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ON THE THEORIES, TECHNIQUES, AND COMPUTER CODES USED IN NUMERICAL REACTOR CRITICALITY AND BURNUP CALCULATIONS

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ABSTRACT

The purpose of this paper is to discuss the theories, techniaues and computer codes that are frequently used in numerical reactor criticality and burnup calculations. It is a part of an integrated nuclear reactor calculation scheme conducted by the Reactors Department, Inshas Nuclear Research Centre. The crude part in numerical reactor criticality and burnup calculations includes the determination of neutron flux distribution which can be obtained in principle as a solution of Boltzmann transport eqation. Numerical methods used for solving transport equations are discussed. Emphasis are made on numerical techniques based on multigroup diffusion theory. These numerical techniques include nodal, modal, and finite difference ones. The most commonly known computer codes utilizing these techniques are reviewed. Some of the main computer codes that have been already developed at the Reactors Department and related to numerical reactor criticality and burnup calculations have been presented.

1. INTRODUCTION AND BASIC BACKGROUND

Reactor criticality and burnup calculations form an extremely important part in nuclear reactor analysis work. The key parameters in these calculations are the neutron flux and power distributions. In principle, the neutron flux can be obtained as the solution of Boltzmann transport equation. However, it is impossible to solve neutron transport equation exactly for general energy dependent reactor problems. This is mainly due to the complications of the representation of the form of cross sections dependence on neutron energy[1].

So; generally; approximate methods are used for solving the energy dependent neutron transport equation, most commonly: Monte Carlo and Multigroup methods.

It can be referred to Honeck[2] for solution of the integral transport equation using numerical or approximate kernels.

Monte Carlo method[3,4] has proved to be useful in some areas of reactor physics and cases of complex geometries. Results obtained by this method can serve as standards for the assessment of the results of other approximate methods.

Monte Carlo method is in principle a numerical procedure that is based on probability or statistical theory. In the application of this method for neutron transport calculations, neutron macroscopic cross sections are defined as the probability of interactions per unit distance travelled by a neutron and so a set of neutron histories is generated by following neutron successive collisions. The locations of actual collisions and the results of such collisions (direction and emerging neutron energy) are determined from the range of possibilities by sets of random numbers.

Multigroup methods are the most commonly used for the solution of energy dependent reactor problems.

In this method, the angular dependence of neutron flux is represented by an expansion; most commonly; in spherical harmonics. In case of axial symmetry of the angular flux distribution, the expansion reduces to a sum of legendre polynomials, denoted by $P_n(\mu)$, where μ is the direction cosine. Since the spherical harmonics (or Legendre polynmials) form a complete set, there is no approximation in the neutron flux representation. The approximation stems from the fact that in practice the expansion has to be terminated after a finite number of terms. The so called P_N approximation is that in which the series is terminated after N + 1 terms.

The next step in the solution is to define the energy groups by dividing the neutron range of interest into a finite number of intervals or groups and then integrating over the energy group to obtain the multigroup P_N equations.

When the angular distribution of the neutron flux is represented adequately by the first two terms of Legendre polynomials; $P_0(\mu)$ and $P_1(\mu)$; the multigroup P_1 approximation is obtained which according to certain assumptions are equivalent to multigroup diffusion theory[5,6].

The second class of multigroup methods is known as the discrete ordinates or discrete S_N (or simply S_N) method.[7] In this method the neutron transport equation is solved in a set of directions only. Angular integrals are then approximated by sums over discrete directions and angular derivatives by differences.

2. MULTIGROUP DIFFUSION THEORY APPROXIMATION

It has been long recogenized that the multigroup diffusion theory appoximation to the transport equation gives sufficient accuracy for various reactor types. A steady state neutron chain reactor problem in the multigroup diffusion theory model is mathematically equivalent to an eigen boundary value problem for the multigroup diffusion theory equations which forms a system of coupled olliptic partial differential equations of second order supplemented by group dependent logarithmic boundary conditions.

The solution of this eigen boundary value problem has been accomplished by applying various numerical techniques, most commonly[8-12]:

a - nodal techniques,
b - modal techniques, and
c - finite difference techniques.

The nodal methods including the finite element technique and modal methods including various synthesis techniques may be combined among themselves and with the finite difference techniques and may finally result in computer time saving when large cores in two and three dimensional geometry are dealt with.

a - Nodal Techniques

In these Techniques the reactor is divided into a number of zones or meshes with volumes much larger than that of the finite difference techniques. Each of these zones,represented by a space point is assumed uniform flux and nuclear properties. Coupling among the zones (or nodes) is evaluated in a way which is a compromise between accuracy and simplicity. Nodal techniques are most commonly applied for solution of reactor kinetics problems. A well known example of the application of nodal techniques is FLARE computer code[8]. It is a three dimensional code written for boiling water reactors and allows a maximum of 14 by 14 by 12 nodes. Another nodal technique is that proposed by Aoki Shimizu called the Response Matrix Method[9]. The finite element method[10]

may be considered belonging to the category of coarse mesh technique rather than to that of nodal techniques. The use of coarse meshes for the three dimensional two-group diffusion calculations has also been suggested by Borresen[11].

b - Nodal Techniques

In these techniques the flux is expanded in a set of orthogonal eigenfunctions. Other sets may be considered for approximate solutions[12]. Examples for the application of modal techniques are LOUISA computer programs[13]. CONDOR[14,15] is two dimensional four group computer code for neutron diffusion and depletion calculations. In this code a coupling of modal and finite difference methods is carried out to allow reasonably good criticality search and a rough flux shape calculation within a limited number of harmonics. Such a calculation is then followed by finite difference calculations with few number of iterations to get the good flux shape and the correct value of criticality. This coupling of the modal and of the finite difference methods results in a substantial computer time saving.

The flux synthesis technique is a relatively new modal method for which the theoretical foundation has not yet been completed[16]. For details it can be referred to the work done by Meyer[83], Wachspress[18 - 20], Kaplan[21 - 23], Nakamura[24 - 25], and others[26 -31]. SYNTRON[32] is an example of the three dimensional burnup programs based on flux synthesis technique. Larsen[33] has discussed the accuracy of flux synthesis and how to select trial functions.

c- Finite Difference Techniques

These techniques are by far the most employed for one, two and three dimensional computer programs developed up to the present time. In the computer codes based on finite difference techniques, the convergence of the numerical solution of the resulting

discretized equations is accelerated through the use of various inner-outer iteration strategies and overrelaxation techniques[34,35]

The most commonly known computer codes used for the solution of criticality and burnup problems and based on the solution of neutron diffusion equations with finite difference techniques in one, two and three dimensions will be reviewed in the following three sections.

3 - One Dimensional Diffusion Codes Based On Finite Difference Techniques

Examples for one dimensional computer codes are WANDA[36] WANDA-5[37], AIM-5[38], and FOG[39], Each can be used for slab, cylindrical, or spherical geometry. In FOG and WANDA series of codes, a maximum of four groups is permitted and slowing down is permitted only from each group to the next lower group. AIM5 code is more flexible as the complete downscatter matrix is allowed as well as up to 12 energy groups can be specified (it is 18 energy group in AIM AIM-6 code). CANDIE[40], and CNCR[41] are one dimensional diffusion depletion codes based on WANDA spatial calculations. For more one dimensional diffusion codes, it can be referred to references[42] through [46]

4 - Two Dimensional Diffusion Codes Based On Finite Difference Techniques

Examples for two dimensional computer codes are CURE[47]; PDQ-2[48], PDQ-3[43], PDQ-4[50], and PDQ-5[51], The only significant mathematical difference between PDQ codes is in the inner iteration techniques, Point, one line, two lines, and block overrelaxation methods are used in respectively PDQ-2, PDQ-3, PDQ-4, and PSQ-5 Optimum overelaxation factors for each group are determined in an auxiliary computer routine which preceeds the solution of the problem using a priori iteration scheme. PDQ codes permit downscatter to only the

next lower group. In CURE code, the inner iteration process is carried out using the alternating direction method[52]. The depletion of PDQ is called TURBO [53,54] and is based on the approach of isotopes depletion calculations adopted in CANDIE[55](a one dimensional, few group diffusion theory depletion code). The depletion version of CURE is developed through the combination of CURE and BOX[56] codes.

EXTERMINATOR[57] and EXTERMINATOR-2[58] are multigroup codes that allow downscatter from any of up to 50 energy groups to any other groups. These two codes are improvements over the slower few group diffusion code TWENTY GRAND[59]. The depletion version of EXTERMINATOR code is the ASSAULT code[60] where the nuclide irradiation chains are specified by the user. CRAM[61] and FTD-2[62] codes are developed especially for gas graphite reactors. In CRAM code, both one and two dimensional problems can be considered with up to one hundred energy groups and neutrons are allowed to scatter from any group to another. In FTD-2 code, a one- or two-group two dimensional flux calculations followed by a heat transfer calculations can be carried out. Inner iterations in FTD-2 code are accelerated by using the extrapolation method with a constant extrapolation factor determined experimentally.

FUEICYC[63-64] is a two dimensional code based on the modified two group diffusion theory. It works for fuel cycle studies allowing for a maximum of seven mesh points in any direction. Outer iterations in this code are accelerated by Aitken's δ^2 process while the inhomogeneous flux equations are solved analytically with Crout reduction method. This code serves well for survey-type calculations and study of different fuel management schemes.

The code developed by Goto[65] for natural uranium graphite moderated reactor is a two-dimensional one-group diffusion code for depletion calculations in r-z cylindrical coordinates. It allows a maximum of 12 by 5 mesh points and treats the reflector by the one-group reflector saving approximation.

EQULPOISE[66] is a two-group two-dimensional computer code with a maximum of 625 mesh points. The inner iteration process in the code is accelerated by the point overrelaxation method with the extrapolation factor determined by an empirical formula. EQULPOISE-3[67] is an improvement of EQULPOISE and allows for up to 2100 mesh points.

For more examples of two dimensional computer codes based on finite difference numerical techniques, it can be referred to GAMBLE-5[68] and GAMTRI[69] (with 10 groups and 20000 mesh points), the companion programs BUG-2 and BUGTRI[70] (with 60 groups and 20000 mesh points and including fuel deletion routine[71], ERBUS[72] (with 15 group and 10000 mesh points and including fuel depletion routine), and TWODIM[73] code with its depletion version DBU[74-75].

5. Three Dimensional Diffusion Codes Based on Finite Difference Techniques

In the review of three dimensional diffusion codes based on finite difference numerical techniques, it can be referred to TKO[76] and TRIXY[77] codes. TKO code is used as a component part of the depletion code DRACO[78].

Among other three dimensional codes, there are WHIRLAWAY[79] (with two groups and 12750 mesh points), TRITON[80] (with ten groups and 16000 mesh points and including fuel depletion routine), and GATT[81] (for hexagonal geometry, 14 groups, and 100000 mesh points).

6. Some Locally Developed Reactor Criticality and Burnup Computer Codes

As an example for the computer codes developed locally for reactor criticality and flux distribution calculations a multigroup multiregion one dimensional diffusion code was developed[45].

This code, which applies for ether slab, cylinderical or spherical geometry uses the finite difference numerical ttechnique for solution of the problem. The resulting inhomogeous flux equations are solved by the factorization method whereas the convergence of source iterations are accelerated by using point overrelaxation methods with a constant acceleration factor used as input.

Another example is the one dimensional computer program "UAFCC[82]" designed for survey-type fuel management calculations. It solves analytically the one energy group neutron diffusion equation for a multiregion infinite cylindrical reactor system with axial symmetry. Although this code allows for multiregion core calculations it only applies for reactor cores with single leading fuel enrichment. Irradiation dependent nuclear properties and fuel composition are introduced as polynomials in the single variable "fluxtime". These polynomials are generated by the application of the point model burnup computer code "UABUC"[83] on the assumption that nuclear and composition properties are strongly dependent on fluxtime and approximately independent on the time dependence of neutron flux. It can be referred to references[84] and[85] for some of UABUC code applications. UAFCC code is used in the study of different strategems of incore fuel management schemes including " In-Out","Out-In",and "Batch" loading schems. The criteria of comparison are the maximum burnup level, flux and power radial form factors, and average incore residence time. It can be referred to reference[87] for the results of this study.

The computer code "CAIRO"[88] is a two dimensional multiregion one group neutron diffusion code for criticality and flux calculations in axial and radial cylindrical coordinates using finite difference numerical techniques. A nonuniform grid of horizontal and vertical lines is allowed such that all internal surfaces and external boundaries lie exactly on mesh lines. The inner iteration process is carried out using point overrelaxation method and outer -

iteration process is solved by the power method accelerated by application of extrapolation techniques. CAIRO code has been used in the study of major numerical factors affecting convergence rates of iteration processes[89].

The depletion version of CAIRO computer code is called AMON2[90] and is based on point model depletion calulations adopted in AMON[91] computer code. AMON2 code has been designed for the purposes of determination of neutron flux and power distributions as functions of space and burnup level as well as the study of poison management and different strategems of incore fuel management. AMON2 code has been designed in a way that permits the user a virtual unlimited choice in carrying out the type of calculations he needs. The usual power method used in outer iteration process is accelerated by either a fixed extrapolation factor or a set of extrapolation factors to be generated internally by the code using Chebyshev polynomials and updated automatically with progress of irradiation. The successive overrelaxation factor to be used in the acceleration of inner iteration process can be either given as input or calculated internally by the code. The output of AMON irradiation dependent nuclear and composition properties are used as inputs to AMON2 code in the form of fitted polynomials of suitable degree in burnup, evaluated using a least square computer routine developed for this purpose and named " POLFIT" [92]. This routine uses orthogonal polynomials and avoids the problems associated with direct methods of least squares.

For further examples of locally developed computer codes; related to lattice cell calculations, reactor criticality and burnup calcuations, and fuel management calculations; it can be referred to the work of M.Michaiel and other colleagues (93).

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