>
<th>fuel type 1 without rod</th>
<th>fuel type 2 with rod</th>
<th>fuel type 2 without rod</th>
<th>reflector constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.255</td>
<td>1.268</td>
<td>1.259</td>
<td>1.234</td>
<td>1.257</td>
</tr>
<tr>
<td>2</td>
<td>0.211</td>
<td>0.1902</td>
<td>0.2091</td>
<td>0.1935</td>
<td>0.1592</td>
</tr>
<tr>
<td>1</td>
<td>0.008252</td>
<td>0.007181</td>
<td>0.008002</td>
<td>0.007122</td>
<td>0.0006034</td>
</tr>
<tr>
<td>2</td>
<td>0.1003</td>
<td>0.007047</td>
<td>0.08344</td>
<td>0.06552</td>
<td>0.01911</td>
</tr>
<tr>
<td>1</td>
<td>0.004602</td>
<td>0.004609</td>
<td>0.004663</td>
<td>0.004668</td>
<td>--------</td>
</tr>
<tr>
<td>2</td>
<td>0.1091</td>
<td>0.08675</td>
<td>0.1021</td>
<td>0.08792</td>
<td>--------</td>
</tr>
<tr>
<td>1,2</td>
<td>0.02533</td>
<td>0.02767</td>
<td>0.02617</td>
<td>0.02805</td>
<td>0.04754</td>
</tr>
</tbody>
</table>

\( \nu = 2.43 \) \hspace{1cm} \text{mean number of neutrons per fission}
\( \Sigma_p = 0.010116 \text{ cm}^{-1} \) \hspace{1cm} \text{equivalent poison cross-section}
\( \nu_1 = 3.0 \times 10^7 \text{ cm.s}^{-1} \) \hspace{1cm} \text{mean neutron velocity in fast group}
\( \nu_2 = 3.0 \times 10^5 \text{ cm.s}^{-1} \) \hspace{1cm} \text{mean neutron velocity in thermal group}

Delayed neutron parameters

<table>
<thead>
<tr>
<th>group</th>
<th>( \beta_i )</th>
<th>( \lambda_i (\text{s}^{-1}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>.0054</td>
<td>.00654</td>
</tr>
<tr>
<td>2</td>
<td>.001087</td>
<td>1.35</td>
</tr>
</tbody>
</table>
Appendix 2

\[ H = 300 \text{ cm} \]  \hspace{1cm} \text{active core height}

\[ B^2 = 1.0 \times 10^{-4} \text{ cm}^2 \]  \hspace{1cm} \text{equivalent buckling for 2D case}

\[ \varepsilon = 0.3204 \times 10^{-10} \text{ Ws/p.f.} \]  \hspace{1cm} \text{energy conversion factor}

\[ d = 1.0 \times 10^{-6} \text{ W.cm}^{-3} \]  \hspace{1cm} \text{mean power density for static solutions}

\[ T_0 = T_f(\hat{r},0) = 300 \text{ } ^\circ \text{K} \]  \hspace{1cm} \text{initial temperature distribution}

\[ \alpha = 3.83 \times 10^{-11} \text{ } ^\circ \text{K.cm}^3 \]  \hspace{1cm} \text{conversion factor in feedback model}

\[ \gamma = 3.034 \times 10^{-3} \text{ } ^\circ \text{K}^{-1} \text{cm}^2 \]  \hspace{1cm} \text{feedback constant}

\[ v = 150 \text{ cm.s}^{-1} \]  \hspace{1cm} \text{velocity of rod}
Appendix 3: Core Description

- Fuel element type 1 with rod
- Fuel element type 1 without rod
- Fuel element type 2 with rod
- Fuel element type 2 without rod
- Fuel elements type 2 where rod is moved
- Fuel element with monitor 1 in central position
- Fuel element with monitor 2 in central position

--- dashed line for evaluating power shapes
active height 300 cm
or $B^2 = 1.0 \times 10^{-4}$ for 2D case
DISCUSSION

G. Williams

Could you explain the discrepancy in the eigenvalue for each submission both for the rod in and rod out states? What is the effect on the transient and what error is associated with the \( \Delta K \) values used by each contributor (i.e. 2D case)?

W. Werner

Errors in eigenvalues are directly related to the mesh sizes used. Specifically, \( \Delta K \) increases with increasing mesh size. The \( \Delta K \)-errors directly influence the transient as is exhibited by the graph of the time history of fluxes in the range from 0 - 1.4 sec; also, the peak powers and temperatures reached in the course of the transient are proportionally affected by the \( \Delta K \)-errors.

J.J. Dorning

I should like to address a question to Dr. Werner. Dr. Werner, in commenting on the ADI method applied to problems with feedback you indicated that very small time steps would have to be used or one would have to go to a predictor-corrector method. Have you examined the use of predictor-corrector methods and do you have any opinion concerning the value of these methods.

W. Werner

Since both predictor- and corrector steps require about the same amount of computing, it is presumably cheaper to use
only predictors, together with a smaller step size.

J.J. Dorning

I should like to suggest a more detailed discussion of the initial static K-calculation. I believe that the transient calculations will be very much affected by this renormalization of K. Perhaps, the contributors could state whether they have done any systematic convergence studies in their static calculations, what the convergence criteria on their source iteration calculation of K was, etc., and, in general, their own subjective view of the credibility of their static calculation. I believe that the inadequate convergence of some of the K-calculations might account for some of the discrepancies in the transient calculations.

W. Werner

There is strong evidence that the discrepancy can be explained by mesh size effects, rather than by poor convergence of static calculations. The mesh size effect is exhibited very strikingly by CITATION-calculations which showed acceptable accuracy only when the mesh size came down to 3.5 cm.

M.J. Bridge

I have noticed that there are significant differences between the reactivity worth shape when poison cross-section is changed linearly between cell-centred and interstitial mesh codes. Could this account for some of the differences observed?
W. Werner

During the rod-withdrawal period of the transient, this could account for some of the observed differences, but the major portion of the observed differences is certainly caused by different (and too large) mesh sizes.

H. Küsters

Have any of the submissions received here been made on programs which are used for actual reactor fault studies?

M.J. Bridge

The 1D submission by the DEGB was made using the KINAX code which has been used for all the MAGNOX reactor fault studies in the UK by the DEGB. I would like to comment at this point that we are encouraged by the fact that our 1 group code KINAX appears to agree well with the average answers from all the 2 group codes. This result is not, however, due to luck as great care is taken in KINAX calculations to make the rod worths and initial flux shapes agree with 2-group static calculations.
COMMENTS

A.R. Dastur

The correlation between $\Delta k$ and mesh size used in the CITATION calculation would perhaps be more understandable if the mesh size is expressed in units of absorption and/or transport mean face paths, or some other convenient neutronic parameter in case of multigroup formulations.

W. Werner

At first sight, we have found considerable disagreement between the solutions of the various contributors.

There is strong evidence that a major portion of the disagreement may be traced down to the spatial discretisation error.

I would like to suggest that the contributors rerun their problems using refined meshes. Hopefully, these solutions should converge and should provide a better estimation of the correctness of the solutions.
Session IV/2

REVIEW OF KINETICS BENCHMARK CALCULATIONS

Chairman: D.A. Meneley, Canada

A. Buffoni, J.K. Fletcher, A. Galati,
F.N. McDonnell, A. Musco, L. Väth

SURVEY OF THE RESULTS OF A TWO-DIMENSIONAL
KINETIC BENCHMARK PROBLEM TYPICAL FOR A FAST
REACTOR
I. Introduction

In 1973 the NEACRP posed a number of kinetic benchmark problems intended to be solved by different groups. The results were to be compared leading to estimates on the accuracy and efficiency of the different codes. This was felt to be of great value since the codes involved become more and more important in the field of reactor safety.

Most of the benchmark problems are typical for thermal reactors, but it was deemed necessary to include one problem typical for a fast reactor. The results for this two-dimensional reactor kinetics benchmark problem are analyzed in this paper.

In formulating the problem two aims were followed. First, the problem was intended to be sufficiently easy to be solved by a large number of codes, putting a strong weight to the neutronics and using a very simple feedback model, which could be easily incorporated in any code. The feedback is therefore independent of
space, using a mean core temperature for computing the Doppler effect. Two nearly equivalent feedback versions were submitted, one acting on the cross sections, the other directly changing the reactivity. A 2-group formulation was chosen so that typical 2-group thermal reactor codes could be used, but furthermore, a more realistic 6-group formulation was submitted, too. Thus the 4 benchmark problems are, in reality, only one problem.

The second aim was to have reactor dimensions and a transient typical for the fast reactor predisassembly phase of a hypothetical core disruptive accident. The reactor geometry and group constants were derived from the German SNR-300 design with a number of simplifications. The very high ramp rate is typical for the rates produced by slumping or fuel-coolant interaction. The total reactivity inserted was limited to less than 3 $\rho$ so as to stay within reasonable bounds for the fuel temperature. Therefore, it was not attempted to model one of the feedback phenomena just mentioned, which result in a much bigger total reactivity. Instead the ramp was produced by a simulation of control rod movement. For further information on the benchmark, see appendix.

Unluckily, the effort at producing a relatively simple problem did not bring the desired result in the form of a great number of contributions. There are only four, none of which is able to act as a reference solution. Thus, there is no standard against which to compare the solutions, and one is not able to obtain a picture of the state of the art, since a big number of methods different of the ones employed by the participants exist.
In section II of this paper a list of the participants and summaries of the methods employed in their codes is given. In section III, the results are presented and compared. The final conclusions will be summarized in chapter IV.

II. List of Contributions

1. UK - RIS
   Submissor: J.K. Fletcher
   Central Technical Service
   UKAEA
   Risley
   Warrington
   Lancs
   England
   Cases submitted: 1, 2, 3, 4
   Computer: ICL 470
   Code: SPARK
   Methods: SPARK uses the improved quasistatic method
   Reference: FRCMWP P(72)71

2. CRNL
   Submissor: P.N. McDonnell
   Applied Mathematics Branch
   Chalk River Nuclear Laboratories
   Chalk River
   Ontario
   Canada
Cases submitted: 1
Computer: CDC 6600
Code: ADEP
Methods: The alternating direction explicit method is used. In addition, an exponential transformation of the flux is used. The program called ADEP was written at Batelle Columbus Labs. It has been modified at CRNL to incorporate a variety of feedback models. Automatic time-step size is not used in this program.


3. CSN
Submissor: G. Buffoni, A. Galati, A. Musco Centro Studi Nucleari della Casaccia C.N.E.N.
Via Anguillarese km 1 + 300
S. Maria di Galeria
Roma
Italy
Cases submitted: 1, 2
Computer: IBM 370/165
Code: NADYP-A
Methods: This program provides for the calculation of neutron fluxes and temperature distribution during an operating or accidental transient. The reactor is described in r-z geometry and few-groups ($\leq 5$) diffusion model, the macroscopic cross sections depending on the Doppler temperature and coolant density. The thermodynamic model involves an appropriate subdivision of reactor in any number of radial shells, any one of which is described by a single channel model. The mass, energy and momentum conservation equations in the fuel, clad and coolant are solved for each channel, where the material properties are temperature dependent.

The stationary diffusion equations are solved by assuming fluxes as sum of trigonometric and/or Bessel functions; the time-dependent diffusion equations are solved by the metastatic method; finally, the heat equations are solved by the characteristics method.

References: A. Galati - N.S.E. 37, 30-40 (1969)
G. Buffoni, A. Galati, A. Musco: "DIFF-2, un programma di diffusione a 2 dimensioni" CNEN RTI(FCR)(74)8

G. Buffoni, A. Galati, R. Mosiello, A. Musco, F. Norelli, C. D. Stanescu: "NADYP, un codice di dinamica per reattori veloci: descrizione del modello fisico matematico" - CNEN RT/PI(74)8

4. GfK

Submissor: L. Väth
Institut für Neutronenphysik und Reaktortechnik
Gesellschaft für Kernforschung
D-7500 Karlsruhe
Postfach 3640
West Germany

Cases submitted: 1, 2, 3, 4

Computer: IBM 370/168

Code: KINTIC-1

Methods: KINTIC-1 may use the normal quasi-static, adiabatic or point kinetics method and has a detailed thermo-hydraulics part.
For the benchmark calculations, the adiabatic model has been used and the simple feedback model was incorporated.

Reference: L. Mayer, H. Bachmann: KINTIC-1
A program for the calculation of two-dimensional reactor dynamics of fast reactors with the quasi-static method. KfK 1627 (1972).
III. Results and Comparison

Case 1

Benchmark case 1 will be analyzed in some detail, since this is the only case which has been solved by all contributors. Furthermore, comparison of the other cases yields similar results requiring only a few additional remarks.

Some of the main results are depicted in fig's 1-5. The development of power vs. time is shown in fig's 2 and 2.1 with good qualitative agreement of UK-RIS, CRNL, and GfK, but markedly different results from CSN. This is astonishing since UK-RIS, GfK and CSN all employ factorizing methods. Nevertheless, there are some peculiarities to the metastatic method which may account for the differences:

1. The method uses different iteration schemes depending on whether the reactor is above or below prompt critical. The marked deviation occurs at 6 msec, the point around which the reactor should go prompt critical, and is finished at 15 msec, the point at which the ramp ends and the reactor goes below prompt critical.

2. There is no information about time step lengths and the way time dependent cross sections are handled. Errors could occur if big time steps are combined with stepwise alterations of the cross sections or if no sufficient iteration between power development and cross section alteration is assured.

The other three solutions (fig.2) agree qualitatively, but the heights of maxima and minima vary about 25 %, their position on the time scale about 10 % or more. The
difference in the initial ramp rates (fig. 1) is 10%.
The resulting temperature behaviour is shown in fig. 3.
In an attempt to find out possible reasons for this,
initial and final flux shapes and spectra have been investigated. Fig's 4 and 5 show that small but distinct
differences exist in the radial flux distribution near
the reactor midplane. Especially these differences can
be found in the region of the movable absorber and thus
may account for the different ramp rates. As an indicator
for the time dependent flux shape the quotient \( \phi_q (r=20, z=88.25,t) / \phi_q (r=38, z=88.25,t) \), \( r=20 \) and \( r=38 \) being the
position of the initial total flux minimum resp. maximum,
has been calculated for each group and different times
(table 2). It shows small but marked differences in the
initial value as well as in its time dependent change.
The time dependent 2-group spectra at two points in the
reactor, one of which is located in the movable absorber
region, has been evaluated too. There is no difference
between the results of all three contributors within
the available accuracy (table 1).

The use of different numerical methods in the transient
part may play a role in explaining the difference between
the CRNL results and the other two contributions in the
feedback part of the transient (\( t > 8 \) msec). This
assumption is supported by the initial contribution
of CRNL, which had used larger time steps with far
worse results (see fig. 2.2). Smaller time steps subse-
quently produced the better results presented, but
it is not clear whether these steps are fully adequate
since CRNL employs no automatic step adjustment.

The difference of the UK-RIS and GfK results cannot be
explained by the different numerical methods. The two
methods - the improved quasistatic and the adiabatic
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<tr>
<th>t[msec]</th>
<th>Author</th>
<th>Group 1</th>
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<th>Group 1</th>
<th>Group 2</th>
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<td>14.0</td>
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</tr>
<tr>
<td></td>
<td>CRNL</td>
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<td>14.0</td>
<td>86.0</td>
<td>14.0</td>
</tr>
<tr>
<td></td>
<td>CSN</td>
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<td>14.2</td>
<td>85.8</td>
<td>14.2</td>
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<tr>
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<tr>
<td>100</td>
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<td>-</td>
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<td>GfK</td>
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<td>13.8</td>
<td>84.5</td>
<td>15.5</td>
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</table>

Table 1: Case 1. 2-group spectra [%] at z = 88.25 cm for start and end of transient in centre of reactor and at position of movable absorber.
<table>
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<tr>
<th>t[msec]</th>
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<th>Group 1</th>
<th>Group 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>UK-RIS</td>
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<td>.90</td>
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<td></td>
<td>GfK</td>
<td>.88</td>
<td>.89</td>
</tr>
<tr>
<td>100</td>
<td>UK-RIS</td>
<td>.96</td>
<td>1.12</td>
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<tr>
<td></td>
<td>CRNL</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>CSN</td>
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<td>1.05</td>
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<tr>
<td></td>
<td>GfK</td>
<td>.93</td>
<td>1.12</td>
</tr>
</tbody>
</table>

Table 2: Case 1. Time and group dependent flux shape indicator, $\phi_g (r = 20, z = 88.25,t) / \phi_g (r = 38, z = 88.25,t)$
approximation - both employ flux factorization. A recalculation of case 1 by GfK with the improved quasistatic method did not change the results appreciably.

In trying to understand the different results for the transient one probably has to start with an examination of the differences for the steady state results. The mesh does not seem to play an important role since UK-RIS has re-run the problem with a bigger mesh, GfK with a smaller one, both without significant changes of results. Nevertheless there are differences in the steady state flux distribution. Probably the underlying multigroup diffusion codes should be compared for an explanation.

In table 3 computer time and storage used by the codes are compared. Such comparisons are problematical not only because different computers may very much influence the performance of a particular code. In addition, two dimensional transients, especially those using approximate methods tend to have a lot of data transfer which may be organized in different ways. This shows up very clearly in the performance of the GfK code, which relies heavily on external storage and accordingly stays for a long time in the computer. CPU-times for UK-RIS and GfK are equivalent, since the ICL 470 is a factor slower than IBM 370/168, but GfK used a factor 4 more mesh points than UK-RIS. The higher CPU-time for the NADYP-A-code probably results from the recalculation of the adjoint in addition to the shape function. The CPU-time quoted for CRNL is the one used for the initial calculations with bigger time steps. It compares unfavorably with the two other methods, indicating that this code would have to be speeded up appreciably if it was to be used for fast reactor accident analysis. Due to the few contributions a more general comparison of the efficiency of fully numerical and approximate methods cannot be made.
Table 3: Case 1. Comparison of code performance. ICL 470 is a factor 4 slower than IBM 370/168, CDC 6600, IBM 370/165, and IBM 370/168 are equivalent.

*CRNL values for solution with bigger time steps than those for final solution.

<table>
<thead>
<tr>
<th></th>
<th>UK-RIS</th>
<th>CRNL *</th>
<th>CSN</th>
<th>GfK</th>
</tr>
</thead>
<tbody>
<tr>
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<td>ICL 470</td>
<td>CDC 6600</td>
<td>IBM 370/165</td>
<td>IBM 370/168</td>
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<tr>
<td>Mesh size</td>
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<td>1036</td>
<td></td>
<td>1320</td>
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<tr>
<td>Elapsed time [min]</td>
<td>13</td>
<td></td>
<td>44</td>
<td></td>
</tr>
<tr>
<td>CPU [min]</td>
<td>9</td>
<td>57</td>
<td>15</td>
<td>6</td>
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<tr>
<td>Storage [K]</td>
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<td>20</td>
<td>192</td>
<td>210</td>
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</table>
Case 2

Cases 2 - 4 have been calculated by UK-RIS and GfK only. The difference between case 1 and case 2 is in the feedback only, which in case 2 directly alters the reactivity. It is dimensioned in such a way that the feedback effect is approximately the same as in case 1. Fig. 6 shows the time dependent reactivity for case 2. The picture is nearly identical with fig. 1 for case 1 and does not lead to any new conclusions.

Case 3

This case is the 6-group version of case 1 and gives qualitatively the same, but quantitatively slightly different results. This shows up in fig's 7 - 9. The initial ramp rates of UK-RIS and GfK agree excellently, but later on slight differences in reactivity turn up. This leads to differences in the power and, consequently, a quite sizable difference of the temperatures at the end of the transient.

As in case 1, spectra and flux distributions have been compared and some details are given in tables 4 and 5. The spectra at the centre of the reactor agree excellently within the limits of accuracy (table 4). The same holds true for the spectra at initial time in the region of the movable absorber, whereas the change of the spectra in this region shows a marked difference in group 5. Furthermore, table 5 shows differences in the flux distributions at initial time and at the end of the transient with GfK consistently producing higher values of $\phi_g(r = 20, z = 88.25, t) / \phi_g (r = 38, z = 88.25, t)$.
<table>
<thead>
<tr>
<th>$r \text{ cm}$</th>
<th>Group</th>
<th>$t = 0$</th>
<th>$t = 100$ msec</th>
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<td>4.1</td>
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</tr>
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<td></td>
<td>3</td>
<td>31.4</td>
<td>31.6</td>
</tr>
<tr>
<td></td>
<td>4</td>
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<td>.2</td>
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<tr>
<td></td>
<td>6</td>
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<td>.2</td>
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</table>

Table 4: Case 3. 6-group spectra $\bar{\phi}$ at $z = 88.25$ cm for start and end of transient in centre of reactor and at position of movable absorber.
<table>
<thead>
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<th>Group</th>
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<td>6</td>
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</table>

Table 5: Case 3. Time and group dependent flux shape indicator, \( \phi_g (r = 20, z = 88.25, t)/\phi_g (r = 38, z = 88.25, t) \).

<table>
<thead>
<tr>
<th>Computer</th>
<th>Mesh size</th>
<th>Elapsed time [min]</th>
<th>CPU [min]</th>
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<td>25</td>
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<tr>
<td>GfK</td>
<td>IBM 370/168</td>
<td>1320</td>
<td>104</td>
<td>19</td>
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</tbody>
</table>

Table 6: Case 3. Comparison of performance. ICL 470 is a factor 4 slower than IBM 370/168.
than UK-RIS. Taking into account the results of the comparison for case 1, it seems that the excellent agreement of the initial ramp rates for case 3 is fortuitous. As in case 1, one should examine the differences of the steady state results for clues to the discrepancies in the transient.

Table 6 shows a comparison of storage and computer time for case 3. The pattern is the same as in case 1.

Case 4

The time dependent reactivity as calculated by UK-RIS and GfK is shown in fig. 10 and is nearly identical to case 3 (fig.6). Since case 4 is related to case 3 in the same way as case 2 is related to case 1, no further discussion of the results is needed.

IV. Conclusions

With only a few contributions it is very difficult to reach definite and many conclusions. Nevertheless, two may be ventured:

1. The performance of the approximate methods looks very good compared to the only finite difference method. A comparison with other finite difference methods would be very desirable, especially with one that could act as a reference solution.
2. A more detailed analysis of the steady state diffusion codes is warranted to find out about causes and effects of the differences in spatial flux distributions.

3. A second 2d fast reactor benchmark problem with more realistic feedback should not be submitted before the differences of the solutions to this first benchmark have been fully understood.
Fig. 2.1: 2d fast reactor benchmark 1 power(t)
Fig. 2.2: CRNL-results for benchmark 1, power (t), for different time step lengths.
Fig. 3: 2 d fast reactor benchmark 1 temp(t)
Fig. 4: 2D fast reactor benchmark 1 $\Phi(t=0, r, z=88.25)$ Group 1
Fig. 5: 2 d fast reactor benchmark 1 $\phi(t=0,r,z=88.25)$ group 2
Fig. 8: 2D fast reactor Benchmark 3, power(t)
Fig. 10: Fast reactor benchmark 4 $\rho(t)$
APPENDIX

Benchmark Source Situation

Descriptive Title: 2D Cylindrical Model
Suggested Functions: Test 2D Neutron Dynamics Solutions

Configuration:
Benchmark Problem

Identification: 1

Descriptive Title: Superprompt critical transient with feedback, 2 group neutron diffusion problem in fast reactor

Reduction of Source Situation:
1. Two group diffusion theory
2. Six delayed neutron precursor groups
3. Feedback through changing cross sections
The equations to be solved are

1. Neutron kinetics:
\[
\frac{1}{v_g} \frac{\partial \phi}{\partial t} = \nabla \cdot \left( \frac{1}{\Sigma_{tr}} \nabla \phi \right) + \chi_g S (1-\beta) \nu E^f \phi_g - \nu_{rem} \phi_g
\]

\[
+ \sum_{g'} S_{g' \rightarrow g} \Sigma_{sc} \phi_{g'} + S \chi_i \lambda_i C_i \quad g = 1, 2
\]

\[
\frac{3C_i}{\partial t} = S \chi_i \nu E^f \phi_g - \lambda_i C_i
\]

with boundary conditions

\[
\frac{\partial \phi}{\partial n} = -\frac{\Sigma_{tr}}{0.71} \phi_g
\]

on all outer surfaces (fig. ); e.g. for the upper surface with

\[
z = 170, \phi_g (r, z + \frac{0.71}{\Sigma_{tr}}) = 0
\]
2. Power and heat source

\[ P = 7.347 \times 10^{-12} \int_{\text{Zone 1+2+3}} dV \frac{S}{S} \vec{F} \phi \left[ \frac{\text{cal}}{\text{sec}} \right] \]

\[ \bar{q} = 7.347 \times 10^{-12} \int_{\text{Zone 1+2}} 0.335 dV \frac{S}{S} \vec{F} \phi \left[ \frac{\text{cal}}{\text{sec cm}^3} \right] \]

\[ P \text{ total power, } q \text{ average power per cm}^3 \text{ of fuel} \]

3. Temperature \( T \) in zone 1 and 2

\[ \rho c \frac{dT}{dt} = \bar{q} (t) - \bar{q} (t = 0) \]

4. Feedback: Identical cross section changes in zone 1 and 2 given by

\[ \frac{\partial \Sigma_i}{\partial T} = a \frac{i}{S} \frac{300}{T} \quad i = \text{capture, fission} \]

The transport cross section is not affected. For \( \Sigma_{\text{rem}} \), the change is the sum of the changes for capture and fission cross section.
Data: Two group constants \( \text{cm}^{-1} \)

<table>
<thead>
<tr>
<th>Region</th>
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<th>4</th>
<th>5</th>
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<td>( v_{E^c} )</td>
<td>( v_{E^f} )</td>
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<td>2</td>
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</table>

Prompt and delayed neutron spectra and \( 1/v \) [sec/cm]:

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<th>Group 2</th>
</tr>
</thead>
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<td>0</td>
</tr>
<tr>
<td>X delayed</td>
<td>1.</td>
<td>0</td>
</tr>
<tr>
<td>( 1/v )</td>
<td>( 1.851 \times 10^{-9} )</td>
<td>( 1.088 \times 10^{-8} )</td>
</tr>
</tbody>
</table>
Delayed neutron parameters:

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<th>Decay constant $\lambda_i$ $[\text{sec}^{-1}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>0.0129</td>
</tr>
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<td>2</td>
<td>0.87 &quot;</td>
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</tr>
<tr>
<td>3</td>
<td>0.12 &quot;</td>
<td>0.134</td>
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<td>11.38 &quot;</td>
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<td>5</td>
<td>5.12 &quot;</td>
<td>1.26</td>
</tr>
<tr>
<td>6</td>
<td>1.70 &quot;</td>
<td>3.21</td>
</tr>
</tbody>
</table>

$\beta = 0.0032$

Parameters for power and temperature calculation:

- $\rho = 9. g/cm^3$
- $c = 0.07 \text{cal/(g}^0\text{K)}$
- $T (t=0) = 1000^0K$
- $P (t=0) = 1000 \text{MW} = 2.39 \times 10^8 \text{cal/sec}$

Parameters of cross section derivatives

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<th>Group</th>
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</thead>
<tbody>
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</tr>
<tr>
<td></td>
<td>2</td>
<td>$2.8906 \times 10^{-7}$</td>
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</table>
Initiating perturbation: The control rod bank (region 4) is to be axially withdrawn by 6.5 cm in 15 msec and to be replaced by sodium (region 5). Transient should be followed for 100 msec.

(The initial configuration is exactly critical; deviation from the exact value \( k = 1.000 \) is eliminated by dividing the fission cross sections by \( k \), and the initial precursor concentrations are in equilibrium with the initial flux distribution. The initial flux is given by the initial power \( P(t = 0) \).)

Expected primary results:
1. Reactivity (\( \Phi \)) vs. time (0...20 msec and 0...100 msec)
2. Temperature (\( ^{\circ} \text{K} \)) vs. time (0...20 msec and 0...100 msec)
3. Power (MW) vs. time (0...20 msec and 0...100 msec)

Possible additional results:
1. Group fluxes vs. time (0...100 msec) at the following points: 
   \( (r = 47.5 \text{ cm}, z = 85 \text{ cm}) \); \( (r = 21.5 \text{ cm}, z = 88.25 \text{ cm}) \).
2. The following spatial flux distributions: \( \phi (r, z = 88.25, t) \);
   \( \phi (r = 21.5, z, t) \); \( \phi (r = 47.5, z, t) \) for \( t = 0, t = 7.5 \text{ msec and } t = 100 \text{ msec.} \)

Further information wanted: Type of computer, storage and time used, size of mesh, method of solution.

Presentation of results:
Please use translucent paper for the graphs containing the primary results and take the following scales (linear if not stated otherwise):

Abscissa:
- Time a) 10 mm \( \equiv \) 1 msec (0...20 msec)
b) 10 mm \( \equiv \) 5 msec (0...100 msec)

Ordinate
- Power 50 mm \( \equiv \) 1 log decade, starting with \( 10^3 \text{MW} \)
- Reactivity 100 mm \( \equiv \) 1 \( \Phi \)
- Temperature 50 mm \( \equiv \) 1000\( ^{\circ} \text{K} \)
As for the additional results, we would appreciate if they would be presented in the following form:

a) Group fluxes vs. time

**Abscissa:**
- Time \(10 \text{ mm} \equiv 5 \text{ msec}\)
- Ordinate \(50 \text{ mm} \equiv 1 \text{ log decade; flux in } \left[ \text{ cm}^{-2} \text{ sec}^{-1} \right]\)

b) Spatial flux distributions: The distributions for \(t > 0\) should be multiplied by the factor \(P(t = 0) / P(t)\) so that the different shapes could be compared. Please present the shapes for the three different values of time in one graph.

**Abscissa:**
- Space \(10 \text{ mm} \equiv 10 \text{ cm}\)

**Ordinate**
- Flux
  - \(20 \text{ mm} \equiv 10^{16} \text{ cm}^{-2} \text{ sec}^{-1}\) for group 1 in 2-group case
  - \(10 \text{ mm} \equiv 10^{15} \text{ cm}^{-2} \text{ sec}^{-1}\) for group 2, 3, 4 in 6-group case
  - \(20 \text{ mm} \equiv 10^{15} \text{ cm}^{-2} \text{ sec}^{-1}\) for group 2 in 2-group case and group 1, 5 in 6-group case
  - \(20 \text{ mm} \equiv 10^{14} \text{ cm}^{-2} \text{ sec}^{-1}\) for group 6 in 6-group case
Benchmark Problem

Identification: 2

Descriptive Title: Superprompt critical transient with feedback, 2D cylindrical 2 group neutron diffusion problem in fast reactor

Reduction of source situation: Same as for problem 1, but with feedback through reactivity

Feedback: Reactivity change given by

$$T \left( \frac{1}{k} \frac{\partial k}{\partial T} \right) = \gamma$$

$$\left( k: \text{multiplication factor}, \gamma: \text{Doppler constant} \right)$$

The resulting reactivity $\Delta \rho_{\text{dopp}}$ is to be added to the reactivity effected by the initiating perturbation.

The feedback models of problem 1 and 2 are equivalent.

Data: Same as for problem 1, except for

$$\gamma = -0.007$$

Initiating perturbation: Same as for problem 1

Expected results: Same as for problem 1
Benchmark problem

Identification: 3

Descriptive title: Superprompt critical transient with feedback, 2D cylindrical 6 group neutron diffusion problem in fast reactor

Reduction of source situation: Same as for problem 1, but with 6 energy groups

Data: Six group constants $[\text{cm}^{-1}]$

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Six group constants \([\text{cm}^{-1}]\)

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Six group constants \( \left[ \text{cm}^{-1} \right] \)

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Prompt and delayed neutron spectra and \( 1/\nu \left[ \text{sec cm} \right] \)

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Delayed neutron parameters: Same as for problem 1
Parameters for power and temperature calculation: Same as for problem 1
Parameters of cross section derivatives:

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Initiating perturbation: Same as for problem 1
Expected results: Same as for problem 1
Benchmark Problem

Identification: 4

Descriptive Title: Superprompt critical transient with feedback, 2D cylindrical 6 group neutron diffusion problem in fast reactor

Reduction of source situation: Same as for problem 2, but with 6 energy groups. The feedback models of problem 3 and 4 are nearly equivalent.

Data: Same as for problem 3, except for 
\[ \gamma = -0.007 \]

Initiating perturbation: Same as for problem 1

Expected results: Same as for problem 1
DISCUSSION

A. Siebertz

1) Could some discrepancies between the results given by codes using QS or IQS method be explained with the difference in reactivity history?

2) Could the difference, if any, in reactivity history be explained by the differences in the way of calculating the reactivity (use of a unique weighting adjoint function calculated once at initial time or use at each time step of a recalculated time independent asymptotic adjoint weighting function)?

D.A. Meneley

1) Yes. They could be resolved by reduction of time steps if the different methods are internally consistent.

2) The differences in "reactivity" values can be explained in this way, differences in total power cannot.

A.F. Henry

The use of what is in effect a time dependent weight function requires that changes in the conventional point kinetics equations (extra terms) be made.

G. Forti

The weighting by the right adjoint fluxes seems to me an important point in the reactivity history determination and, to be more precise, the lifetimes parameters are of
the same importance - the transient evaluation may be effected remarkably by these factors, and Galati's approach to the problem has many advantages from this point of view.

J.J. Dorning

I believe that Prof. Henry was referring to the problem of the additional term which arises in the point kinetics equations when a time-dependent adjoint function (or any time-dependent weight function) is used. In the case at hand, you effectively have piecewise constant adjoint weighting functions which when inserted into the time derivative of the inner product of the adjoint function and the shape function will lead to delta-function terms at time corresponding to the time points at which the adjoint functions are changed (recalculated). I think it is the question of whether these terms were accounted for in your calculation which Prof. Henry was raising rather than the recalculations of lifetimes, reactivity, etc.

COMMENTS

J.K. Fletcher

Although the agreement between SPARK and KINTIC is satisfactory on the 2D FR benchmark calculations it is not as good as one would expect. Therefore over the next few weeks the benchmark problems will be further investigated and any significant results will be communicated to Dr. Väth.
As a general comment on the meeting; the impression is that the quasi-static method will continue, over the next few years at least to be as good a way of solving neutron kinetics problems as any other.
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