Journal of the Korean Nuclear Society
Volume 11, Number 3, September, 1979

<Review>

Review of Computational Methods for Space-time Reactor Kinetics

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(July 9, 1979)

Abstract

The current status of the computational methods and computer codes for the analysis of reactor kinetics is reviewed. Computational methods which have been developed for space-dependent transient analyses are presented and recent progress in the development of methods is discussed.

1. Introduction

Nuclear reactor kinetics is the study of the time-dependent behavior of the neutrons in a reactor core. The prediction of the time behavior of the neutron population induced by various changes in reactor multiplication is essential to safe design and operation. However, the accurate prediction is very difficult to obtain.

One can roughly distinguish between two different types of kinetics analysis depending on the time scale characterizing changes in core properties. In this overview, methodology for treating transient phenomena with time constants on the order of hours or days, such as isotopic depletion and xenon spatial oscillations, is not included. The specific areas of reactor kinetics to be treated here are computational methods for analyzing relaively short-term changes such as operational transients, off-normal transients, and hypothetical accidents in power reactors for operational and safety purposes.

The subject of space-time nuclear kinetics is extensively treated in Stacey's book.[1] In recent years, excellent and comprehensive reviews of the space-time reactor kinetics were made by Henry[2], Stacey[3], Stewart[4], and Ferguson[5].

There has been growing need for development of solution methods for more than one spatial dimension in order to insure accurate predictions of transient flux and power distributions, because the power reactors are growing in size and there is an increasing economic incentive to be able to set operational safety limits in reactors as realistically as possible. With the advent of today's high-speed scientific computers, it became practical to implement solution methods for treating multidimensional transient analysis.

2. Mathematical Models

The neutron population in a reactor can

be modeled mathematically by the Boltzmann transport equation. Solving this equation analytically is usually impossible, and approximate numerical solutions are often time consuming.

A simpler mathematical description of the neutron behavior is that of point kinetics for which angular and spatial neutronic properties are assumed constant in time. For many problems angular effects may be neglected, but spatial effects may not. Hence point kinetics is usually inadequate for describing the detailed behavior of neutrons in a reactor, especially in a large one.

The neutron population of a reactor may be described by diffusion theory in which complicated angular effects are neglected. Space, time, and energy are treated with sufficient accuracy so that approximate solutions of the diffusion equation are satisfactory for most kinetics problems.

The well-known multigroup diffusion form of the reactor kinetics equations may be written as follows[6,7]:

$$\frac{1}{v_g}\frac{\partial}{\partial t}\phi_g(r,t)=\nabla\cdot D_g(r,t)\nabla\phi_g(r,t)$$
$$+\sum_{g'=1}^{G}\Sigma_{gg'}(r,t)\phi_{g'}(r,t)+\sum_{i=1}^{I}f_{gi}C_i(r,t),$$
$$g=1,2\cdots\cdots\cdots G \qquad (2.1a)$$

$$\frac{\partial}{\partial t}C_i(r,t)=\sum_{g=1}^{G}p_{ig}(r,t)\phi_g(r,t)-\lambda_i C_i(r,t),$$
$$i=1,2,\cdots\cdots\cdots I \qquad (2.1b)$$

where $\phi_g(r,t)$ = neutron flux in g'th energy group (n/cm² sec)
$C_i(r,t)$ = concentration of i'th precursor group (atoms/cm³)
v_g = group speed (cm/sec)
$D_g(r,t)$ = group diffusion coefficient (cm)
$\Sigma_{gg'}(r,t)$ = intergroup transfer cross section, $g'\neq g$ (cm^{-1})
$\Sigma_{gg}(r,t)$ = group removal cross section in g'th energy group (cm^{-1})
f_{gi} = fractional yield of i'th-group precursors into group g (sec^{-1})
$p_{ig}(r,t)$ = production factor i'th precursor by fission in g'th energy group (cm^{-1})
λ_i = decay constant of i'th precursor group (sec^{-1})
g = index of neutron energy group, $g=1,2,\cdots\cdots,G$
i = index of precursor groups, $i=1,2,\cdots\cdots I$

The (G+I) Eqs. (2.1) can be compacted into matrix form as

$$\frac{\partial}{\partial t}\Phi(r,t)=M(r,t)\Phi(r,t) \qquad (2.2)$$

where Φ is (G+I) element vector and M is (G+I) × (G+I) operator matrix. Eq. (2.2) is a convenient way of expressing the multigroup neutron diffusion quation without specifying the method of solution. Other forms are possible depending upon the ordering of unknowns, the method of solution, and the discretization of space and time.

Let a reactor be modeled by a grid of spatial mesh points. Then spatial discretization of multigroup neutron diffusion equation leads to the semi-discrete form of the kinetics equation

$$\frac{\partial\Psi}{\partial t}=A\Psi \qquad (2.3)$$

Much effort has been devoted to the development of methods that numerically solve the multigroup neutron diffusion euqation as efficiently as possible. These methods are reviewed in the next section.

Numerica solution algorithms for the time-dependent nutron transport equation have been reviewed by Ise and others.[8] At present, only a few transport kinetics codes have been developed for one[9,10,11] and

two dimensional applications.[12,13] The detailed discussion on the transport kinetics is beyond the scope of this report.

3. Computational Solution Methods

Since a general solution of the multigroup diffusion equation in terms of continuous parameters r and t is impractical for most reactor problems of interest, numerical solution techniques are usually employed. A nuclear reactor may be numerically modeled as a grid of mesh points. Associated with each mesh point are the values of the dependent variables of the neutron diffusion equation: G group fluxes and I precursor concentrations. For a total of N mesh points there are then $(G+I)\times N$ unknowns. Furthermore, the time dependence is discretized and the unknowns must be solved at each step in time.

Solution techniques for the multigroup form of the timedependent diffusion equation in one or more space dimensions can be divided into two broad categories: direct solution techniques and indirect solution techniques such as synthesis methods. For purposes of reviewing their status in this paper, comptatioal methods are grouped into five classes. These are: finite difference (direct integration) methods, synthesis (modal) methods, quasistatic (factorization) methods, nodal (coupled-core) methods, and coarse-mesh methods.

In finite difference methods the neutron diffusion equation is solved by direct numerical integration. These mothods are direct solution techniques and other ones belong to indirect solution techniques.

In synthesis methods the fluxes are expanded as sums of spatial modes with expansion coefficients to approximate the unknown function of space and time by a linear combination of known space functions with unknown time-dependent cofficients. Quasistatic methods may be thought of as synthesis methods with only one spatial mode.

In nodal methods a reactor is divided into large subregions. A single node is then associated with each of these subregions and assigned gross values that are characteristic of the nuclear properties of the subregion.

While the first four classes utilize a fine-mesh spatial discretization procedure, coarse-mesh methods use a variety of techniques to increase the size of the reactor regions which are used in the discretization procedure.

3.1 Finite Difference Methods

The direct finite difference methods are the most straightforward approach to the solution of space-time problems. The general theory of these techniques has been discussed in some detail.[1,7,14]

In finite difference methods, the neutron diffusion equation is solved directly: fluxes are not approximated by piecewise polynomials, coupled black boxes, or spatial modes as in other methods. The only assumption made is that differential operators in the diffusion equation may be adequately represented by finite differences. A consequence of this lack of major approximations is that finite difference methods are characterized by a large number of unknowns. In favor of finite difference methods is the applicability of mathematical analysis which makes fairly definite error estimates possible.

Because of the large storage requirements and long computing times, until recently this approach has been impractically expensive for multidimensional problems. But

increased computing power in the past several years has permitted serious consideration of direct solutions to multidimensional problems.

3.1.1 Explicit method

Explicit time-differencing of Eq. (2.3) leads to

$$\frac{\Psi^{n+1}-\Psi^n}{h}=A\Psi^n \tag{3.1}$$

where $\Psi^{n+1}\equiv\Psi(t^{n+1})$=flux vector at time t^{n+1}

$\Psi^n\equiv\Psi(t^n)$=flux vector at time t^n

$h\equiv t^{n+1}-t^n$=time step size,

or $$\Psi^{n+1}=(I+hA)\Psi^n \tag{3.2}$$

The explicit method represents the absolute minimum computational effort at each time step, but is numerically unstable unless h is undesirably small.

3.1.2 Implicit method

Implicit time-differencing of Eq. (2.3) leads to

$$\frac{\Psi^{n+1}-\Psi^n}{h}=A\Psi^{n+1} \tag{3.3}$$

The solution is

$$\Psi^{n+1}=(I-hA)^{-1}\Psi^n \tag{3.4}$$

Implicit solutions are unconditionally stable and therefore permit the use of relatively large values of h. The allowable time-step size is limited only by truncation error. However, the solution of Eq. (3.4) requires a very expensive matrix inversion at each time step.

Recently TRIMHX code[15], a direct implicit method analyzing three-dimensional problems, has been developed and shown to be accurate at reasonable computing costs.

3.1.3 Semi-implicit method

Although fully explicit and fully implicit integration algorithms have been employed to some extent, numerical stability problems associated with the former and truncation errors associated with the latter have motivated the study of semi-implicit algorithms.

The best known of the semi-implicit methods is the so-called "θ-method," which is employed in the widely used WIGL[16,17] (one-dimensional) and TWIGL[18] (two-dimensional) codes. In θ-method, the matrix A is divided into two parts as follows:

$$\frac{\Psi^{n+1}-\Psi^n}{h}=\theta A\Psi^{n+1}+(I-\theta)A\Psi^n \tag{3.5}$$

where θ is a diagonal matrix of elements, θ_{ii}, such that $0\leq\theta_{ii}\leq 1$, The θ_{ii}'s are chosen to improve the accuracy of the approximation. In the limits $\theta\rightarrow 0$ and 1, the algorithm becomes fully explicit and fully implicit, respectively.

The solution of Eq. (3.5) is

$$\Psi^{n+1}=[I-h\theta A]^{-1}[I+h(I-\theta)A]\Psi^n \tag{3.6}$$

Proper selection of θ makes it possible for semi-implicit methods to solve the neutron diffusion equation efficiently by using large time step sizes. However, at each time step, the matrix $(I-h\theta A)$ must be inverted. In two or three space dimensions, this would require quite expensive interative procedure.

A particular method has been investigated to reduce truncation error without the expense of complicated inversions as in the previous technique, making use of an "exponential transformation,"

$$\Psi(t)=exp[\Omega t]T(t) \tag{3.7}$$

where Ω is a diagonal matrix. Since the behavior of $\Psi(t)$ is basically exponential in nature, $T(t)$ should be relatively slowly varying, provided that Ω is properly chosen. Hence, the time derivative of $T(t)$ can be represented adequately by a low-order difference approximation.

The idea of exponential transformation along with matrix splitting techique was employed in the one-dimensional GAKIN code[19] and its revised version GAKIN II[20]. This algorithm was applied to two-dimen-

sional problems by McCormick and Hansen,[21] and extended to treat higher spatial dimensions by coupling with the alternating direction methods.

"Alternating direction methods" use a two-step partitioning. A-matrix is splitted as

$$A=A_1+A_2=A_3+A_4$$

For even time steps one partitioning is employed, and for odd time steps the other partitioning is employed, so that temporal discretization of Eq. (2.3) leads to

$$\frac{\Psi^{n+1}-\Psi^n}{h}=A_1\Psi^n+A_2\Psi^{n+1}$$

$$\frac{\Psi^{n+2}-\Psi^{n+1}}{h}=A_3\Psi^{n+1}+A_4\Psi^{n+2} \qquad (3.8)$$

where Ψ^{n+2}=flux vector at time t^{n+2}

$$h=t^{n+2}-t^{n+1}=t^{n+1}-t^n$$

The two-step finite difference solution in

$$\Psi^{n+2}=[I-hA_4]^{-1}[I+hA_3][I-hA_2]^{-1}[I+hA_1]\Psi^n \qquad (3.9)$$

Alternating direction methods are two-step finite difference methods for which A_1, A_2, A_3, and A_4 are chosen such that Eq. (3.9) is numerically stable and yet $(I-hA_2)$ and $(I-hA_4)$ are easily inverted. These methods may be divided into three categories differentiated by the treatment of diffusion terms: alternating direction explicit (ADE), alternating direction implicit (ADI), and alternating direction checkerboard (ADC).

ADE method (MITKIN code) by Reed and Hansen[22] and ADI method by Wight and others[23] were successfuly applied to the solution of diffusion equations in two space dimensions. The MITKIN method was subsequently extended to treat three-dimensional geometries by Ferguson and Hansen[6] with 3DKIN code. The checkerboard method[7], a recently proposed alternating direction method, was shown to be competitive with other alternating direction methods.

3.2 Synthesis Methods

A varity of methods, having the expansion of part or all of the spatial dependence in known functions with undetermined expansion coefficients that depend upon the remaining spatial variables (if any) and time, have been developed in an attempt to obtain an economical, but accurate, spatial approximation. These methods have been labeled as modal-expansion[24] or synthesis methods.[25,26]

Synthesis techniques can be broadly categorized as being either time synthesis or space-time synthesis. Methods in which all the spatial dependence is expanded, resulting in ordinary differential equations for the time-dependent expansion coefficents, are known as "time synthesis" methods. "Space-time synthesis" is the term used for those methods in which only part of the spatial dependence is expanded, resulting in partial (space and time) differential equations.

In time synthesis methods the fluxes are expanded as sums of spatial medes with time varying coefficients

$$\phi_g(r,t)=\sum_{k=1}^{K}\phi_{gk}(r)\,T_{gk}(t) \qquad (3.10)$$

where $\phi_g(r,t)$=multigroup flux

$\phi_{gk}(r)$ =k'th spatial mode or "trial function"

$T_{gk}(t)$=coefficient of k'th mode.

Space-time synthesis scheme is capable of dealing with problems of much greater detail than is the time synthesis. The space-time techniques utilize expansion functions which represent flux shapes over subregions of a reactor. A standard approach is to use two-dimensional flux shapes representing all or part of a cut through the reactor perpendicular to the z-axis

$$\phi_g(r,t)=\sum_{k=1}^{K}\phi_{gk}(x,y)\;T_{gk}(z,t) \qquad (3.11)$$

where $\phi_{gk}(x,y)$=two-dimensional trial function

$T_{gk}(z,t)$ =mixing coefficient.

The spatial modes decribe the flux behavior over large portions of the reactor, therefore, fewer spatial mesh points are required and the total number of unknowns is substantially decreased. The choice of modes (expansion functions) is an important aspect of the application of modal expansion methods. Various attempts[1,3] utilizing several types of modes have been successfully applied to reactor models. Two variants of space-time synthesis have been found to be the most accurate; the multichannel synthesis[27,28] and the discontinuous space-time synthesis[29,30]. The space-time synthesis with axially discontinuous trial functions treating BWR rod drop accident[31] showed accurate results of calculation with fairly large time step sizes relative to the ADE finite difference method.

Modal methods are characterized by a lack of definitive error bounds. For the analysis of operational transients, where safety is not an important issue, space-time synthesis methods are generally satisfactory and are often the most practical. When safety issues become important, such as in the analysis of the more severe off-normal transients and hypothetical core disruptive accidents in LMFBRs, the fact that no procedure exists for establishing an error bound on the solution provided by a synthesis method becomes a serious drawback. This fact has served to spur the development of more exact quasistatic methods.

3.3 Quasistatic Methods

The quasistatic methods proposed by Ott[32] and improved by Ott and Meneley[33], factorize the neutron flux into a time-dependent amplitude function and a space- and energy-dependent shape function which is assumed to be slowly varying in time. The amplitude function is obtained as the solution to the point kinetics equations; shape function is to be recomputed at intervals throughout the transient. Quasistatic methods may be though of as time synthesis with only one spatial mode. The total flux $\Phi(r, E, t)$ can be separated into a product of a "shape" function and an "amplitude" function

$$\Phi(r,E,t)=\Psi(r,E,t)N(t) \qquad (3.12)$$

where $\Psi(r,E,t)$ =shape function

$N(t)$ =amplitude function; $N(0)=1.0$

The factorization approach has been the basis for the onedimensional computer program QX-1[34] for the "quasistatic treatment of excursions." It has been demonstrated that the quasistatic solution converges to the solution obtained by direct numerical integration for both fast reactor[35] and thermal reactor problems.[36,37,38] Although the accuracy of quasistatic method is adequate for both reactor problems, the accuracy of the method is much better for fast reactors than for thermal reactors.

Because the quasistatic method was developed primarily for fast reactor transient analysis, it has been employed in two production-oriented two-dimensional multigroup fast reactor transient analysis codes, FX2[39,40] and KINTIC-1[41]. Some variation of the quasistatic method will surely be utilized in three-dimensional fast reactor transient analysis code which is to be developed at Argonne Natonal Labora tory[5].

Quasistatic method has also been proved to be an accurate and practical tool for use in CANDU reactor transient calculations[42]. At present all routine CANDU transient analyses requiring multidimensional neutron kinetics calculations are carried out using this method[43,44].

3.4 Nodal Methods

The extension of the modal expansion to actual reactor is often unsatisfactory because too many modes are required to describe the complex configuration in two or three dimensions. These practical reactor problems may be solved by applying the nodal method first proposed by Avery[45] for a system of coupled reactors.

In nodal methods[1,46] a reactor is divided into large subregions. A single "node" is then associated with each of these large subregions and assigned gross values that are characteristic of the nuclear properties of the subregion. The number of spatial points at which a solution is sought is thus greatly reduced. The group flux within each node j is written as the product of a shape function and an amplitude function,

$$\phi(x,y,z,t)=\Psi_j(x,y,z)N_j(t) \qquad (3.13)$$

where $\Psi_j(x,y,z)$ = shape function

$N_j(t)$ = amplitude function.

The nodal approximation is actually a special case of a modal approximation in which only a single expansion mode is used in a given region. The nodes in nodal approximation are then coupled together by coupling coefficients and may be treated as "black boxes" once the coupling coefficients between them are specified.

The principal difficulty encountered in using the nodal model is associated with determining the couling coefficients. The essential problem is that the coupling coefficients are not constant but rather depend on the flux levels and shapes, both of the nodes directly coupled and of neighloring nodes. The most successful nodal schemes[47] account for this fact by updating the coupling coefficients as the calculation proceeds or by dealing with the currents between nodes explicitly.

The application of nodal methods has been primarily to reactors composed of physically separated cores, such as those proposed for rocket propulsion or for fast breeder reactor. Recent investigations[48,49,50] have demonstrated that the response matrix technique, which is included among nodal methods, can significantly reduce the computational effort for solution without loss of accuracy.

3.5 Coarse-Mesh Methods

The most obvious stratagem for reducing the computing time associated with the multigroup method is to reduce the number of mesh points. This reduction may be done simply without modifying the computational algorithm, or it may be done in conjunction with a redefinition of the algorithm.

A number of methods have been proposed for arriving at an algorithm for coarse-mesh difference equations which is more accurate than the conventional type of difference algorithm. A generalization of the finite difference approximation method by Alcouffe and Albrecht[51] allowed the possibility of significantly reducing the number of mesh points necessary to achieve an accurate solution over that required by the conventional finite difference method. The coarse-mesh method[52,53], the principle of which has been introduced by Birkhofer and Werner[54], requires considerably smaller number of unknowns and consequently less computing time than the finite difference method at comparable accuracy.

A second coarse-mesh techique which has only recently been applied to transient problems is the well-known finite element method[55,56]. Kang and Hansen[55] first treated the two-dimensional time-dependent diffusion equations with this method.

In finite elment methods the spatial flux

shape is approximated by piecewise polynomials defined over subregions of the problem domain, the "finite elements." Finite element methods tend to reduce the number of spatial points at which the flux must be calculated for results of a certain degree of accuracy. The time dependence of the flux may also be approximated by polynomials to increase the time step size. These methods are amenable to computer analysis which guarantees convergence; rigorous error bounds are readily determined. Rohan and others[57] designed HERMITE code for use in PWR transient analysis and extended finite element solution technique to three-dimensional calculations with promising results.

4. Summary

Solution methods for the multigroup space-dependent reactor kinetics equation are divided intot wo broad categories: direct solution methods and indirect solution methods such as synthesis, quasistatic, and nodal methods. Direct methods are characterized by fairly definitive error bounds and thus valuable as numerical standards against which the more rapid but more approximate indirect techniques can be compared. Major shortcoming of the direct methods is the large storage requirements and long computing time. With the recent increase in computing power, the direct integration methods, among which alternating direction methods are most promising, are now feasible for use in routine production calculations.

Indirect solution methods have characteristically small computing time requirements. But their main drawbacks are no existance of rigorous error bounds and strong influence of the accuracy by the choice of trial functions. Space-time synthesis scheme is more capable of dealing with problems of much greater detail than other indirect methods. Quastatic methods have been used in transient analyses of fast breeder reactors and heavy water reactors. The response matrix technique, which is included among nodal methods, significantly reduces the computational effort and are undergoing development as an efficient analysis tool. Coarse-mesh mothods such as the finite element method show promise of allowing a reduction in the number of unknowns without loss of accuracy.

A solution technique should be as economical as possible while still providing a sufficiently accurate solution. In order to accomplish this, one should reduce the number of unknowns and/or should minimize the number of times that the unknowns must be determined. The methods which permit either a reduction in the number of unknowns and/or large time step sizes will deserve further attention.

The day when the three-dimensional multigroup time-dependent diffusion-theory treatment of realistic reactor transients can be routinely used is not far long way in the future.

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