CALCULATION OF 3-DIMENSIONAL RATING DISTRIBUTIONS IN OPERATING REACTORS

CALCUL DES DISTRIBUTIONS TRIDIMENSIONNELLES DE DENSITÉ DE PUISSANCE DANS LES REACTEURS EN COURS D’EXPLOITATION

Proceedings of a Specialists’ Meeting
Compte rendu d’une réunion de spécialistes

PARIS
26-28 NOVEMBRE 1979

NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT
AGENCE POUR L’ENERGIE NUCLEAIRE
ORGANISATION DE COOPERATION ET DE DEVELOPPEMENT ECONOMIQUES
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Paris, 26-28 novembre 1979

Sponsored by the
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Organisé sous l’égide du
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NUCLEAR ENERGY AGENCY
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FOREWORD

New calculation methods for reactor power rating distributions had been discussed in detail at the 20th and 21st Meetings of the OECD/NEA Committee on Reactor Physics in 1977 and 1978. Sponsorship of a specialist meeting on this topic was decided in order to bring together a wide range of experts from NEA Member countries, from scientific research, development, reactor vendors and utilities operating nuclear reactors.

Discussions at this meeting concerned the verification of the new and much faster 'nodal' or 'coarse mesh' computer calculation techniques for three-dimensional power rating distributions in operating power reactors. The emphasis of the papers included in these proceedings is on the comparison of calculations with measured operating data in order to demonstrate the validity and accuracy of these new methods for predicting power peaking and for fuel management. The increase in speed of calculation offered by these methods, as compared to existing 'fine mesh' diffusion and transport techniques, is of great importance in the potential it offers for 'on-site' computer guidance to plant operators, and perhaps in the future as an 'on-line' tool in the reactor control room.

AVANT-PROPOS

De nouvelles méthodes de calcul des distributions de puissance dans les réacteurs avaient été discutées en détail pendant les 20 et 21èmes réunions du Comité OCDE/AEN sur la Physique des Réacteurs, en 1977 et 1978. Le Comité a décidé de patronner une réunion de spécialistes sur ce thème, dans le but de rassembler des experts de domaines très différents, tels que : la recherche scientifique, le développement, la construction et l'exploitation des réacteurs nucléaires de puissance.

Les discussions au cours de cette réunion ont porté sur la vérification de nouvelles et puissantes techniques de calcul, sur ordinateur (dites de mailles grossières) des distributions de puissance en trois dimensions dans les réacteurs en cours d'exploitation. Les articles reproduits dans ce rapport concernent principalement la comparaison de ces calculs avec les données de mesures opérationnelles, faisant ainsi la démonstration de la validité et de l'exactitude de ces nouvelles méthodes de prévision pour les excursions de puissance et pour la gestion du combustible. Les gains en vitesse de calcul que promettent ces méthodes sont d'un très grand intérêt pour les responsables de centrales nucléaires désirant se faire guider directement par ordinateur pour le fonctionnement du réacteur, et ouvrent même pour l'avenir des perspectives de pouvoir faire ces calculs en temps réel dans les salles de commande des réacteurs.
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Summary of the Meeting
Résumé de la réunion

J. Askew

The meeting was held at OECD Headquarters in Paris over the three days 26th-28th November 1979. There were 59 participants, representing utilities, reactor vendors and research laboratories, one from IAEA and three from non-OECD countries.

Twenty-four papers were presented. In almost all cases copies of these were available at the beginning of the meeting, and this greatly facilitated discussion. The contributions reflected the practical importance of the topic to all concerned with the exploitation of nuclear power.

Almost all the papers related to Light Water Reactors, but the two exceptions, one on heavy water moderated, boiling light-water cooled, pressure tube reactors and the other on sodium cooled fast reactors, showed that very similar considerations arose in the operation of these reactors.

The session chairmen summarized at the meeting the salient points to emerge from the papers and from the discussions following their presentation, and I attempted an overall summary which I was agreed reflected the state of the art. The following notes are an edited version of this summary.

1. Types of Calculation in Use

The calculations reported were predominantly of a coarse mesh type in which the whole reactor was represented by one or 2 x 2 nodes per assembly in the xy plane and by a mesh of broadly similar size in the axial direction. There was, however, a great deal of detailed difference between the methods, both in the treatment of energy as one, 1/2 or 2 groups and in the derivation of the equations representing a node, which ranged from simple finite difference forms deduced from a homogeneous theory to more elaborate finite element or within node expansion solutions in which more than one degree of freedom per node was allowed. Some use of synthesis methods was reported, especially for representing the axial dimension in cases where control rod strategies were such as to permit a simplification in modelling. No use of the more complex variational synthesis methods was reported.

2. Lattice Calculations

All the methods assumed the use of rather detailed models of the fuel assemblies. It was at this level that the heterogeneities due to different pin enrichments, the incorporation of burnable poisons and of control absorbers were treated in some relatively fine space/energy model. The homogenization techniques used to reduce these to a smeared, few-group, form had been the subject of a recent meeting in Lugano, sponsored by NEACRP, and were not discussed in detail. It could, however, be deduced from comparisons between different sets of core follow data that some significant contributions to the observed discrepancies in rating distribution arose from either the nuclear data or the models being used by some
contributors at this stage of the calculation. Because of the importance of neutron spectra and heterogeneity on the depletion of burnable poisons, a burnup calculation is usually performed using the assembly model. In many cases it is sufficient to generate a library of macroscopic cross-sections as a function of irradiation and other salient variables to service the whole reactor calculation, but in some cases microscopic cross-sections are used and individual nuclides are identified at the reactor level. This is most common in the treatment of transient effects due to variation in xenon concentration.

3. **Within Assembly Variations in Depletion**

The whole reactor calculation leads to the prediction of significantly different flux levels in different parts of a fuel assembly, and hence to different burnup levels. Although it is possible to devise nodal models which give a good representation of the solution in a large mesh of constant properties, this variation will set a limit to the accuracy achievable unless the smooth within-mesh changes of cross-section are accounted for. Most contributors followed burnup separately for each quadrant of an assembly, and the conclusions on achievable accuracy include any residual errors due to this approximation. The point was not, however, explicitly addressed in papers to the meeting.

4. **Experimental Evidence**

Many contributors were able to cite evidence from "in-reactor" scans using fission chambers or aeroballs, occasionally supplemented by flow and temperature data, to substantiate the performance of their chosen methods. It was noted that measurements at one location in an assembly can be interpreted as assembly ratings only with the aid of a subsidiary model, and that the uncertainty introduced at this step of the comparison is not negligible. It is therefore most desirable that, wherever possible, the reactor and lattice model be used directly to predict the quantity actually measured rather than some derived quantity perhaps obtained using an inconsistent model. Reference was made to the ANSI standard recommending such a procedure. Very little evidence on the relative rating of individual pins was presented. The only type of evidence easily obtained is that from gamma scanning, and it was not clear how much data was available. As pin ratings are the quantity of most direct interest in a safety argument, and hence in determining operating limits, it is desirable that attention be focused on the requirement for more data of this type. An associated question is that of deducing consistent pin ratings from coarse mesh models of the reactor. There is some evidence that a simple synthesis, in which the macroscopic rating distribution is imposed upon the original lattice cell distribution, may be insufficiently accurate, and other methods in which the pin rating was recalculated using some imposed quantity such as fast flux or fission-source distribution, or assembly boundary conditions deduced from the whole reactor calculation, were discussed. No definitive evidence on the accuracy achieved by such models was presented.

5. **Current Measurement Accuracies**

Participants were of the view that ion chamber measurements would be expected to have an RMS error of the order of ± 2% including statistical and positioning effects, although some participants considered that higher precision was achieved. At this level the problems of interpreting the measurements are likely to be the dominant source of uncertainty in comparisons, and will contribute about ± 3% for a PWR and a larger uncertainty, dependent upon coolant conditions, in a BWR. Gamma scanning of pins should give 1 - 2% depending upon the technique and the cooling period, but the resulting data is not directly related to rating at a point.
in time and so is of limited resolution. It appeared that measurement accuracy was not at present the most severe limitation or prediction.

6. **Accuracy of Calculation**

It appeared that calculations on a simple 2 x 2 mesh per assembly scheme in 2 energy groups could reproduce measured distribution of fission chamber signals to a peak error of 6% at the worst point in the fuel cycle, equivalent to an RMS error of better than ± 3%. The use of a more refined model for each of the nodes would give a systematic improvement in prediction, as could be shown by comparison with finer mesh calculation and from reactor comparisons, and in this case RMS errors of less than ± 2% were possible with careful representation of reflectors and other physical features of the system. Differences in model and data could, however, give contributions to error which were large compared to this, and it would be necessary to accumulate an extensive body of validating evidence before such precision could be assumed for a particular calculational route.

7. **Adaptive Models**

Two papers referred to adaptive models, and it was clear from the discussions that other participants were actively interested in this topic. The basic idea is that once a model and data set has been developed to give a prediction to an uncertainty of the same order as that of measurement - a situation which was close to realization for a number of the models discussed at the meeting - comparison with observation over a long period of time and systematic adaptation of the codes to agree with the measurements will produce a better prediction capability. A particular application considered is that of developing even simpler models, either on existing computers or on more advanced machines, to the point that they could give reliable indications to reactor operators of the current status of the reactor core in real time. One facet of such a concept is its possible role in assisting the operator to reject the readings of failed instruments in a statistically justified manner.

8. **Future Developments**

Coarse mesh methods have been demonstrated to be a reliable and useful tool for both reactor designers and operators in predicting the assembly to assembly variations of rating for operating reactors. The most advanced models appear to be capable of doing this with an RMS error of the order of ± 2%. There is scope for further refinement in the modelling of reflectors and shrouds, and in the representation of variations of burnup within an assembly, especially at the core edge or following shuffling of edge assemblies. With improvements of this kind the models will be capable, given good nuclear data and lattice calculations, of a predictive accuracy of the same order as that of the measurements.

It is important, however, that further data on pin power is obtained, and there is still scope for improving the ways in which this is deduced from the coarse mesh reactor solution.

It is to be expected that adaptive procedures will be more widely pursued, both in the further refinement of the methods already in use and in the important area of developing simpler and more efficient models suitable for on-line computation as an aid to the reactor operator, either on existing mini-computers or possibly on novel machines based upon microprocessor hardware.
Session 1

Chairman - Président
Dr. J. ASKEW
(United Kingdom)

Séance 1
THE PERFORMANCE OF UK COARSE MESH PWR CALCULATIONS IN COMPARISON WITH REACTOR DATA

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ABSTRACT

LWR physics calculation methods have been under development in the UK since 1969. A sophisticated lattice code, LWR-WIMS, is used to derive cross-sections for use in the core simulator JOSHUA. JOSHUA is a three-dimensional two-group coarse mesh diffusion code. The codes are briefly described in the paper. Validation has also proceeded for many years and the results and conclusions from this work are discussed. Specific sections cover reactivity, radial power and flux distribution, axial power shape, control rod worths and reactivity coefficients. The primary source of data for validation is from power reactors and results from ten operating cycles are included. The paper provides a basis for establishing the accuracy of the methods and also points out those areas where coarse mesh correction techniques could give small improvements in accuracy.

1. INTRODUCTION

Methods of calculation specifically suited for LWRs have been developed in the UK since 1969. The two primary codes used are the lattice code LWR-WIMS and the core simulator code JOSHUA, both of which were based on earlier developments and in particular the WIMS family dates back to 1964. LWR-WIMS and JOSHUA are briefly described in Sections 2 and 3 of this paper.

Validation of this code package has proceeded for many years by comparison with more elaborate calculations, by comparison with zero energy experiments and by comparison of measured and calculated composition of discharged fuel. It was recognised early on that the most important test would be in the simulation of operating LWRs, although the precision of the data obtained in this way would not be great. There are no LWRs in the UK so steps were taken to obtain data from elsewhere. So far we have obtained data from steel clad PWRs Trino Vercellese and Haddam Neck, from the Zircaloy clad PWRs Beznau 1 and Tihange 1 and from the PWRs Dodewaard and Montecello. In this paper we concentrate on Zircaloy clad PWR data on which most work has been done. JOSHUA embodies a simple coarse mesh, finite difference diffusion formulation. We examine the accuracy which can be achieved with such a simple route and provide a basis against which to assess the improvements offered by more advanced coarse mesh treatments.

In 1977 NOK, the operators of the Beznau reactors, became licensees of the LWR-WIMS/JOSHUA code package and have continued the validation work of the Beznau 1 reactor from Cycle 6 onwards.

Simulation has now been carried through 14 cycles of PWR operation including 4 cycles from the steel clad reactors. The amount of data produced is very
large, particularly on power and flux distributions. In this paper we have not attempted to present all the data but have tried to present sufficient to give a good overall impression of accuracy and to draw attention to those areas where improvement in methods can be expected to give real benefits to reactor operators.

2. DESCRIPTION OF LWR-WIMS

2.1 PURPOSE

LWR-WIMS performs reactor physics lattice calculations on LWR fuel assemblies and associated regions such as control rods, shrouds and water gaps. Output includes reactivity, fluxes and reaction rates and few-group averaged cross-sections for whole core static and transient codes. The physics of LWR-WIMS is fully described in /1/.

2.2 THE NUCLEAR DATA LIBRARY

The 69-group data library is common to all the members of the WIMS family of codes and has been used in connection with light water, heavy water and graphite lattices loaded with all types of uranium, plutonium and thorium fuel. Thus any improvements made to the library as the result of comparisons between integral experiments and WIMS calculations must be shown to be valid for the whole range of lattice types. This adds greatly to confidence in the library.

For LWR-WIMS, it has been found convenient to use a sub-set of the 69-group library, obtained by group condensation using typical LWR fuel and moderator spectra. The code is able to accept libraries with any number of groups but extensive optimisation studies have established a standard 28-group structure with only 4 fast, 4 resonance and 20 thermal energy groups. Comparisons of the reaction rates of all nuclides computed with 69 and 28-group libraries have demonstrated the viability of the 28-group library in all cases ranging from uranium enrichment to heavy loadings of recycled plutonium. The corresponding differences in reactivity between the two sets is generally less than 0.001 for irradiation of operational interest.

2.3 RESONANCE TREATMENT

Homogeneous resonance cross-sections are tabulated as a function of temperature and effective scattering cross-section. These WIMS group cross-sections were obtained from calculations using 120,000 energy groups with data generated from the resonance parameters. In a heterogeneous cell an effective homogeneous scattering cross-section is determined using equivalence theorems and this is used to interplate between the tabulated resonance cross-sections. The infinite lattice Dancoff factor is computed by the Carlyik method and corrected where necessary for the effects of water gaps and empty lattice sites. Goldstein Cohen λ-values are used to eliminate the narrow resonance assumption and Bell factors are introduced to correct the rational approximation of the fuel self-collision probability. Corrections are also made for the interaction between resonant absorbers, and group removal cross-sections are adjusted to account for the distortion from a 1/B flux within each resonance group.

2.4 LATTICE DATA INPUT

The input to the code was designed to be straightforward without requiring subsidiary calculations. All the geometric data are in terms of dimensions as they might appear on engineering drawings.

2.5 FLUX CALCULATION

This is a two stage process in which the spectrum in the full number of library groups is first calculated in as many distinct regions as the user requires. This calculation allows for full interaction between these regions. Condensation is made to few groups (normally six) and a calculation of flux distribution in the precise geometry of the assembly is carried out. The options for this are either diffusion theory (GOO), Carlson Sn transport theory (TWOTRAN) or integral transport theory (CLWGR), where the pin cell may be represented heterogeneously.
2.6 BURNUP

The burnup equations are integrated by a simple finite difference method with automatic time step selection. Relative isotopic reaction rates and their renormalisation to the required power level are evaluated with the aid of an homogeneous few group flux criticality calculation that is made at intervals between the full lattice calculations. The normal burnup routine assumes the same reaction rates for all pins of a given pin cell type, but the code does have an option to compute power maps with an allowance for the differences in rating between such pins. A special adjustment is also made to the Pu-240 cross-section to allow for the strong dependence of self-shielding on atomic number density.

Subsidiary transport calculations permit the flux depression in burnable poison pins to be followed without recourse to frequent full lattice calculations.

2.7 TYPICAL MODE OF USE

The normal mode of use of the programme has been designated as the design calculation and uses the GOG diffusion theory main transport option. Normal calculations for PWRs are carried out using the following specification of data:

- Pin cell mesh:
  - 1 mesh point in fuel
  - 1 mesh point in can
  - 1 mesh point in coolant
  - 1 mesh point in control pins

- Main transport mesh:
  - 1 point per pin cell

- Main transport group structure: 6 groups with energy cuts at 821 KeV, 9.118 KeV, 4 eV, 0.625 eV and 0.14 eV.

3. DESCRIPTION OF JOSHUA

3.1 PURPOSE

JOSHUA is a computer program that simulates, in two or three dimensions, the neutronics, hydraulics and burnup of water cooled reactors.

3.2 BACKGROUND

The JOSHUA series of programs were developed originally on SGRWRs. JOSHUA III was the first to use the neutronics calculation of the program BASHAN, which uses diffusion theory with an in-channel mesh point representation and was developed for use with LWRs. In JOSHUA, it is limited to two energy groups. The thermal hydraulics routine is general enough to deal with pressure tube and pressure vessel reactors. Optional features include soluble poison and the reactivity feedback effects of xenon poisoning and fuel temperature, as well as control rod or interlattice tube representation. A number of core simulation and fuel management options are available. A full description of JOSHUA III with many additional references is given in /2/. The versions have recently been combined into a single program capable of dealing with LWRs and SGRWRs and known simply as JOSHUA /3/.

3.3 DESCRIPTION

3.3.1 Physics

Nuclear data are in the form of libraries of two group cell data derived from WIMS calculations. The libraries are stored as functions of irradiation and current coolant density, either on cards or on library discs. Reactivity feedback effects are included in the calculation by modifying the library cross-sections. Such modifications normally vary with time. However, the library cross-sections will have been generated on the assumption that the fuel was irradiated in a constant environment. This is not normally true in practice, especially when the fuel has been shuffled within the reactor. The recommended method of overcoming this is to use the nuclide follow options. In this method the concentrations of the two
fissile nuclides U-235 and Pu-239 are followed, and cross-section corrections made on the basis of the difference between current values and library values. This correction is not normally necessary for PWR calculations.

Control rods are represented by complete libraries in which the control rod has been included explicitly in the WIMS calculations. Soluble poison is represented by additions to the absorption cross-sections at each mesh point using separate input effective cross-sections for each material which are tabulated as a function of irradiation. The boron absorption cross-sections are given for each coolant density in the library and linear interpolation is used for all other values.

The two energy group version of the three-dimensional diffusion program BASHAN is employed for the flux solution. The diffusion equations for each group are approximated by finite difference equations within the core region. Mesh spacing is uniform but may be different in each direction. In calculating neutron currents the diffusion coefficient at a mesh boundary is the harmonic average of the coefficients at either side since this is the relationship derived from the condition of continuity of neutron current at the boundary. At the axial boundaries the boundary condition is a linear extrapolation distance and this is normally applied directly at the end of the core region without explicitly representing any of the axial reflector. For FWRs the extrapolation distance has been obtained by first carrying out a fine mesh transport calculation of a fuel channel and its adjacent end regions, and then adjusting the top and bottom extrapolation distances in a coarse mesh JOSHUA calculation to give a good fit to the fine calculation. The coarse mesh corresponds to that of the proposed core calculation and has normally 16 nodes in a standard length fuel channel. This procedure has an element of a coarse mesh correction, since by it, the coarse mesh method is constrained to fit a more detailed calculation. The radial boundary condition is a matrix albedo one. The albedos used are directly calculated from the currents through the core/shroud interface in a transport solution, using LWR-WIMS, of a section of core and its neighbouring reflector. Allowances are made for the effect of varying boron level in the reflector both axially and radially. The albedos are, in principle, properties only of the reflector including the steel shroud and their formulation includes a simple allowance for the stepped nature of the core reflector interface. The method is fully described in /4/.

The solution proceeds with inner iterations on the flux for each group within outer iterations on the fission source. The line form of the Liebmann successive over-relaxation method is used for the solution of the inner problem with the axial flux solved by the forward elimination/backward substitution technique. The outer problem is accelerated by the Chebyshev extrapolation method.

The libraries of cross-sections used by JOSHUA are calculated at the mean reactor rating and fuel temperature so that the effects of xenon and Doppler at this library rating are included in the cross-sections. At each mesh point, corrections to these cross-sections are made depending on the difference between the local and library ratings.

For xenon, a simple correction is made to the thermal absorption cross-section, based on a library value for the microscopic xenon cross-section, and \( \Delta X \), the difference between the cell atomic number density of xenon at each mesh point and the value for the library rating. \( \Delta X \) is calculated from a simple one-group equation. It is found that \( \Delta \) needs to be known only approximately for accurate results to be obtained.

To represent the Doppler (fuel temperature) feedback effect at each mesh point, a correction is applied to the fast group removal cross-section. The logic of the correction is based on a \( \sqrt{T} \) broadening law for U-238 resonance absorptions. The difference between the effective fuel temperature and the mean coolant temperature is calculated internally by JOSHUA on the basis of a simple algorithm shown to have validity for a wide range of LWRs. JOSHUA uses 'X8 factors' produced by the WIMS calculations which generated the library data. The 'X8 factor' is the ratio of the U-238 resonance absorptions to the total fast absorptions occurring in the cell.
3.3.2 Thermal Hydraulics

The thermal hydraulic routines solve the equations of momentum and energy conservation using simplified methods. Each channel has the same outlet pressure and iterations proceed until the flow pattern is such as to achieve the same input pressure for each channel. Alternatively, iteration proceeds until the inlet pressure is such as to achieve the input flow data.

Each channel can be represented by feeder, core and riser sections (to suit SDMR geometry) but for LMR calculations the feeders and risers are omitted. Each channel may have an inlet gag and there is representation of the flow restriction caused by spacer grids. Channel inlet sub-cooling or enthalpy is specified in the data input. Sub-cooled voids can be represented optionally. For BWRs, each channel is independent but for PWRs the additional complication of inter-channel mixing is represented. Interchannel mixing is computed by JOSHUA using an approximate method which has been shown to yield close agreement with the more sophisticated methods of HAMBR0 /5/, the UKAEA thermal hydraulics sub-channel program for the steady state. Two libraries of thermal hydraulics properties for water are included in JOSHUA - one for pressures around 1000 psi (for BWRs) and one for 2200 psi (for PWRs). JOSHUA selects one of the two from the input pressure data.

3.3.3 Mode of Solution

The iterative procedure starts with a first estimate of the three-dimensional rating distribution and from this an initial coolant flow and enthalpy distribution is derived. From the resultant coolant density at each mesh point, nuclear cross-sections can be looked up in the library. The rating distribution also yields the corrections for the xenon and Doppler effects. The neutron flux solution is carried out, and a new rating distribution derived. The whole procedure is then repeated until the maximum fractional change in the point rating at any given mesh point in successive computations of the rating distribution falls below an input value (usually 0.01). It is found that under-relaxation on the rating changes is necessary.

JOSHUA then produces the fully converged flux distributions, a two-dimensional radial power map, a two-dimensional irradiation map and a two-dimensional flow map, followed by a three-dimensional map of the rating, irradiation coolant density and voidage distributions. Finally, a three-dimensional point rating and burnup map is produced for every mesh point. This information may be written to magnetic tape or disc which may be used either as a record of the calculation for other programs to read, or as a restart tape or disc.

The burnup of the core is simulated by advancing the irradiation at each mesh point by the product of the rating and a given time step, recalculating the cross-sections, including interpolation in the new irradiation, and repeating the calculation. At each new burnup step, control rod insertion, boron level (in a PWR), inlet sub-cooling or enthalpy, flow, inlet pressure, outlet pressure and core power can be specified anew. This option is called the 'core following' mode. Alternatively, a burnup option can be used with fixed thermal hydraulic data where the program adjusts the poison level to achieve an input eigenvalue. With both options a fuel change at the end of the cycle can be performed and JOSHUA can carry on with the next cycle of core operation automatically.

3.4 COARSE MESH CORRECTION

An option in JOSHUA permits some degree of coarse mesh correction as an operation carried out after convergence of the main flux solution. Average fluxes are obtained from the mesh centre flux and gradients between it and its neighbours. The method may be applied optionally to only the x and y directions or to all three. For the purpose of this averaging when the albedo option is used, it is at present assumed that the flux between the outermost mesh point and the boundary is constant. This coarse mesh correction is referred to as the NOAV procedure.
4. **Reactors for Which Results are Quoted**

Most of the results in this paper are from the Beznau 1 and Tihange 1 reactors. Beznau 1 is an 1130 MW(th) reactor with 121 fuel channels. The fuel array is 14x14 with 10.72 mm pins. Figure 4.1 shows the arrangement in the assembly and the positions of burnable poison pins. Figure 4.2 shows the core layout including control rod groups and positions of burnable poison in the first cycle.

Tihange 1 is a 2652 MW(th) reactor with 157 fuel channels. The fuel assembly has the same size pins as Beznau but in a 15x15 array. Figure 4.3 and 4.4 show the assembly and core layout in a similar way to Figures 4.1 and 4.2 for Beznau.

Validation studies up to Cycle 4 on Beznau 1 have been reported in /6/ and /7/ and Cycle 1 results for Tihange 1 in /8/.

5. **Reactivity Results**

The simulation calculations have been carried out by feeding into JOSHUA the critical reactor conditions during each cycle. These are the power, boron level, control rod positions, total coolant flow and inlet enthalpy. The output from JOSHUA includes the eigenvalue appropriate to the reactor conditions and nuclear data supplied. Reactivity is not particularly sensitive to the coarse mesh modelling technique but for the purpose of this paper it provides a useful comment on the overall accuracy of the nuclear data being used.

Figure 5.1 gives a plot of many of the results for the Zircaloy clad fuel cycles. In general all the results are consistent and lie within a band. The width of the band is indicative of the overall accuracy of the reactor data fed into these calculations. There is a decreasing trend from a near zero error for fresh fuel to an error in the region of 0.6% low at the end of a typical PWR equilibrium cycle. There is an error of about 0.1% in K due to representation of spacer grids by smearing them along the outside of the fuel cans. Corrections for this could raise the curves uniformly by 0.1%. It is known that the worth of boron is underestimated by about 10%. The cause of this is not known, but if it were corrected, the band would be almost horizontal but still showing an underprediction of about ¾.

A simple method of correcting for this error in making predictions of boron concentration using the boron search option in JOSHUA is to specify a target eigenvalue of 0.995. NOK have carried out such calculations and comparison of predicted and observed boron concentrations show good agreement as shown in Figure 5.2 for Cycles 7 and 8 of Beznau 1.

There are anomalies in the curves which represent departures from the overall trend. The most striking of these is the large positive reactivity at the start of Cycle 1 in Beznau. We believe this must be due to some defect in specification of the reactor data but have not been able to identify it. At the start of some cycles there are excessively low points possibly due to inclusion of equilibrium samarium in the nuclear data before it has had time to build up in the reactor. In spite of these anomalies, however, there appears to be a well established trend which could be reliably used to correct reactor design calculations. Except in the presence of burnable poisons, it is believed that neither the trend, nor the anomalies, will be significantly improved by coarse mesh correction techniques.

6. **Radial Power Distributions**

Both Beznau and Tihange are equipped with travelling incore fission chambers which can be inserted up the instrument tubes in a number of assemblies. For Tihange, the positions are shown in Figure 4.4. These chambers provide U-235 relative fission rates as continuous axial scans at the instrument tube position. They thus provide a reasonably complete flux map especially when account of the core symmetries is taken. The most direct use of this data for validation purposes is to calculate these fission rate distributions directly and make comparisons between calculation and measurement.
Reactor operators use various procedures to deduce assembly power maps from the in-core measurement data. These procedures involve various assumptions and often involve some sort of a fit to a calculated distribution. The results depend on the assumptions made in formulating them. Where small discrepancies between JOSUHA calculations and 'experimental' power maps occur, there is always some doubt as to whether the error lies in JOSUHA or the fitting procedure or both. However, such maps have been more readily available than the flux map data and many JOSUHA/measurement comparisons have been made on the basis of them.

The problems of deriving point fluxes at the centre of an assembly on the basis of JOSUHA coarse mesh results have been recently investigated. Some recent work on flux comparison is also presented in the following sections.

A large number of power map comparisons have been made and it is fair to say that the overall agreement is very good. It is not possible to present it all in this paper but we have tried to give a sufficient number of results to show the overall agreement and to illustrate the patterns of discrepancies which remain.

Figures 6.1 and 6.2 show two typical maps in Beznau taken from cycles 3 and 8. Many maps show agreement to this standard where the majority of assemblies show discrepancies of not more than 2%. Note that all discrepancies are expressed as a percentage or fraction of mean assembly power, rather than as a percentage of local assembly power. Both these maps are taken well into the cycle and it is certainly true that discrepancies diminish during each cycle - the well known phenomena of irradiation flattening. Figure 6.3 shows a result early in Cycle 8, where agreement is almost as good. Note that channel 15 in Cycle 8 is a fresh mixed oxide fuel assembly. The experimental standard deviation has not been well quantified but it must be of the order of 5% so that the observed discrepancies are within this uncertainty.

On many of the maps, various systematic error trends are apparent. Figure 6.4 shows the situation late in cycle 1 of Beznau where the calculation has a tendency to be low in the core centre and higher at the edge. Most of the other cycles show a tendency to overcalculate power in the centre and edge and undercalculate in an intermediate annulus. This is shown in Figure 6.5 and is typical of Beznau 1 results. The same trend is apparent in Figure 6.3 which includes a mixed oxide assembly in the intermediate annulus. Figure 6.6 shows a situation where the errors on and near the diagonal are unusually high. The discrepancies shown in Figures 6.1 to 6.6 are still small compared with the experimental standard deviation but their systematic nature shows that they do illustrate real trends. Whether these trends are due to the experimental power map fitting procedure or whether they are inherent in the JOSUHA procedure is hard to say. It is possible that an overall improvement in performance could be obtained by a modification of the albedo treatment although many people would say that the errors we have are already of no importance. They are certainly not large enough on their own to justify the development of more complex calculation procedures.

It is notable in Figures 6.2 and 6.3 that there is no detectable additional error in the region of the mixed oxide fuel assembly (Channel 15).

When burnable poison was present during the first cycles, there is a different picture giving a pattern of discrepancies which could be eliminated by a coarse mesh correction treatment /9/. Figure 6.7 shows the situation near the start of Cycle 1 in Beznau where burnable poison was loaded as shown in Figure 4.2. The calculated powers are high in all burnable poison channels, the difference being about 2% overall. Figure 6.8 shows a similar effect in Tihange at 1540 Mwd/t where the discrepancy averages about 3%. Figure 6.9 shows that this discrepancy would be reduced, by using a 4 x 4 mesh instead of a 2 x 2 one since the power in the poisoned channels is reduced by about 2% relative to the surrounding unpoisoned channels. We return to this point later when discussing flux maps.

7. RADIAL FLUX DISTRIBUTIONS

The in-core measurement system obtains the U-235 fission rate in an essentially non-self-shielded U-235 sample. Furthermore, the measurement is made along a particular axial line in a fuel assembly. The ratio of flux at that line
to average flux in the assembly varies with irradiation, enrichment and the presence of burnable poison or control rods. There will also be variations in the local neutron spectrum which will affect the two group cross-sections. In comparing measurements and calculations these factors should be taken into account. In the comparisons which follow, the data in the radial flux maps refer to axial averages of both calculation and measurement.

The simplest course is to assume that the fission chambers measure thermal flux and that this can be obtained from the calculation by averaging the four adjacent mesh points. In the results shown in Figures 7.1 to 7.3 the fluxes used were those obtained after using the NOAV procedure which is strictly appropriate for average rather than point parameters. Figure 7.1 shows the discrepancies between calculation and measurement obtained on this basis early in Cycle 5 of Bezau 1 and compares them with the discrepancies in the power map. In the centre of the core there is good agreement between the two sets of discrepancies but near the edge of the core, the flux map shows greater discrepancies.

Tihange 1 Cycle 2 had a non-symmetric core loading and it was necessary to carry out whole-core JOSHUA calculations. A comparison of flux measurements is shown in Figure 7.2. The flux calculated at the edge of the core is again low compared with measurements.

Flux comparisons during the first cycle have the checkerboard pattern of discrepancies shown by the power maps. Figure 7.3 shows an illustration of this for Tihange.

The estimation of detector reaction rates from coarse mesh calculations can be improved in a number of ways and some recent work has been done in this area. These improvements are to include instrument tube cross-sections in the calculation and to quantify the coarse mesh errors in the central region with burnable poison, and in the edge region.

Instrument tube cross-sections were calculated by including a small amount of U-235 in the central instrument tube in the LWR-WINS calculation. From this, two group cross-sections were derived from the fission rate in the tube, the number density of U-235 and the assembly average flux. These cross-sections therefore include a relative local flux factor. The resulting cross-sections for Tihange 1 Cycle 1 fuel are shown in Table 7.1.

**Table 7.1**

<table>
<thead>
<tr>
<th>Assembly Type</th>
<th>Effective Cross-Section (barns)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0 MWD/t</td>
</tr>
<tr>
<td>3.1% Unpoisoned</td>
<td>252</td>
</tr>
<tr>
<td>3.1% 12 burnable poisons</td>
<td>285</td>
</tr>
<tr>
<td>2.5% 12 burnable poisons</td>
<td>294</td>
</tr>
<tr>
<td>1.9% Unpoisoned</td>
<td>264</td>
</tr>
</tbody>
</table>

There is a variation of up to 12% with irradiation, up to 5% with enrichment and up to 15% for the effect of poison. These results have been used in JOSHUA, taking as the flux the average of the four surrounding points but without using the NOAV procedure. Results interpolated for 1000 MWD/t are shown in Figure 7.4. The checkerboard error remains with the difference between poisoned and unpoisoned assembly errors at about 4%. This is consistent with the power map errors. It is also consistent with errors shown in Figure 7.3 where use of the NOAV procedure fortuitously has an effect only slightly less than the use of the instrument tube fission cross-sections. The good agreement in Figure 7.3 is thus fortuitous.
The chequerboard error was investigated in further detail by the use of supercell calculations. The results of Figure 6.10 show that coarse mesh errors are significant in contributing to this error, but it was important also to establish whether there were spectrum interaction effects as well. A supercell representation of an infinite chequerboard of unpoisoned 1.95% and poisoned 2.55% enriched assemblies was set up on an LMR-WIMS (Case A), on a JOSHUA coarse mesh representation (Case B) and a fine mesh case like Case B but with 10 x 10 meshes per assembly rather than 2 x 2 (Case C). Results at BOL are shown in Table 7.2.

**Table 7.2**

<table>
<thead>
<tr>
<th>Case</th>
<th>Channel Power</th>
<th>Instrument Tube Flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.987</td>
<td>0.817</td>
</tr>
<tr>
<td>B</td>
<td>1.024</td>
<td>0.861</td>
</tr>
<tr>
<td>C</td>
<td>0.994</td>
<td>0.827</td>
</tr>
</tbody>
</table>

For both power and flux, the coarse mesh results (Case B) are about 4% higher than the definitive Case A results. The fine mesh (Case C) reduces these errors to about 1%. It is clear therefore that spectrum effects are not very important but that a coarse mesh correction has the potential to greatly reduce the chequerboard error.

The flux maps all show larger errors at the edge of the core than do the power maps. Errors at the edge of the core were investigated with the help of a detailed LMR-WIMS simulation of a few assemblies at the edge of the core with detailed modelling of the shroud and reflector. The flux distribution through the outer assembly (Channel 1 on the Tihange quarter core maps) is shown by the continuous line on Figure 7.5. The peaks, due to the water gaps in the assembly, have been removed in the dotted line using factors based on a single assembly calculation with reflecting boundary conditions. The resulting flux has a convex shape and the flux at the middle of the assembly is about 5% higher than the mean. This would account for 5% error in instrument tube flux calculations in JOSHUA.

In the NOAV coarse mesh averaging method in JOSHUA, it is assumed that the flux is constant between the outer mesh point and the cell boundary. This would be a reasonable assumption with no shroud present but, from Figure 7.5, is clearly not appropriate for a PWR. The resultant error in power is about 2%. The two effects therefore give a net difference of about 7% in the local errors expected from power and flux calculations in edge assemblies. In terms of the way errors are quoted in this paper (i.e. as fractions of mean assembly power rather than local power) the error difference would be 5.5% which is similar to the results observed. These errors would be larger in corner channels such as 2, 6 and 11, as shown in Figure 7.4.

From this analysis, it would appear that where coarse mesh corrections are appropriate, that is with burnable poison or control rods and at the edge of the core, effects of about 5% in calculated channel power distribution can be obtained and these are in the right direction. The issue of determining peak pin power wherever it may occur in an assembly has not yet been tackled in JOSHUA.

**8. AXIAL POWER DISTRIBUTION**

A very large number of axial plots are available and have been compared with JOSHUA calculations and the comparison with measurement is normally good. Note that the three dimensional calculations for the comparisons are always carried out with the operational data of the time including the current control rod insertion. The dips in the experimental power shape in Figures 8.1 to 8.3 are due to the presence of grids but the coarse mesh model cannot show such local grid effects. In the presentation of results, both the calculated and measured curves
have been normalised to unity for the channel concerned so that any errors in radial power calculation have been eliminated.

Figures 8.1 to 8.3 show results taken from Cycle 7 of Beznau 1. Figure 8.1 is for fresh fuel at the edge of the core in Channel 2 and at the beginning of cycle. The axial form factor is well predicted but the discrepancy around Mesh 4 is as big as has been observed on any plots. Figure 8.2 shows one year old fuel near the centre of the core, in Channel 25, and at the end of cycle. Figure 8.3 shows the start of cycle result for mixed oxide fuel in Channel 15. It is very similar to Figure 8.1 which showed an enriched uranium fuel channel at the same time.

The pattern of results is typical. There is a tendency to underpredict in the lower half of the channel at the start of cycle and in the upper half at the end of cycle. The maximum discrepancy is normally of the order of 5% although occasionally there are small regions (such as in Figure 8.1) which have a 10% discrepancy. There is no detectable additional error in the region of partially inserted control rods nor in the presence of mixed oxide fuel.

9. CONTROL ROD WORTH

JOSHUA calculations have been compared with measurements of control rod worth at the beginning and end of Beznau Cycle 1 and BOL for Tihange. The conditions were hot zero power with reactivity held down by boron.

The reactivity scale used in the measurements is presumed to be based on interpretation of doubling time measurements, whereas the reactivity in the calculations is based on eigenvalues. To eliminate errors which might arise from differences in these scales, results of both measurements and calculations of rod worth were expressed in terms of boron changes using the measured or calculated values of boron worth as appropriate. Calculations were made using LWR-WIMS data generated with HZP temperatures and with a boron level appropriate for criticality with control rods out.

The calculated total rod worths are always low, as summarised in Table 8.1 below:

<table>
<thead>
<tr>
<th>Identification</th>
<th>% Error in Control Rod Worth Based On Boron Levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beznau Cycle 1 BOL Group A</td>
<td>-7%</td>
</tr>
<tr>
<td>Beznau Cycle 1 BOL Group B</td>
<td>-7%</td>
</tr>
<tr>
<td>Beznau Cycle 1 EOL Group A</td>
<td>-11%</td>
</tr>
<tr>
<td>Beznau Cycle 1 EOL Group B</td>
<td>-11%</td>
</tr>
<tr>
<td>Tihange Cycle 1 BOL Bank D</td>
<td>-14%</td>
</tr>
</tbody>
</table>

Note that a 10% error is equivalent to about 10 ppm boron. These errors persist over the range of insertion except for Beznau BOL where the error is near zero between fully out and two-thirds total insertions.

The presentation of control rod worth results in terms of boron worth represents the real situation where boron can be traded for rod insertion to maintain criticality. As discussed in Section 10, there is an error in calculation of boron worth which is different for the two reactors. If this difference is allowed for the errors in Table 8.1 would be more uniform and around -10%.

The sign of this error is consistent with the chequerboard error in the power and flux map comparisons. Too high a flux in the poisoned regions implies too little absorption in the burnable poison. The results in this section also show
too little absorption in a strongly absorbing region and it is expected that a coarse mesh correction treatment would reduce the error in calculated control rod worths.

10. REACTIVITY COEFFICIENTS

It is not expected that the whole core calculation method would have much effect on the estimates of reactivity coefficients. They are dependent primarily on nuclear data and neutron spectrum. Results of comparisons are included here for completeness.

Boron worth has been compared in both Tihange and Bezmau reactors and gives inconsistent results. For Bezmau Cycle 1 calculations were 11% low at BOL and 8% low at EOL. For Tihange Cycle 1 BOL the calculations were 4% high. Earlier results for the stainless steel clad reactor Trino Velcelles were in good agreement but results for the different geometry of the Winfrith SGHW Reactor are a few percent low. On balance, it is assumed that the calculations are a few percent low and this is consistent with the downward trend of reactivity results discussed in Section 5.

The moderator temperature coefficient has also been compared for BOL and EOL in Bezmau and BOL in Tihange. In the latter case comparisons were made for two control rod states including all rods withdrawn where the measured coefficient was positive at 1.5 x 10^{-5}/K. The Bezmau calculations were 2.5 x 10^{-5}/K low whereas the Tihange cases are approximately 4 x 10^{-5}/K low. Earlier calculations on the steel clad Haddam Neck reactor showed an underestimate of 2.7 x 10^{-5}/K with 2300 ppm of boron and a slight overestimate at 1700 ppm. These latter results were at BOL Cycle 1 at zero power and with varying control rod insertions to maintain criticality.

Some part at least of this error is believed to be due to non-representation of the variation of capture to fission ratio in U-235 in the thermal region.

11. CONCLUSIONS

Simulations of PWR operating cycles using the codes LWR-WIMS and JOSHUA have been compared with measurements and the results have been shown to be generally satisfactory. LWR-WIMS is a code which includes a sophisticated calculation of spatially dependent neutron spectrum in a fuel assembly and condensation to cell averaged two group cross-sections which are used in JOSHUA. JOSHUA, by contrast, uses a simple finite difference approximation to the diffusion equation. It has been shown that only in the effects of strong absorbers is there any need for a more sophisticated core calculation. Without such sophistication, errors remain in the range of 5-10%.

ACKNOWLEDGEMENTS

The authors are grateful to Electrolux SA for data from the Tihange 1 reactor.

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Fig. 6.8 Tihange I Cycle 1
FRC 49040. JOSHA - EXPERIMENT 9%.
Shading indicates poisoned assemblies.

Fig. 6.9 Tihange I Beginning of Cycle 1
Effect of mesh size in JOSHA.
Shading indicates poisoned assemblies.

Fig. 7.1 Beznaul Cycle 5
49044.19 Comparison of errors on channel power and instrument tube flux calculated with now procedure.
FIG. 8.1 NORMALISED AXIAL POWER DISTRIBUTION CYCLE 7 AT 209 MWFD LHA
FIG. 8.2 NORMALISED AXIAL POWER DISTRIBUTION CYCLE 7 AT 7484 MWFD LHA
FIG. 8.3 NORMALISED AXIAL POWER DISTRIBUTION CYCLE 8 AT 200 MWFD LHA
TRILUX NODAL SYSTEM FOR IN-CORE FUEL MANAGEMENT STUDIES

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ABSTRACT.

The TRILUX code, initially designed by CUNF, has been extensively improved at BELGONUCLEAIRE. Several new options have been added, enabling the code to compute the variation versus time of xenon and iodine concentrations when they are rapidly changing, to compute water outlet temperature, and fuel inventory. Another option allows to perform a fine mesh, two group diffusion calculation on part of the core, using the coarse mesh information to obtain boundary conditions. This allows a more accurate determination of the form factor, and an accurate treatment of local thermal flux gradient, resulting in a better power distribution in case of cores partially fuelled with plutonium.

1. INTRODUCTION.

For the design of LWR's fuel reloads, the reactor physicist has to contribute to a safe, flexible and economical operation of the reactor. Fulfilling these goals require not only the physicist's experience, but also computational tools having to be accurate, flexible, easily usable and fast running. Moreover, within a short delay, physicists must answer to problems arising in design or operation. They have also to supply data required by others.

The TRILUX nodal system was developed and validated to fulfil these objectives.

2. TRILUX CODE SYSTEM.

The relationship between the various calculation steps and the flow of data through the whole calculation is illustrated in figure 1.

The computer codes PANTHER /1/, EREEBUS /2/ and TRILUX /3/4/ form the skeleton of the in-core fuel management calculation system. The few group nuclear constants of each fuel type and core composition are calculated using the PANTHER cell code. The 2D diffusion depletion code EREEBUS calculates the main assembly nuclear characteristics such as $k_e$, migration area, homogenized macroscopic cross-sections, ..., in function of power level, water temperature, boron concentration and exposure. Those characteristics are correlated with polynomial coefficients.

Recently, the LWR-WIMS /5/ code has been incorporated in the TRILUX system as assembly constant generator.

The TRILUX and XENOLUX codes calculate the three-dimensional power distribution and the critical boron concentration using a modified one group nodal coupling model. The reactivity feedback effects of variations in the xenon density, Doppler effect, moderator temperature and boron concentration, are included in those codes. The TRILUX code is used for depletion calculations where the xenon distribution is the equilibrium distribution that is consistent with the power distribution. The XENOLUX code computes the power distribution and the critical
boron concentration during load following operation where the xenon distribution
is rapidly changing.

The MICROLUX code determines the pin power distribution in a reactor core
on the basis of the TRILUX results.

3. TRILUX CODE.

TRILUX calculates a three-dimensional \((x,y,z)\) \((34 \times 34 \times 24)\) nodal power
density distribution using a modified one-group nodal coupling calculation in
which each fuel node is characterized by the infinite multiplication factor \(K\infty\) and
the migration area \(M_i^2\). In this approach, thermal neutrons are absorbed within the
boundaries of the node where they are thermalized and epithermal and fast neutrons
are allowed to migrate to adjacent nodes and beyond.

The neutron interchange between nodes is treated with coupling coeffi-
cients which are function of :

\[
\Delta X, \Delta Z \quad \text{node sizes;}
\]

\[k_i\] \quad \text{infinite multiplication factor of node } i \text{ which is function of water den-
sity, power, exposure, soluble poison and presence or absence of the}
control rods;

\[M_i^2\] \quad \text{migration area;}

\[\sigma_i\] \quad \text{probability that a neutron born in node } i \text{ is thermalized there directly;}

\[r_{ij}\] \quad \text{fraction of neutron in node } i \text{ and leaking to node } j

\[
\sum_{j=1}^{6} r_{ij} = 1 ;
\]

\[\rho_{ij}\] \quad \text{fraction of neutrons leaking from node } i \text{ to node } j \text{ and reflected back to}
node } i ;

\[\beta_{ij}\] \quad \text{fraction of neutrons leaking from node } i \text{ to node } j \text{ and immediately}
thermalized in node } j ;

\[\mu_{ij}\] \quad \text{fraction of neutrons leaking from node } i \text{ to node } j \text{ and joining the fast}
neutron population in node } j \text{ "forgetting" its origin}

\[\rho_{ij} + \beta_{ij} + \mu_{ij} = 1\]

\[\alpha_i = \frac{\beta_{ji}}{\mu_{ji}}\]

The basic equations solved in TRILUX are as follows :

\[
\begin{bmatrix}
\sum_{j=1}^{6} \nu_{ij} + \gamma_i \\
\sum_{j=1}^{6} \nu_{ji}L_j + k_i \gamma_i L_i
\end{bmatrix}
\lambda^{-1} =
\begin{bmatrix}
\sum_{j=1}^{6} \nu_{ij}L_j + k_i \gamma_i L_i
\end{bmatrix}
\]

where \(L_i\) represents the rate at which fast neutrons are crossing out of node \(i\)

\[
\nu_{ij} = \frac{r_{ij}(1 - \rho_{ij})}{1 - \rho_{ij}\rho_{ji}}
\]

\[
\gamma_i = \frac{\alpha_i + \sigma_i}{(1 + \alpha_i k_i)(1 - \sigma_i)}
\]

The relationship between node power \(P_i\) and \(L_i\) is as follows :

\[
P_i = \frac{K}{\nu} k_i \gamma_i L_i
\]
where $\nu$ is neutron yield per fission;
$K$ is energy per fission.

After a specific number of source iterations or a converged source distribution, a water density iteration is performed and consists of the determination of the average water quality at each node based on the coolant flow, inlet enthalpy and power integrated from the bottom of the channel to the node of interest. The water density is calculated by a numerical fit to a void-quality correlation curve. From this new water density distribution, new values of $k_{\text{ef}}$ and $H^2$ are then calculated and the code proceeds to new source calculations. The calculation is terminated when the specified convergence criterion on the eigenvalue is satisfied. Then TRILUX can process for a new time step calculation.

The non-multiplying nodes such as reflector can be taken into account by assigning appropriate albedos at the boundaries or can be explicitly treated by the determination of coupling coefficients relative to that kind of nodes.

The Becker's power correction /8/ can applied when a steep thermal flux gradient appears between two adjacent nodes.

The main outputs of TRILUX are:
- nodewise and assembly wise arrays for power, exposure, water density;
- multiplication factor;
- critical boron concentration;
- coolant outlet temperature distribution;
- fuel inventory.

TRILUX initially developed by GUNF /6/ has been improved and extended by BELGONUCLEAIRE /7/.

4. XENOLUX OPTION.

The XENOLUX option computes the local variation versus time of xenon and iodine concentrations when they are rapidly changing, simulates the xenon induced spatial transients and can evaluate load-following ability of water reactors.

The differential equations relating Xe and I concentrations to power are numerically integrated to obtain concentrations at a given time, assuming that the power distribution remains constant during the time step. The 3D Xe distribution is input or calculated by XENOLUX after a preliminary TRILUX-3D calculation. On the basis of this Xe distribution, a TRILUX calculation is performed for modified operating conditions such as power level, control rod pattern, ... For successive time increments, XENOLUX determines the modified Xe distribution from which TRILUX recalculates the power distribution. The calculation can be interrupted to change control rod pattern or power level as desired and then can be continued for those new operating conditions. The insertion of part length control rods can be treated by TRILUX.

5. MICROLUX OPTION.

The MICROLUX option calculates the rodwise power map and can determine the nuclear form factor $P_N$ and its accurate location. Moreover, MICROLUX treats more accurately the local thermal flux gradients (e.g. at the interface of plutonium and uranium assemblies) and the strong local absorbers (e.g. control rods, burnable poison pins).

The information provided by TRILUX is used to furnish boundary conditions to a fine mesh diffusion computation performed over part of the core or over an "average" plane of the whole core. As in the MICROLUX use, the nodal calculation is performed with four nodes by assembly, a part of the core consists in the selected node with the three neighbours in the same plane which are part of a different assembly. The boundary of the region thus constructed will coincide with the median planes of the assemblies and the coupling between assemblies will be

- 38 -
treated by the fine mesh diffusion calculation.

The diffusion equations are solved in two groups with the boundary conditions:

\[ \alpha^i \psi^i + \beta^i \frac{\partial \psi^i}{\partial n} = \gamma^i \]

where

- for a boundary coinciding with a symmetry plane
  \[ \alpha^i = 0 \quad \beta^i = 1 \quad \gamma^i = 0 \]

- otherwise
  \[ \alpha^i = 0.25 \quad \beta^i = 0.5 \quad \gamma^i = J_{in} = \text{in-current} \]

Following the procedure described in /9/, the values of the flux and currents in the X and Y directions at the corner of each node is approximated by polynomials of the form:

\[ \psi^k(x,y) = \sum_{i=0}^{4} \sum_{j=0}^{4} b_{ij}^k \frac{x^i}{a} \frac{y^j}{a} \quad k = 1, \ldots, 4 \]

where

- \( a \) is the node width;
- \( b_{ij}^k \) are constants deduced from 32 equations solved with information provided by TRILUX and with macroscopic cross-sections of nodes.

The variation of the in-current along the boundaries of the nodes is computed using a fourth degree interpolating polynomial in X and Y for the flux:

\[ \psi(x,y) = \sum_{i=0}^{4} \sum_{j=0}^{4} C_{ij} \left( \frac{x^i}{a} \right) \left( \frac{y^j}{a} \right) \]

setting

\[ C_{33} = C_{34} = C_{43} = C_{44} = 0, \]

the remaining 21 constants are evaluated using the twelve local quantities just computed, plus the nine integrated quantities calculated by TRILUX.

With proper choice of the co-ordinate system, the only constants of interest are the \( C_{0j} \), \( C_{1j} \), and \( C_{11} \) and the in-currents are given by:

\[ J_{in}^{\text{fast}}(X) = \sum_{i=0}^{4} \left( \frac{1}{4} C_{10} - \frac{1}{2} \frac{D}{a} C_{11} \right) \left( \frac{x^i}{a} \right) \quad \text{at} \ Y = 0 \]

\[ J_{in}^{\text{fast}}(Y) = \sum_{j=0}^{4} \left( \frac{1}{4} C_{0j} - \frac{1}{2} \frac{D}{a} C_{1j} \right) \left( \frac{y^j}{a} \right) \quad \text{at} \ X = 0 \]

These in-currents are then integrated over each fine mesh interval and passed to the diffusion calculation as boundary conditions for the fast group.

As the nodal calculation does not consider explicitly thermal neutrons, the code approximates the thermal in-current by the relation:

\[ J_{in}^{\text{th}} = \frac{\Sigma_r^{\text{fast}}}{\Sigma_r^{\text{th}}} J_{in}^{\text{fast}} \]

This relation is, of course, exact only in an infinite medium. However, it is a fair approximation as long as thermal flux gradients are not too high. That is the reason of the choice of a region with boundaries coinciding with the median planes of assembly.
Fig. 2 Configuration 184 MWd/TU - 50% PN
Axial power distribution

POWER

1.5
1.0
0.5
TOP

CB: 888 ppm Expér.
875 ppm Trilux (Sm éq.)

- Expér.
- Trilux

Axial Position
Bottom
The fine mesh diffusion calculation can be performed over selected nodes or over an "average" plane of the whole core. In this last case, the nodal power distribution can be corrected by the diffusion power distribution because of the consistency of all node diffusion calculations.

The MICROLUX option combines the best features of the coarse mesh codes (e.g., fast running, 3D distribution, thermal hydraulic feedbacks) and those of the fine mesh codes (e.g., more accurate treatment of local heterogeneity, detailed power distribution).

6. CODE VALIDATION.

Already checked by GUNF on US reactors, TRILUX has also been validated on Belgian reactors by comparison with fine mesh diffusion results and with experimental data. The accuracy of TRILUX has been checked on the SENA core with cruciform control rods and on the THANGÉ and DOEL cores with RCC assemblies. A few results of this validation are illustrated hereafter for the cycle 1 of the THANGÉ reactor.

The TRILUX nodal code and the CONDOR 3 /10/ diffusion code represent the two types of methods used for core calculations: with TRILUX, the calculations are more economical and with CONDOR 3, the finite difference calculation is more accurate at the beginning of life. But, with the exposure, the depletion of the burnable poison becomes important and a three-dimensional evolution calculation is necessary to take into account the axial buckling variations. CONDOR 3 and TRILUX have given almost the same results for the beginning of the first cycle. This analysis has demonstrated the ability of TRILUX to calculate the radial power distributions as well as a fine mesh calculation.

Moreover, the representation of each assembly by four nodes improves the calculation of the power distribution namely at the core periphery and allows the optimization of the orientation of the assemblies in the refuelling pattern for the following cycles.

Figure 2 gives the axial power distributions measured and calculated by the TRILUX code and shows a good agreement. The measurement conditions are 184 MWd/TH with a critical boron concentration of 888 ppm at half power. The critical boron concentration calculated by TRILUX in these conditions is 875 ppm; this shows the good estimation of the reactivity by TRILUX. A very good agreement has been also obtained on the radial distribution of activations as shown in the figure 3.

The average error is 1.6 % for a maximum discrepancy smaller than 4 %.

The reactivity lifetime of the first cycle has been estimated by the TRILUX code at 14,000 MWd/tU and 7 ppm, the experimental value was 13,887 MWd/tU and 4 ppm.

Other verifications have been made in order to verify the ability and the accuracy of the nodal calculations for the DOEL core and namely the comparison with experimental results obtained during the operation of the first cycle. An example of this comparison is given at the figure 4 and shows the good agreement between TRILUX predictions and experimental values on the relative burn-up distribution at the end of the first cycle.

The MICROLUX option was tested on a very severe case, a checker board pattern of uranium and plutonium assemblies because of the thermal flux gradients. Results obtained with TRILUX, with TRILUX and the Becker's power correction, with MICROLUX and with EREBUS diffusion code, have shown the very good agreement between MICROLUX and diffusion calculations as well for the power sharing as for the fine power distribution (figure 5).
|   | -0.15 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| -3.04 | 0.30 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 0.93 | -2.15 | 1.73 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| -2.54 | 0.11 | -2.37 | 1.18 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 0.64 | -2.08 | 1.09 | -0.64 | 2.60 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| -1.19 | -0.24 | -3.37 | -3.92 | -1.66 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 1.88 | -0.99 | 3.41 | 0.95 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 2.94 | 0.0 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |

$\bar{\epsilon} = 11.621$

$\epsilon = \frac{\text{TRILUX-Exper.}}{\text{Exper.}} \%$

**TIHANGE REACTOR. CYCLE 1.**

184 MWD/TU . 50% PN

ACTIVATION COMPARISON

FIG. 3
<table>
<thead>
<tr>
<th></th>
<th>1.06</th>
<th>1.03</th>
<th>1.10</th>
<th>1.22</th>
<th>1.07</th>
<th>1.04</th>
<th>0.80</th>
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<td>1.12</td>
<td>1.23</td>
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<td>1.01</td>
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<td></td>
</tr>
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<td>1.15</td>
<td>1.06</td>
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<td></td>
</tr>
<tr>
<td>1.11</td>
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<td>1.04</td>
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<td>1.10</td>
<td>1.18</td>
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<tr>
<td>1.02</td>
<td>1.01</td>
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<td>0.74</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**DOEL REACTOR: RELATIVE BURNUP DISTRIBUTION AT THE END OF THE FIRST CYCLE**

*Fig. 4*
POWER SHARING (Pu ass., Power/Average Power)

TRILUX : 1.108
TRILUX with Becker's correction : 1.197
MICROLUX : 1.181
EREBUS (diffusion) : 1.184

□ UO₂ 3.3%  
◯ PuO₂-UO₂ 3.22% Pu fiss.
● PuO₂-UO₂ 2.62% Pu fiss.  
◊ PuO₂ - UO₂ 2.12% Pu fiss.

ASSEMBLY PuO₂-UO₂ - POWER DISTRIBUTION.
7. TRILUX USE FOR RELOAD DESIGN.

A. SENA reactor.

The BCR groupement (BELGONUCLEAIRE - C E A - R BU) has to supply the re-
loads 10, 11 and 12 to the SENA reactor located at Chooz. TRILUX code has been
successfu9ly used for the nuclear design of cycle 8 and is now well qualified to
perform the fuel management of the next SENA cycles.

A preliminary validation performed by the follow-up of cycles 4,5,6 and
7 have demonstrated the TRILUX system ability to analyse this reactor type using
cruciform control rods.

After the first qualification, the obtained accuracies were :
+ 2 % on the cycle length (figure 6) for the 4 studied cycles ;
+ 5 % on the assembly-wise exposure and power map (figure 7) between a fine mesh
diffusion calculation and the nodal computation with TRILUX, the greatest discrep-
cancies occurring at the core periphery.

Furthermore, the validation of this method has been continued by an ex-
tensive investigation of the main physics parameters that could be encountered in
such design calculations. Taking cycle 7 as reference the following characteris-
tics of which a few ones have been compared with measurement results, have been
calculated :
- temperature diagram of the core versus power ;
- cold and hot critical boron concentrations ;
- differential and integral rod worth ;
- axial power versus rod insertion level ;
- power defect ;
- xenon effect ;
- fuel and moderator coefficients in various operating conditions.

TRILUX was then used for the cycle 8 nuclear design and has allowed to
determine the in-core fuel management, the cycle length, the reactivity coeffi-
cients, the control rod and the procedures for a safe and efficient operation.
The start-up physics measurements have shown the accuracy of the predicted values
(figure 8) and proved the TRILUX ability to analyse this reactor type.

In order to follow the power start-up step of the SENA core, power dis-
tribution can be controlled by the aeroball system. The deduced theoretical activ-
ities from TRILUX have been compared during these start-up experiments with the
reduced activities of each aeroball channel. A comparison of normalized theore-
etical and experimental activities is indicated at figure 9 showing the good accu-
rracy which was obtained for the beginning of cycle 8. The mean deviation is 0.7 %
for a maximum deviation of 5.5 %. Moreover, at the utility request, a series of
cycle calculations has allowed to select the best enrichment for reaching a larger
equilibrium cycle length.

The outlet temperature measured by thermocouples are now investigated in
order to provide supplemental nuclear data and to deduce the power map inside the
core. Those temperatures could be compared with the temperatures calculated by
TRILUX.

B. Tihante reactor.

In the frame of accident analysis /12/ for Tihange reactor partially
fuelled with all Pu assemblies, the TRILUX system has allowed to perform the in-
core fuel management and to determine easily the nuclear characteristics of ura-
nium equilibrium cycle and those of transition cycles to reach 30 % and 70 % plu-
tonium fuelled cores, to verify the various nuclear criteria of operation and to
compared U cores and Pu partially fuelled cores.
## Length of 4 successive cycles of SENA reactor with Trilux

<table>
<thead>
<tr>
<th>Cycle</th>
<th>Exper. natural cycle length (MWd/tM)</th>
<th>Natur. cycle length from utilities (MWd/tM)</th>
<th>Trilux estimate</th>
<th>Error Tr - Ref. (°/o) Ref.</th>
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<td>4</td>
<td>9450</td>
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<td>9360</td>
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<tr>
<td>5</td>
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<td></td>
<td>8110</td>
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<tr>
<td>6</td>
<td></td>
<td>8750</td>
<td>8840</td>
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<tr>
<td>7</td>
<td></td>
<td>10000</td>
<td>9980</td>
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<td>Relative power distribution</td>
<td>Comparison TRILUX (nodal) - Condor (diffusion)</td>
<td>SENA REACTOR - CYCLE 5 - BOC</td>
<td></td>
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<tr>
<td>-----------------------------</td>
<td>-----------------------------------------------</td>
<td>-----------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x</td>
<td>x x</td>
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<td>-6.5</td>
<td>+1.6</td>
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</tbody>
</table>

**FIG. 7**
Comparison of experimental results and Trilux predicted values (Sena Core)

<table>
<thead>
<tr>
<th>Characteristics</th>
<th>Trilux</th>
<th>Experiment</th>
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</thead>
<tbody>
<tr>
<td><strong>BOL - Cycle 7</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Critical boron concentration at 283°C and zero power (ppm)</td>
<td>1966</td>
<td>1954</td>
</tr>
<tr>
<td>Critical boron concentration at 283°C, Xe-Sm equil., $P_N$ (ppm)</td>
<td>1270</td>
<td>1250</td>
</tr>
<tr>
<td>Boron worth (pcm/ppm)</td>
<td>6</td>
<td>6,9</td>
</tr>
<tr>
<td>Equival. boron concentr. between $P=0$ and $R_N$ at Xe-Sm equil. (ppm)</td>
<td>696</td>
<td>704</td>
</tr>
<tr>
<td>Control rod worth (12 rods) at zero power (pcm)</td>
<td>3210</td>
<td>3080</td>
</tr>
<tr>
<td>Maximum differential rod worth (pcm/step)</td>
<td>29,2</td>
<td>29</td>
</tr>
<tr>
<td><strong>BOL - Cycle 8</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature coefficient at $P=0$, 284°C, 1530 ppm (pcm/°C)</td>
<td>-16,0</td>
<td>-16,5</td>
</tr>
<tr>
<td>Control rod worth at zero power: 12 rods (pcm)</td>
<td>2780</td>
<td>2742</td>
</tr>
<tr>
<td>30 rods (pcm)</td>
<td>7600</td>
<td>7742</td>
</tr>
<tr>
<td>Maximum differential rod worth (pcm/step)</td>
<td>25</td>
<td>23,5</td>
</tr>
</tbody>
</table>
In the UO₂-PuO₂ fuel, the plutonium oxide is blended with natural uranium oxide (i.e. with 0.7 % U235). The basic criteria for selecting the Pu average enrichment and the number and repartition of enrichments inside the assembly were:

- to obtain a reactivity lifetime equivalent to the reference uranium assembly;
- to produce the same power as in the uranium assembly;
- to achieve acceptable local power distributions (local form factors similar to those of uranium assembly).

The average enrichment of U rods has been fixed to 3.3 w/o U235 and the average Pu fissile enrichment of plutonium assemblies is 3.0 w/o Pu fissile. Three Pu enrichments were needed to satisfy the criterion on the form factor.

As illustrated in figure 10, the reloading patterns have been chosen avoiding the loading of plutonium assemblies under controlled positions because of the reduction of control rod worth when they are inserted into plutonium assemblies.

The MICROLUX option has been used in the calculations of power and burn-up maps because of the important gradients of the thermal flux at the interface of uranium and plutonium assemblies.

Figure 11 illustrates this effect by comparing the TRILUX results with the MICROLUX results for a BOC calculation. It appears that if the thermal flux gradient is not taken into account between assemblies, the power released by a plutonium assembly is underestimated by about 5 %. This comparison illustrates very well the accuracy gain of MICROLUX. Similar effects have been found for the power distribution in controlled assemblies. The reactivity coefficients, the shut-down margin, the control rod worth, the kinetic characteristics, ..., have also been determined with the TRILUX system.

It appeared that THANGRE reactor fuelled with 30 % Pu assemblies could operate safely without modification of the control rod number, all nuclear design criteria being satisfied for the chosen Pu assembly and for the in-core fuel management selected.

8. CONCLUSIONS.

The TRILUX system is a powerful tool for the nuclear design of fuel reloads. Being fast running, accurate, flexible and easily usable, TRILUX system can also simulate any core configurations at any time and provide for all situations the nuclear core characteristics required by the nuclear design. It is used for nuclear design studies of fuel reloads and for core follow-up studies.

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**Microlux - Trilux %**

**Trilux**

**Pu Assembly**

**TIHANGNE REACTOR 30 % Pu CORE**

**COMPARISON BETWEEN MICROLUX AND TRILUX.**

FIG. 11
Session 2

Chairman - Président
Dr. H. FINNEMANN
(Federal Republic of Germany)

Séance 2
NEPTUNE : LES MODULES ELECTRE ET CRONOS POUR LES CALCULS STATIONNAIRES ET TRANSITOIRES DE DISTRIBUTION DE PUISSANCE AVEC PRISE EN COMPTE DES CONTRE-REACTIONS THERMOHYDRAULIQUES

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Développés au cours des dernières années, les systèmes de code ELECTRE et CRONOS permettent le calcul des distributions de puissance stationnaires et transitoires dans les réacteurs nucléaires, par résolution de l'équation de la diffusion à trois dimensions avec prise en compte des contre-réactions thermohydrauliques. Les temps de calcul de diffusion ont été fortement réduits par l'utilisation de la méthode des éléments finis pour la discrétisation spatiale du flux. Les calculs thermohydrauliques sont effectués par le code FLICA. Un langage algorithmique ARIANE permettant un enchaînement simplifié des processus de calcul a été également développé, ainsi qu'un ensemble de logiciels facilitant le développement et l'utilisation de systèmes de code.

INTRODUCTION

Le calcul de la gestion du combustible et du suivi des réacteurs électrogènes de puissance à eau légère pressurisée doit nécessairement être réalisé en représentant correctement les contre-réactions dues aux effets de puissance (densité du modérateur, températures, xénon...) ; de plus, la représentation du cœur entier en géométrie tri-dimensionnelle est généralement obligatoire.

L'ensemble ELECTRE du système NEPTUNE a été conçu pour effectuer tous les calculs nécessaires à la conception des réacteurs PWR avec la meilleure précision possible, mais aussi avec la meilleure efficacité informatique.

ELECTRE est basé sur l'utilisation de la méthode des éléments finis pour la résolution à deux et trois dimensions de l'équation multigroupe de la diffusion des neutrons ; grâce à des algorithmes spécifiques, les coûts de calculs sont très largement réduits à précision égale par rapport aux méthodes classiques : l'ensemble de ces méthodes numériques est décrit au § 1.

L'ensemble CRONOS a été développé à partir d'ELECTRE pour traiter la cinétique neutronique en conservant le traitement spatial par la méthode des éléments finis : la discrétisation temporelle est basée sur une méthode à un pas ; les méthodes numériques de CRONOS sont décrites au § 2.

La prise en compte des contre-réactions thermohydrauliques peut être délicate dans le cas d'un grand réacteur à réseau ouvert : nous avons choisi d'utiliser le code d'analyse thermohydraulique par sous-canaux FLICA 3 qui a été introduit dans NEPTUNE : basé sur un modèle thermohydraulique à quatre équations, FLICA permet le calcul des températures, du taux de vide et de toutes les grandeurs thermohydrauliques utiles : le modèle de FLICA est décrit au § 3.
Le § 4 est dédié à la présentation de l'algorithme de couplage neutronique-thermohydraulique en régime transitoire qui a été introduit dans NEPTUNE.

La programmation d'un système aussi complexe que NEPTUNE serait lourde si des outils informatiques efficaces n'étaient utilisés : le § 5 décrit les logiciels particuliers développés pour assister la programmation de NEPTUNE et permettre à l'utilisateur un emploi facile du système, tant pour les calculs de conception que pour les calculs raffinés de l'analyse du physique des réacteurs.

1/ LA METHODE D'ELEMENTS FINIS UTILISEE DANS ELECTRE

La méthode des éléments finis a été récemment appliquée à la résolution de l'équation de diffusion : elle permet de résoudre cette équation en utilisant un maillage large lorsque les sections efficaces le permettent. Ainsi le nombre d'inconnues est considérablement réduit par rapport aux méthodes classiques de différences finies et le temps de calcul est lui-même fortement réduit.

1.1. Formulation faible de l'équation de diffusion

Considérons l'équation de la diffusion monocinétique à source : celle-ci s'écrit:

\[ H \phi - V D V \phi + \Sigma \phi = S \quad \text{sur} \quad \Omega_i \cup \Omega_j \]

(1)

\( D \) et \( \Sigma \) sont des fonctions \( C^0 \) sur chaque \( \Omega_i \) et strictement positives.

A cette équation sont associées un certain nombre de conditions aux limites :

\[
\begin{cases}
D \frac{\partial \phi}{\partial n} + Y \phi = 0 & \text{sur} \quad \Gamma_1 \cup \Gamma_2 = \partial \Omega = \Gamma \\
\phi = 0 & \text{sur} \quad \Gamma_2
\end{cases}
\]

(2)

\[
\begin{cases}
D_i \frac{\partial \phi_i}{\partial n} = D_j \frac{\partial \phi_j}{\partial n} & \text{sur} \quad \Gamma_{ij} = \overline{\Omega_i} \cap \overline{\Omega_j} \\
\phi_i = \phi_j
\end{cases}
\]

(3)

Soit \( \psi \) une fonction suffisamment régulière. Si nous multiplions (1) par \( \psi \) et intégrons sur \( \Omega \), il vient :

\[ \int_{\Omega} (- V D V \psi + \Sigma \psi) \psi = \int_{\Omega} S \psi \, d\Omega \]

Supposons l'application de la formule de Green justifiée dans le premier membre de l'équation précédente, on obtient :

\[ \int_{\Omega} D \nabla \phi \nabla \psi + \Sigma \phi \psi = \int_{\partial \Omega} \frac{\partial \phi}{\partial n} \psi - \int_{\Omega} S \psi \]

Si \( \psi \) vérifie la condition \( \psi = 0 \) sur \( \Gamma_2 \) en remplaçant \( \frac{\partial \phi}{\partial n} \) par sa valeur il reste :

\[ a(\phi, \psi) = \int_{\Omega} D \nabla \phi \nabla \psi + \Sigma \phi \psi + \int_{\Gamma_1} \gamma \phi \psi = \int_{\Omega} S \psi = f(\psi) \]

On voit que les intégrales précédentes sont maintenant parfaitement définies si on choisit :

\[ \phi, \psi \in V = \left\{ \phi \in L^2(\Omega) \mid \nabla \phi \in L^2(\Omega) \ , \ \phi = 0 \ \text{sur} \ \Gamma_2 \right\} \]
Le problème (4) :

trouver $\phi \in V$ tel que $a(\phi, \psi) = f(\psi)$ $\forall \psi \in V$ \hspace{1cm} (4)

est la forme variationnelle du problème (1), (2), (3). Compte tenu des conditions sur $D$ et $\Sigma$ on peut démontrer l'existence de l'unicité de la solution de (4).

1.2. La méthode des éléments finis

Si on considère un sous-espace $V_h$ de $V$ de dimension finie, il est possible de poser le problème (4) sur l'espace $V_h$.

Trouver $u_h \in V_h$ tel que $a(u_h, \psi_h) = f(\psi_h)$ $\forall \psi_h \in V_h$ \hspace{1cm} (5)

Ce problème admet une solution unique qui s'obtient facilement par résolution d'un système linéaire. En effet, si $(w_i)$ est une base de $V_h$, toute fonction de $V_h$ s'écrit :

$$\phi_h = \sum \alpha_i w_i$$

Mais on doit avoir $a(\phi_h, w_j) = f(w_j)$ $\forall j$, donc :

$$A_{ij} \cdot (\alpha_i) = f_j$$

avec $A_{ij} = a(w_i, w_j)$ et $f_j = f(w_j)$

On rappelle le théorème de convergence : si $V_h \to V$, alors la solution $\phi_h$ tend vers $\phi$ solution de (4).

On a de plus la majoration d'erreur :

$$||\phi - \phi_h||_V \leq C \inf_{\psi_h \in V_h} ||\phi - \psi_h||_V$$

La méthode des éléments finis consiste à choisir pour $V_h$ l'espace :

$$V_h = \{ \phi \in C^0(\Omega) \text{ avec } \chi_{E_k} \phi \in P_k(E_k) \}$$

$E_k$ étant un recouvrement de $\Omega : \Omega = \bigcup_{k=1}^{L} E_k$

$\chi_{E_k}$ fonction caractéristique de $E_k$

$P_k(E_k)$ espace des polynômes de degré inférieur ou égal à $K$ sur $E_k$

Pour appliquer la méthode décrite précédemment, il est nécessaire de représenter $V_h$ à l'aide de fonctions de base. Celles-ci doivent être continues sur $\Omega$ et être des polynômes de degré inférieur ou égal à $K$ sur chaque élément $E_k$. Pour construire de telles fonctions, la méthode la plus commode est de choisir sur chaque $E_k$ un ensemble de noeuds $n_j$ et de fonctions polynomiales $P_i$ de degré inférieur ou égal à $K$, telle que :

$$P_i(n_j) = \delta_{ij}$$ ($\delta$ symbole de Kronecker)

Considérons maintenant l'ensemble de noeuds ainsi défini sur $\Omega$. Les fonctions de base correspondant à un noeud $n_j$ seront définies comme la réunion des fonctions polynomiales sur chacun des éléments contenant $n_j$.

La condition de continuité à l'interface de 2 éléments implique la condition suivante : le nombre de noeuds sur l'interface de 2 éléments doit être au nombre de $K + 1$. 

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La donnée de l'ensemble de noeuds \( n_j \) ainsi que des polynômes \( P_i \) sur \( E_k \) définit donc de façon univoque l'espace \( V_h(7) \) et donc l'approximation éléments finis.

1.3. Choix des éléments finis dans ELECTRE

1.3.1. Forme des éléments

En physique des réacteurs à eau l'assemblage est de forme parallélépipédique rectangulaire; le choix le plus logique était donc de prendre des éléments de même forme: ces éléments ont en outre l'avantage de conduire à un calcul très rapide au niveau de l'assemblage de la matrice (le jacobien pour le passage d'un élément de référence à l'élément lui-même est très simple).

1.3.2. Calcul de la matrice

On peut détailler le calcul de \( A_{ij} \) dans le cas où \( D \) et \( \Sigma \) sont constants sur \( E_k, k = 1...L \).

Soit \( T = [0 \, 1] \times [0 \, 1] \times [0 \, 1] \) l'élément de référence, soit \( P_i \) la base de polynôme sur \( T \); supposons calculé une fois pour toutes les intégrales:

\[
D_{ij}^x = \iiint_T \frac{\partial P_i}{\partial x} \frac{\partial P_j}{\partial x} \, dx \, dy \, dz \\
D_{ij}^y = \iiint_T \frac{\partial P_i}{\partial y} \frac{\partial P_j}{\partial y} \, dx \, dy \, dz \\
D_{ij}^z = \iiint_T \frac{\partial P_i}{\partial z} \frac{\partial P_j}{\partial z} \, dx \, dy \, dz \\
S_{ij} = \iiint_T P_i P_j \, dx \, dy \, dz
\]

Par homothétie il est facile de se ramener aux polynômes de base sur l'élément \( E_k = h_x^k \times h_y^k \times h_z^k \). Celui-ci s'écrit :

\[
P_i(x, y, z) = P_i \left( \frac{x}{h_x^k}, \frac{y}{h_y^k}, \frac{z}{h_z^k} \right)
\]

Désignons maintenant par \( i_k, j_k \) les numéros internes à \( E_k \) des noeuds \( n_i \) \( n_j \). On peut écrire :

\[
w_i = \sum_{k=1}^{L} x_{E_k}^i \quad w_i = \sum_{k=1}^{L} x_{E_k}^i \quad P_i \left( \frac{x}{h_x^k}, \frac{y}{h_y^k}, \frac{z}{h_z^k} \right)
\]

donc

\[
A_{ij} = a(w_i, w_j) = \sum_{k=1}^{L} a(x_{E_k}^i, x_{E_k}^j) = \sum_{k=1}^{L} A_{i_k j_k}^k
\]

avec

\[
A_{i_k j_k}^k = D_{i_k j_k}^x = h_x^k \frac{\partial x_{E_k}^i}{\partial x_{E_k}^j} + D_{i_k j_k}^y = h_x^k \frac{\partial y_{E_k}^i}{\partial y_{E_k}^j} + D_{i_k j_k}^z = h_x^k \frac{\partial z_{E_k}^i}{\partial z_{E_k}^j}
\]

A ce cas simple (\( D_x, D_y, D_z \) et \( \Sigma \) constants par éléments) s'ajoute des possibilités de calcul plus complexe.
C'est ainsi que le code permet le traitement éventuel d'éléments hétéro-
gènes ($D_x, D_y, D_z$ et $\Sigma$ constants sur des parties de $E_x$ seulement); peuvent également
être traitées des variations polynomiales des fonctions précédentes sur chaque $E_x$.
Nous renvoyons à /1/, pour une description détaillée du cas précédent.

1.3.3. Choix des noeuds et des polynômes de base

Après avoir choisi la forme des éléments, il nous reste à choisir la
base $P_i$ ainsi que la distribution de noeuds $n_i$. L'inégalité (5) nous fournit un
ordre de grandeur de la majoration d'erreur, en effet si on choisit $\psi_h = \Pi_h \phi$
tel que,

$$\Pi_h \phi = \sum_{i=1}^{N} \phi(n_i) w_i$$

on voit que l'on ramène ainsi l'erreur, à l'erreur d'interpolation de la fonction $\phi$
par éléments finis. Ceci nous conduit à 2 familles d'éléments finis ayant des er-
reurs d'interpolation en $h^\alpha$ $h = \max(h_x, h_y)$.

1.3.4. Cas à deux dimensions

a) La famille de Lagrange

Linéaire     LL4

\[ \varepsilon C_1(\phi) h^2 \quad (\phi \in H^2) \]

Parabolique  PL9

\[ \varepsilon C_2(\phi) h^3 \quad (\phi \in H^3) \]

Cubique      CL16

\[ \varepsilon C_3(\phi) h^4 \quad (\phi \in H^4) \]

b) La famille de Serentipity (obtenue à partir de la famille précédente par sup-
pression des noeuds internes et conservation de l'ordre de grandeur de l'erreur
d'interpolation)

Parabolique  PS8

\[ \varepsilon C_4(\phi) h^3 \quad (\phi \in H^3) \]

Cubique      CS12

\[ \varepsilon C_5(\phi) h^4 \quad (\phi \in H^4) \]

1.3.5. Cas à trois dimensions

Pour des raisons de structuration de la matrice $A_{14}$ obtenue, on choisit
des éléments finis 3D, obtenus comme produit tensoriel d'une des bases précédentes
avec une base d'éléments finis Lagrange en $z$, linéaire, parabolique ou cubique.
C'est ainsi que l'on a par exemple:
1.4. Résolution du système linéaire

On distinguerà ici 2 cas, suivant que l'on se trouve en 2 ou 3 dimensions.

1.4.1. Cas à deux dimensions

A 2 dimensions les matrices sont en général d'ordre peu élevé N = 1000 ; on peut donc utiliser une méthode directe. Dans un premier temps on effectue une décomposition de A sous la forme :

\[ A = L D L^t \]

L est une matrice triangulaire inférieure
D est une matrice diagonale

La matrice L est beaucoup plus pleine que la matrice A. Le nombre de termes non nuls de L est égal au profil de la matrice A que l'on définit par :

\[ P = \sum_{i=1}^{N} \left[ i - \min(j) \right] \]

La valeur de P dépend assez fortement de la numérotation des noeuds. Il existe dans ELECTRE un algorithme sous-optimal de minimisation du profil de A /2/.

Dans le cas où ce profil resterait très grand, la matrice L est alors découpée en sous-blocs regroupant un certain nombre de lignes, ceci de telle sorte qu'au cours de l'étape de décomposition, seul 2 blocs successifs sont nécessaires en mémoire centrale.

1.4.2. Cas à trois dimensions

Par le choix des éléments finis 3D, la matrice possède un découpage naturel en blocs de plans, chacun des blocs étant symétriques. L'algorithme d'inversion du système est une méthode de sur-relaxation par blocs de plans (SOR). Le facteur de relaxation optimum est calculé automatiquement au cours des premières itérations. Dans le cas de calcul très volumineux, on utilise éventuellement une méthode SOR ponctuelle.

1.5. Méthodes itératives pour le calcul de la valeur propre

Plusieurs méthodes itératives sont à la disposition de l'utilisateur du programme.
1.5.1. Méthode de minimisation du reste dans $L^2(\mathbb{R}^n)$

La méthode de minimisation successive du reste dans $L^2(\mathbb{R}^n)$ a été développée pour le traitement de problème de valeur propre. Elle nécessite le stockage des vecteurs flux en double précision et également une inversion directe des matrices éléments finis. C'est la raison qui en limite l'utilisation au calcul à 2D.

1.5.2. Méthode de Tchebychev

Elle est surtout utilisée pour les calculs à trois dimensions, elle permet en général une convergence relativement rapide ; mais d'autres méthodes sont utilisées simultanément pour accélérer les convergences : initialisation par un flux de synthèse et rééquilibrage variationnel à mailles larges.

1.5.3. Initialisation du flux par un calcul de synthèse aux éléments finis

Considérons une représentation du flux tri-dimensionnel sous la forme :

$$\phi^q(x,y,z) = \sum_{i=1}^{i=N} a_i^q(z) w_i(x,y) \quad (8)$$

Dans cette forme, les fonctions $w_i(x,y)$ sont supposées connues et représentées sur la réduction à deux dimensions de la base d'éléments finis utilisés à trois dimensions.

Le problème à valeur propre étudié conduit à la stationnarité de la fonctionnelle :

$$J(\varphi, \varphi^*) = \frac{\langle \varphi^*, H \varphi \rangle}{\langle \varphi^*, P \varphi \rangle} \quad (9)$$

En utilisant la représentation (8) du flux et la forme équivalente correspondant au flux adjoint, il est possible d'obtenir une représentation des fonctions $a_i^q(z)$ développées sur la projection sur $z$ de la base tri-dimensionnelle utilisée. On obtient ainsi une approximation du flux tri-dimensionnel qui sert à initialiser le calcul.

1.5.4. Rééquilibrage variationnel à mailles grossières

Soit $\varphi$ le flux obtenu après un certain nombre d'itérations sur un maillage fin éléments finis, définissons un deuxième maillage plus grossier se superposant au précédent, et soit $Q_k$ la base d'éléments finis définie sur ce nouveau maillage.

La méthode de rééquilibrage consiste à modifier le flux fin $\varphi$ par multiplication par une fonction définie sur le maillage grossier, de telle sorte que le nouveau flux fin rende stationnaire la fonctionnelle (9).

Posons

$$\hat{\varphi} = \varphi \sum_{k=1}^{L} \phi_k^* Q_k$$

et

$$\hat{\varphi}^* = \varphi \sum_{k=1}^{L} \phi_k^* Q_k$$

Les conditions de stationnarité par rapport à chaque $\phi_k^*$ nous conduisent à un nouveau problème de valeurs propres dont les coefficients $\phi_k^*$ sont solutions.
1.5.5. Application de ces méthodes au traitement du Benchmark AIEA

Nous avons testé l'efficacité des différentes méthodes précédentes sur le réacteur Benchmark /4/. La figure 4 représente un diagramme (précision relative sur le flux/temp de calcul), 4 courbes figurent sur ce diagramme :
- La première est la courbe obtenue en itération puissance accélérée par une méthode de Tchebychev. Le nombre d'itérations internes par externes est de 3.
- La deuxième représente la même itération mais avec initialisation par synthèse. Le nombre d'itérations internes est seulement de 2.
- La troisième représente l'itération avec rééquilibrage à la 3ème itération externe (2 internes).
- La quatrième représente l'itération avec rééquilibrage à la 3ème itération externe et initialisation par synthèse (2 internes par externes).

On voit que le couplage du rééquilibrage et de l'initialisation par synthèse conduit à un gain très important en temps de calcul, mais également en nombre d'itérations fines (7 seulement).

1.6. Représentation des sections efficaces

Au cours d'un calcul couplé neutronique-thermodynamique la variation des sections efficaces en fonction de nombreux paramètres doit être prise en compte : irradiation du combustible, densité et température du modérateur, température du combustible, densité du Xénon, etc...

Le principe retenu dans NEPTUNE est de tabuler des sections efficaces macroscopiques en fonction des paramètres principaux (densité du modérateur et température du combustible par exemple) et de représenter par des sections efficaces microscopiques les isotopes ayant moins d'influence sur le spectre (par exemple Bore et Xénon).

Dans la version actuelle de l'interface NEPLIB qui est utilisée, le maillage en température et densité d'eau est la même pour tous les états d'irradiation.

Ces NEPLIB sont obtenues automatiquement par le module APOLLO du système NEPTUNE, en utilisant une procédure à deux étapes.

Pour un assemblage donné, on effectue un calcul utilisant la bibliothèque standard à 99 sur une configuration représentant une moyenne approximative des densités en cours d'évolution et l'on condense la bibliothèque à 30. Cette bibliothèque APOLLIB à 30 groupes est utilisée pour réduire considérablement le coût des calculs d'assemblages nécessaires à la création des bibliothèques.

Actuellement cette procédure est en cours d'amélioration pour réduire encore le nombre de groupes nécessaires au cours des calculs où l'on fait varier les derniers paramètres.

2/ CALCUL DE CINETIQUE TRI-DIMENSIONNELLE (ensemble de modules CRONOS)

L'utilisation de la méthode des éléments finis nous a permis de résoudre des problèmes de Keff en 3 dimensions dans des temps de calcul assez courts. Son utilisation a donc été développée pour le traitement des problèmes de cinétique 3D. La méthode développée ici s'inspire assez fortement du travail de KANG /5/, qui employait une méthode d'éléments finis d'hermite en 2 dimensions.

2.1. Equation cinétique

On considère l'équation de cinétique avec intégration exacte des termes de précurseurs. Soit :

\[
\frac{1}{v_g} \frac{\partial \phi_g}{\partial t} = v_D \nabla \cdot \phi_g + \sum_{g'} g' \cdot \Sigma_{tg} \phi_{g'} + \sum_{g'=1}^{g} \phi_{g'} \cdot \Sigma_{fg'} (1 - \beta_{g'}) + \sum_{g'=1}^{G} \Sigma_{fg'} \phi_{g'} \cdot (1 - \beta_{g'}) + \sum_{g'=1}^{G} \Sigma_{fg'} \phi_{g'} \cdot \sum_{k} \chi_{kg} \lambda_k C_k
\]

- 64 -
avec
\[ C_z(r,t) = C_z^0(r) e^{-\lambda_z t} + \int_0^t e^{-\lambda_z (t-s)} \sum_{g'=1}^G \beta_{zg'} g' \Sigma_f g' \phi_{g'} ds \]

A cette équation sont associées des conditions aux limites en espace conditions (2) et (3) et une condition initiale :
\[ \phi_g(r,0) = \phi_g^0(r) \]

\( v_g \) vitesse des neutrons
\( \lambda_z \) constante de décroissance du précurseur
\( \beta_{zg} \) proportion du précurseur \( z \) pour une fission du groupe \( g \)
\( C_z \) concentration du précurseur \( z \)

On peut décomposer l'étape d'approximation d'une telle équation en deux parties.

2.1.1. Approximation spatiale

On utilise ici la méthode décrite au § 1.2. basée sur une représentation éléments finis. Le flux \( \phi_g \) est décomposé sur une base \( P_i(r) \) d'éléments finis sous forme :
\[ \phi_g(r,t) = \sum_{i=1}^N \alpha_{ig}(t) P_i(r) \]  
(12)

Par remplacement de (12) dans (11) et projection sur la base \( P_i \) elle-même (méthode de Galerkin) on est conduit au système différentiel suivant :
\[ M \cdot \frac{d \alpha}{dt} = -K(t) \cdot \alpha(t) + \sum_{z=1}^L e^{-\lambda_z t} S_z^0 + \int_0^t e^{-\lambda_z (t-s)} F_z(s) \cdot \alpha(s) ds \]  
(13)

\( M, K \) et \( F_z \) étant des matrices éléments finis d'ordre \( G \times N \) (\( G \) nombre de groupe, \( N \) nombre de points).

On a :
\[ M = \frac{1}{v_g} \int_\Omega P_i P_j d\Omega \delta_g g' \]
\[ K(t) = \left[ \int_\Omega (D_g \nabla P_i \nabla P_j + \Sigma_{tg} P_i P_j) d\Omega + \int_\Gamma P_i P_j d\Gamma \right] \delta_g g' \]
\[ - \int_\Omega \Sigma_r g' g P_i P_j - \int_\Omega \chi g(1-\beta_{g'}) \nabla \Sigma_f g P_i P_j d\Omega \]
\[ S_z^0 = \int_\Omega \chi g \lambda_z C_z^0(r) P_i d\Omega \]
\[ F_z(t) = \int_\Omega \beta_{zg} g' \chi g \lambda_z \nabla \Sigma_f g P_i P_j d\Omega \]

2.1.2. Approximation temporelle

On introduit ici une discretisation du temps en un certain nombre de pas \( [t_p] \).

Chacune des matrices \( K(t) \) et \( F_z(t) \) sont susceptibles de variations au cours du temps par contre-réaction thermohydraulique ou variation de l'état physique du réacteur. On se limitera ici à des variations linéaires des matrices \( K(t) \) et \( F_z(t) \). On peut donc écrire :

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\[
K(t) = k^p \xi_p(t) + k^{p+1} \xi_{p+1}(t) \quad \text{pour} \ t \in [t_p, t_{p+1}]
\]
\[
F_\xi(t) = F_\xi^p \xi_p(t) + F_\xi^{p+1} \xi_{p+1}(t)
\]
aux
\[
\xi_p(t) = \frac{1}{\delta t_p} (t_{p+1} - t), \quad \xi_{p+1}(t) = \frac{1}{\delta t_p} (t - t_p)
\]

Introduisons d'une manière générale une approximation du flux sous la forme (schéma à un pas) :
\[
\alpha_i(t) = \alpha_i^p \omega_p(t) + \alpha_i^{p+1} \omega_{p+1}(t)
\]

L'intégration de (13) sur le pas de temps \([t_p, t_{p+1}]\), nous conduit à la relation matricielle :
\[
A_{p+1} \alpha^{p+1} = - A_p \alpha^p + R_p^e
\]
aux
\[
A_{p+1} = M + a_{pp+1} k^p + a_{p+1} p+1 k^{p+1} - \sum_{\xi=1}^L (c_{\xi p}^p F_\xi^p + c_{\xi p+1}^e F_\xi^{p+1})
\]
\[
A_p = -M + a_{pp} k^p + a_{p+1} p k^{p+1} - \sum_{\xi=1}^L (c_{\xi p}^p F_\xi^p + c_{\xi p+1}^e F_\xi^{p+1})
\]
\[
R_p^e = \chi_g \sum_{\xi=1}^L \left(1 - \frac{1 - e^{-\lambda_\xi \delta t_p}}{\lambda_\xi}ight) S_{\xi p}
\]

Les coefficients \(a_{pq}, b_{pq}^e, c_{pq}^e\) dépendent du choix des fonctions \(\omega_p, \omega_{p+1}\). Ils s'écrivent :
\[
\begin{align*}
a_{pq} &= \int_{t_p}^{t_{p+1}} \xi_p \omega_q \ dt \\
b_{pq}^e &= \int_{t_p}^{t_{p+1}} \ dt \int_{t_p}^{t} \frac{1 - e^{-\lambda_\xi (t-s)}}{\lambda_\xi} \xi_p \omega_q \ ds \\
c_{pq}^e &= \int_{t_p}^{t_{p+1}} e^{-\lambda_\xi (t-t_p)} \xi_p \omega_q \ dt
\end{align*}
\]

2.1.3. Choix des fonctions \(\omega_p, \omega_{p+1}\)

On rappelle la propriété suivante : considérons un système différentiel du type suivant :
\[
M \frac{d\alpha}{dt} = -K \cdot \alpha
\]
(14)

\(K\) est ici une matrice indépendante du temps.
Supposons le flux représenté sur un intervalle \( t_p, t_{p+1} \) par une fonction polynomial de degré \( p + q - 1 \) vérifiant:

\[
\frac{d^s}{dt^s} \omega(t_p) = \phi(s)(t_p) \quad s = 0 \ldots p - 1
\]

\[
\frac{d^s}{dt^s} \omega(t_{p+1}) = \phi(s)(t_{p+1}) \quad s = 0 \ldots q - 1
\]

Par intégration de (14) sur un pas de temps \( (t_p, t_{p+1}) \), on est conduit à l'équation matricielle:

\[
\hat{\phi}_{p+1} = P_{pq} (\delta_t M^{-1} K) \cdot \hat{\phi}_p
\]

où \( P_{pq} \) n'est autre que la représentation en approximant de Padé de la fonction exponentielle.

En particulier :
- le choix \( \omega_p = \frac{\varepsilon_p}{\varepsilon} \omega_{p+1} = \frac{\varepsilon_p}{\varepsilon} \), nous redonne le schéma de CRANK NIKOLSON classique ;
- le choix \( \omega_p = 0 \omega_{p+1} = 1 \), nous redonne le schéma implicite.

D'une manière générale, si:

\[
\begin{align*}
\omega_p &= (1 - 2\theta) \varepsilon_p + \varepsilon_p \\
\omega_{p+1} &= (2\theta - 1) \varepsilon_p + \varepsilon_{p+1}
\end{align*}
\]

on retrouve le \( \theta \) algorithme.

Les intégrales \( a_{pq}, b_{pq} \) et \( c_{pq} \) sont calculées dans le programme pour un choix \( q \) de \( \theta \), ce qui permet de modifier éventuellement le schéma au cours de l'intégration.

3/ LE MODULE FLICA

Le module FLICA /6/ calcule le régime permanent et transitio d'un fluide en simple ou double phase circulant dans des ensembles de sous-canaux couplés ou non. Le calcul est basé sur un modèle homogène à trois équations avec en plus une équation de déséquilibre liquide et la prise en compte éventuelle d'un glissement entre phases.

Dans le modèle mathématique tous les termes importants des équations fondamentales de l'hydrodynamique sont pris en compte, la turbulence étant représentée par l'utilisation d'une viscosité et d'une conductibilité enthalpique turbulentes.

3.1. Représentation géométrique

Les canaux de même longueur, formés par la réunion de sous-canaux, sont parallèles à l'axe Oz, direction principale de l'écoulement. La section droite perpendiculaire à l'axe Oz, dans laquelle toutes les grandeurs physiques sont homogénéisées, fait apparaître les canaux définis par une section de passage du réfrigérant, un diamètre hydraulique, un périmètre chauffant et un poids dans le cœurs. Une correspondance biunivoque entre la géométrie du réacteur et celle des sous-canaux permet de passer des calculs neutronics aux calculs thermohydrauliques.
3.2. Le modèle mathématique

3.2.1. Equation de conservation de la masse

On définit la masse moyenne du fluide dans la cellule \( \tau_i \) de volume élémentaire \( \tau_i \). En intégrant l'équation de conservation de la masse sur le volume \( \tau_i \), on obtient :

\[
\frac{3}{a} \rho_i + \frac{3}{a} G_i + \frac{1}{a} \sum_{k=i} v_{ik} q_{ik} \delta_{ik} = 0
\]

où \( g_{ik} \) sont les vitesses massiques moyennes mesurées sur les axes \( 0Y_{ik} \) perpendiculaires aux surfaces de communications entre sous-canaux, \( s_{ik} \) et \( e_{ik} \) des sections et largeurs de communications moyennes entre deux niveaux de discrétisation axiale.

3.2.2. Equation des quantités de mouvement en projection sur l'axe OZ

Elle s'écrit :

\[
\frac{3}{a} p_i = \left( K_i \frac{|G_i|}{d} + \frac{f_i}{D h_i} \times d_i \right) \frac{G_i}{G_i} + \rho_i g \cos \theta + \frac{3}{a} \frac{G_i}{G_i}
\]

\[
+ \frac{3}{a} (V_i G_i^2) + \frac{1}{a} \sum_{k=i} v_{ik} V_i g_{ik} q_{ik} \delta_{ik} + \frac{1}{a} \sum_{k=i} \frac{l_{ik}}{l_{ik}} (V_i G_i - V_k G_k) \times u_t
\]

avec :

\[
\sigma_i = (G_i^2 + \frac{1}{n} \sum_{k=1}^{n} g_{ik}^2)
\]

\( n \) = nombre de couplages du canal \( i \)

Les 4 premiers termes de cette équation sont respectivement les pertes de pression par frottement et singularités, par élévation, par accélération transitoire, par accélération permanente.

Le cinquième terme traduit l'échange de quantité de mouvement par transport de fluide entre les canaux \( i \) et \( k \), il fait partie de la perte de pression par accélération permanente.

Le dernier terme fournit les échanges de quantité de mouvement par turbulence. On voit qu'il est représenté sous la forme :

\[
u_t \frac{3}{a} v_{ik}
\]

produit d'une viscosité turbulente par le gradient de vitesse. On a défini cette viscosité par :

\[
u_t = u_x \left( 1 + M_t \left( \frac{G L_t}{u_x} \right)^{1-b} \right)
\]

La distance \( L_{ik} \) qui figure dans (15) et traduit la distance sur laquelle est calculé le gradient de vitesse est la même que celle sur laquelle est défini le gradient de pression entre sous-canaux.

Le terme de perte de pression par accélération permanente représente la somme des pertes de chaque phase pondérées par la section qu'elle occupe :

\[
\frac{3}{a} V_i G_i^2 = \frac{3}{a} (1 - \alpha) \rho_k V_k^2 + \frac{3}{a} \alpha \rho_g V_g^2
\]
donc avec :\[ V' = \frac{(1 - X)^2}{(1 - X_0)} \frac{\alpha}{\rho_g} + \frac{x^2}{\alpha \rho_g} \]

Pour traduire l'augmentation de la turbulence en double phase on a aussi utilisé le volume spécifique \( V' \) dans le terme d'échange turbulent de quantité de mouvement.

3.2.3. Équation de quantité de mouvement en projection sur les axes \( O \ Y_{ik} \)

En présentant les termes dans le même ordre que dans les équations précédentes, l'équation du code est :

\[- \frac{3 \rho}{\rho} \frac{\partial}{\partial t} \frac{1}{y_{ik}} \left[V_{ik} + g_{ik} + \frac{3}{8} \frac{\partial}{\partial t} \left( \frac{\partial V'_g}{\partial y_{ik}} \right) \delta_{ik} + \frac{3}{8} \frac{\partial V'_g}{\partial z} \delta_{ik} \right] = \frac{\partial}{\partial z} \left( G_{ik} \right), \]

avec :

\[ G_{ik} = \left( G_{ik}^2 + g_{ik}^2 \right)^{\frac{1}{2}} \quad \text{ou} \quad G_{ik} = g_{ik} \quad \text{au choix de l'utilisateur.} \]

Par rapport aux équations fondamentales de l'hydrodynamique on voit que les termes de variations de pression liés à l'élévation et aux échanges par turbulence n'ont pas été pris en compte.

Pour l'élévation le terme pourrait être rajouté mais il faudrait définir en données l'angle de \( O \ Y_{ik} \), avec la verticale. Ce terme est nul dans les cas de canaux verticaux.

Le terme relatif à la turbulence est certainement faible car on sait que celle-ci ne se propage pas à l'amont d'un canal, et aussi parce que les \( \Delta z \) sont souvent grands devant les longueurs caractéristiques \( L_{ik} \).

3.2.4. Équation du bilan d'énergie

Pour l'ensemble des phases liquide et vapeur, elle s'écrit :

\[ \frac{\partial}{\partial t} \left( \rho_k h_k (1 - \alpha) + \rho_g h_g \alpha \right) + \frac{3}{8} \frac{\partial}{\partial z} \left( G_{ik} \right) - \frac{1}{S_i} \sum_{i=k}^i L_{ik} (H_i - h_k) = - \frac{P_i \phi_i + q_i}{S_i} \]

Le troisième terme du membre de gauche représente le transfert d'enthalpie du aux débits transversaux, \( H_{ik} \) étant l'enthalpie à l'interface.

Le quatrième terme représente l'échange d'enthalpie par turbulence, il est de la même forme que l'échange de quantité de mouvement.

3.2.5. Équation du bilan d'énergie dans la phase liquide

Pour le calcul de la double phase, le code comporte une équation supplémentaire qui permet le calcul du titre réel en ébullition locale. Cette équation a été écrite en ne tenant compte que de la proportion de liquide et en négligeant les effets de la pression.

\[ \frac{\partial}{\partial t} \left( \rho_k h_k (1 - \alpha) \right) + \frac{3}{8} \frac{\partial}{\partial z} \left( G_{ik} \right) + \frac{1}{S_i} \sum_{i=k}^i L_{ik} \left( h_{ik} - h_{ik} \right) g_{ik} \delta_{ik} + \frac{K_T}{L_{ik}} \left( h_{ik} - h_{ik} \right) \]

\[ = K_v \left( h_{sat} - h_{ki} \right) \left( H_i - h_{ki} \right) + \frac{P_i \phi_i (1 - \chi_{ci}) + q_i (1 - \alpha_i)}{S_i} \]

Les termes d'apport d'énergie dans la phase liquide qui figurent dans le membre de gauche constituent des modèles, ce sont :

- pour le premier l'expression de la recondensation supposée proportionnelle aux écarts entre l'enthalpie liquide et l'enthalpie moyenne et entre l'enthalpie
moyenne et l'enthalpie à la saturation. Le coefficient de proportionnalité \( k_v \)
étant recalé à partir de résultats expérimentaux.
- pour le second, l'apport calorifique provenant du chauffage des parois et du
chauffage directe.

3.3. Méthodes de résolution utilisées

La résolution des équations principales est effectuée par discrétisation
aux différences finies. Quelles que soient les conditions aux limites, les équa-
tions sont résolues à chaque niveau successivement, à partir de l'entrée.

Des itérations d'ensemble permettent de prendre en compte les phénomènes
locaux sur l'amont de l'écoulement et sur tous les canaux. La convergence est réa-
lisée sur les vitesses massiques radiales et sur les pressions.

3.4. L'interface neutronique-thermohydraulique

Le calcul neutronique fournit une distribution de puissance dans tous
les éléments du cœur du réacteur. La correspondance géométrique des éléments et
des sous-canaux permet de calculer la distribution axiale du flux dans chaque sous-
canal, en tenant compte du poids et du périmètre chauffant des sous-canaux.

Le calcul thermohydraulique fournit des distributions axiales de la den-
sité apparente du réfrigérant et de la température moyenne pour chaque sous-canal.
On en déduit la concentration en noyaux du modérateur en tenant compte du facteur
d'homogénéisation de chaque composition du cœur et la température effective de
echaque élément.

4/ INTRODUCTION DES CONTRE-REACTIONS THERMODYNAMIQUES

L'introduction de ces contre-réactions se fait en enchaînant un calcul
CRONOS et un calcul FLICA, selon le schéma que nous allons décrire.

4.1. Calcul CRONOS

L'état neutronique et thermohydraulique du réacteur est connu à l'ins-
tant \( t \), nous le représenterons par le vecteur \( \mathbf{N} \) représentant l'état neutronique
et le vecteur \( \mathbf{T} \) représentant l'état thermohydraulique.

La première phase du calcul est constituée par l'extrapolation de l'état
thermohydraulique au temps \( t + dt \) (c'est le vecteur \( \mathbf{T}(t + dt) \)).

Le calcul neutronique est ensuite effectué en supposant que l'état ther-
mohydraulique pendant le step \( t \), \( t + dt \), varie linéairement entre \( \mathbf{T}(t) \) et \( \mathbf{T}(t+dt) \).

On obtient ainsi l'état neutronique approché \( \mathbf{N}(t + dt) \) et en particulier
une approximation de la puissance totale du réacteur \( P(t + dt) \).

4.2. Calcul FLICA

La moyenne de la distribution de puissance pendant le step \( (t, t + dt) \)
est transmise à FLICA qui calcule l'évolution des conditions thermohydrauliques
avec ces hypothèses.

4.3. Itération

Le résultat de FLICA, c'est-à-dire l'état thermohydraulique au temps
\( t + dt \) est renvoyé à CRONOS et une itération est effectuée jusqu'à convergence.

Pour les transitoires traités, une seule itération suffit en général.
5/ SYSTEME INFORMATIQUE DE CRONOS

5.1. Organisation générale

Le système CRONOS est constitué d'une bibliothèque de modules indépendants et du logiciel général destiné à l'enchaînement de ces modules et à la transmission des informations traitées.

Chaque module remplit une fonction logique définie :
- implantation d'un algorithme d'analyse numérique
- acquisition de données
- transformation de données
- édition d'informations

A chaque module est associé un ensemble de données alphanumériques par l'intermédiaire d'un ou plusieurs arguments transmis à ce module.

Un macro-langage de commande ARIANE a été développé pour permettre à l'utilisateur de programmer l'enchaînement des modules nécessaires à l'exécution de son calcul et le transfert des informations symboliques utilisées par celui-ci. L'ensemble des données forme une structure de données pour le langage ARIANE qui permet à chaque module de traiter, donc d'évaluer, la structure des données de référence.

Un des éléments de la structure des données peut être un fichier d'archivage, ARIANE possédant toutes les fonctions de gestion d'un fichier.

5.2. Méthode de programmation utilisée

Les modules sont programmés dans le langage LAGD qui outre les instructions de FORTRAN IV possède des instructions de gestion de mémoire en relation avec un espace disque. Le langage permet ainsi une simulation de mémoire virtuelle sans limitation d'adressage, autre que la limite de l'espace disque disponible.

Ce langage n'est pas compilé, mais traduit un FORTRAN standard, ce qui assure la transportabilité des produits réalisés. De plus LAGD est compatible avec tout programme directement écrit en FORTRAN.

5.3. Le chargeur dynamique d'ARIANE

Les sous-programmes du système NEPTUNE ne sont pas traités par l'éditeur de liens du système IBM sous lequel l'exécution se fait, mais chargés dynamiquement au cours de l'exécution.

Le processeur de commande ARIANE /7/ détermine au cours de l'exécution les modules à charger, les recherche sur les disques bibliothèques et les charge en mémoire après avoir résolu les références externes nécessaires.

De cette manière, la création d'arbre d'overlay est inutile, la place mémoire à l'exécution est réduite au minimum et la maintenabilité du programme est améliorée.

L'utilisateur de NEPTUNE a ainsi la possibilité d'introduire ses propres programmes écrits en FORTRAN et grâce au langage ARIANE de les faire exécuter.

Toutes les informations nécessaires à ces programmes transitent par les structures des données.
5.4. État actuel du système

La version actuelle du code possède plus d'une centaine de fonctions. A titre d'indication, les principales fonctions permettent :
- d'entrer les informations nécessaires à la description du réacteur ;
- de modifier la description de ce réacteur, par des déplacements d'éléments, d'assemblages, etc... ;
- de créer les matrices d'éléments finis approchant l'équation multigroupe de diffusion ;
- de résoudre les problèmes à valeurs propres associées ;
- d'effectuer le calcul de cinétique CRONOS ;
- d'effectuer le calcul FLICA.

Un macro-programme effectuant un calcul BILAN complet est donné en exemple ci-dessous :

DEFI MAILX COORDX FIND
DEFI MAILY MAILX FIND
DEFI ITE EL2 RMI NE1 NE2 FLUX ICOMP VP EPS FIND
DEFI MAILX COORDX FIND
DEFI MAILSY MAILSX FIND
DEFI SECTION (données d'entrée des sections efficaces)
DEFI GEOT EL1 ICOMP COORDX COORDY GEOTRI FIND
DEFI GEOTRI (données d'entrée de la géométrie)
DEFI COORDY (abscisses des points en x)
DEFI COORDX COORDX FIND
DEFI INITAB (initialisation des Burn-up)
DEFI POLY FICHIER 23 OUVRIR POLO LIRE NE1 APPR FERMER FIND

DEFP ELECTRE LECTURE (: NBURN NBAS TCOMP SECTIONS) ; DESCRIPTION (GEOT) ;
              INIELEM (: TCOMP INITAB) ; FINB ;
DEFP INID SET (POLY) ; ELEM (: TCOMP EL2 MAILX MAILY) ; PROFIL (: EL2
              NE1 NE2 OCTIM PROF) ; INIFLU (: FLUX) ; FINB ;
DEFI MAT MATRICE (: TCOMP EL2 NE1 NE2 RHI) ; CHOL (: NE2 RHI) ; FINB ;
DEFI ITER SI (TYPE = "TCHBEYCHEV") ; ALORS TCHB (ITE) ;
              SINON LIVO (ITE) ; FINB ;
DEFP EDT EDITION (: EL2 NE1 NE2 FLUX TCOMP MAILSX MAILSY) ; FINB ;
DEFP BILAN ELECTRE ; INID ; MAT ; ITER ; EDT ; FINB ;
DEFP MAIN APPROXIMATION = PS8 ; TYPE = "TCHBEYCHEV" ; EPS = 0.001 ;
              BILAN ; FINB ;
ENTREE MAIN
Figure 1

Représentation radiale du flux pour le Benchmark 2D
approximation linéaire (LL4) : découpage 17x17 34x34 68x68
(référence PS8 68x68)

COUPE Y=0. FLUX THERMIQUE
Figure 2

Représentation radiale du flux pour le Benchmark 2D
approximation parabolique (PSB) : découpage 9x9 17x17 34x34
(référence PS 68x68)

COUPE Y=0. FLUX THERMIQUE
Figure 3

Représentation radiale du flux pour le Benchmark 2D
approximation cubique (CS12) : découpage 9x9 17x17 34x34
(référence PS8 68x68)

COUPE y=0. FLUX THERMIQUE
Figure 4

NEPTUNE 0.2
AIEA 3D Benchmark
PPL 17 x 17 x 16
REFERENCES BIBLIOGRAPHIQUES

/1/ A. KAVENOKY, J.J. LAUTARD
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Rapport à paraître.

/3/ M. LIVOLANT
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/6/ R. PLAS
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et de boucles d'essais.
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/7/ M.F. FOURQUET, A. KAVENOKY, D. ROBÉAU
Manuel de référence du langage ARIANE.
Rapport à paraître.
SUIVI D'UN PWR DE 900 MWe PAR CRONOS

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Service d'Etudes des Réacteurs et de Mathématiques Appliquées
Centre d'Etudes Nucléaires de Saclay
B.P. N° 2 91190 Gif sur Yvette FRANCE

Le module CRONOS du système NEPTUNE est constitué du couplage du module TRIDENT qui résout l'équation de diffusion à trois dimensions par la méthode des éléments finis et du module thermohydraulique FLICA III qui résout les équations de la thermique et de l'hydraulique /1/.

Ce système modulaire a été développé pour les calculs de coeur des réacteurs PWR mais peut être utilisé pour les autres types de réacteur.

Pour ces calculs, il est nécessaire de créer des tables de sections efficaces à peu de groupes dépendant de nombreux paramètres qui peuvent être la densité du modérateur, la température combustible, le taux d'irradiation, la concentration xénon, la densité de bore, etc... Ces tables sont créées par le code de transport APOLLO /2/.

Dans une première partie, nous exposons le schéma de calcul pour la création des sections efficaces à peu de groupes paramétrées par le code APOLLO et dans la deuxième partie l'application du code CRONOS au calcul de l'évolution d'un réacteur PWR de 900 MWe.

INTRODUCTION

L'étude entreprise a permis de qualifier le schéma de calcul le plus complet que l'on puisse mettre en œuvre actuellement pour le traitement d'un cœur de réacteur.

Ce traitement est fait par le code CRONOS /1/ développé au CEA à SACLAY.

Le couplage neutronique-thermohydraulique permet de calculer un cœur en tenant compte d'une manière physiquement rigoureuse des contre-réactions liées à la puissance : effet Doppler, effet de température et de densité du modérateur. De plus, CRONOS permet de traiter l'évolution en régime de fonctionnement permanent.

I/ CREATION DES TABLES DES SECTIONS EFFICACES A VARIATION (NEPLIBS) PAR APOLLO

La simulation de l'évolution d'un cœur PWR pose le problème de la préparation des bibliothèques de constantes neutroniques avec le code APOLLO /2/.

En effet les sections efficaces à peu de groupes (2 groupes) à introduire dans CRONOS doivent être tabulées en fonction de la température combustible, de la densité de l'eau, du taux d'irradiation et d'autres paramètres, par exemple le xénon, le samarium, le bore (CRONOS interpolant linéairement dans ces tables).

Avant de présenter le schéma utilisé pour la création de ces bibliothèques d'un cœur de réacteur PWR de 900 MWe, quelques tests préliminaires ont été nécessaires pour représenter et calculer au mieux les constantes neutroniques des assemblages.
### Tableau I
Réactivités de différents assemblages

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>B - A pcm</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 P</td>
<td>2,55 %</td>
<td>0,96480</td>
</tr>
<tr>
<td>12 P</td>
<td>3,10 %</td>
<td>1,02782</td>
</tr>
<tr>
<td>8 P</td>
<td>2,55 %</td>
<td>1,01112</td>
</tr>
</tbody>
</table>

A : les cellules combustibles entourant les poisons ne sont pas distinguées
B : les cellules combustibles entourant les poisons sont distinguées

### Tableau II

<table>
<thead>
<tr>
<th>Cellule</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>N2S8-M8</td>
<td>- 0,17</td>
<td>- 0,09</td>
<td>+ 0,91</td>
<td>- 0,66</td>
<td>- 0,97</td>
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Écarts sur la puissance en %

<table>
<thead>
<tr>
<th>Δ ABSP</th>
<th>Δ KINF</th>
</tr>
</thead>
<tbody>
<tr>
<td>N2S8-M8</td>
<td>+ 47</td>
</tr>
</tbody>
</table>

Écart en pcm sur KINF et l'absorption dans le poison

- 80 -
1. Représentation des assemblages

Du point de vue des hétérogénéités, nous distinguons trois types d'assemblages $15 \times 15$ dans le réacteur PWR étudié :

- assemblage sans poison (figure 1)
- assemblage avec 8 poisons (figure 2)
- assemblage avec 12 poisons (figure 3)

Compte tenu de leur symétrie, il faudrait distinguer 36 cellules pour un huitième d'assemblage ce qui mènerait à un nombre de points de calcul important et, par suite, à des calculs onéreux.

Une représentation des assemblages à 8 types de cellules pour les assemblages avec poisons (figure 4) et à 6 types de cellules pour les assemblages sans poison (figure 5) dans les calculs permettent d'obtenir des résultats intégrés sur l'ensemble de l'assemblage (taux de réactions, sections efficaces) satisfaisants par rapport aux calculs détaillés.

La représentation simplifiée des assemblages apporte un écart de 200 pcm sur la réactivité par rapport à un calcul détaillé à 36 cellules.

Il est à remarquer qu'il est primordial de distinguer les cellules combustibles entourant les poisons (tableau I).

2. Choix du module de calcul de l'assemblage

Différents modules multicellules sont opérationnels dans APOLLO : module MULTICELLULE standard, module NAUSICAA, module CALLIOPE, module MARSYAS /3/.

En vue d'obtenir les propriétés neutroniques des assemblages dans les meilleures conditions (précision, coût, temps de calcul) nous avons effectué une comparaison NAUSICAA-MULTICELLULE sur un assemblage 12 poisons à 8 types de cellules.

La comparaison se réfère aux deux calculs suivants :

- MB : MULTICELLULE
- N2S8 : NAUSICAA avec 8 secteurs dans le modérateur et 4 dans le combustible des cellules entourant les poisons.

(des tests ont prouvé que c'est la meilleure répartition des secteurs dans NAUSICAA).

D'après le tableau II, il ressort que le calcul MULTICELLULE est en bon accord avec le calcul NAUSICAA, grâce à une compensation d'erreur sur les secteurs et d'erreur sur la différentiation des faces.

Les écarts ayant donc été jugés insuffisants pour justifier de l'utilisation de l'option NAUSICAA, les tables de sections efficaces ont été créées en option MULTICELLULE.

3. Condensation à 30 groupes de la bibliothèque à 99 groupes dans APOLLO

Pour réduire le temps et le coût d'un calcul APOLLO MULTICELLULE standard utilisant une bibliothèque à 99 groupes, on crée une bibliothèque à un nombre réduit de groupes.

Un découpage à 30 groupes a été retenu, défini par 14 groupes épithermi ques et 16 groupes thermiques (tableau III).

La condensation se fait de la manière suivante : un calcul à 99 groupes est effectué jusqu'à mi-cycle, les sections efficaces des noyaux lourds et des produits de fission sont condensés à 30 groupes sur le flux à ce taux de combustion, c'est-à-dire dans une situation avec une certaine quantité de plutonium.
<table>
<thead>
<tr>
<th>Tableau III</th>
</tr>
</thead>
<tbody>
<tr>
<td>Structure de la bibliothèque à 30 groupes</td>
</tr>
</tbody>
</table>

<table>
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<td>0,7050</td>
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<td>98</td>
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<td>51</td>
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<td>75</td>
<td>0,6250</td>
<td></td>
<td>99</td>
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<td>76</td>
<td>0,54001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Le tableau IV représente la comparaison du calcul en évolution à 99 groupes et de celui à 30 groupes sur un assemblage typique d’un PWR.

On constate que cette simplification n’introduit que des erreurs minimes :

- les facteurs de multiplication infinis sont calculés (par rapport au calcul à 99 groupes) avec une erreur inférieure à 150 pcm ;
- les écarts sur les sections efficaces d’absorption ne dépassent pas 1 %.

4. Nombre de températures d’évolution nécessaires pour les calculs 2D

Dans les calculs à trois dimensions avec contre-réactions, il est nécessaire de créer des tables de sections efficaces (les Neplins) à peu de groupes dépendant de la température combustible, de la densité d’eau, et du taux d’irradiation pour la prise en compte de la variation axiale de température dans le cœur du réacteur.

Le problème consiste à déterminer le nombre de températures d’évolution nécessaires à ces calculs, c’est-à-dire le nombre de bibliothèques évolutives à créer.

Deux calculs axiaux sur une cellule combustible avec contre-réactions sont faits et comparés :

Calcul 1 : calcul sur la cellule formée d’une seule composition axiale dont la bibliothèque évolution est créée et paramétrée à partir d’un calcul APOLLO caractérisé par une température modérateur $T_1$ et une densité d’eau correspondante $N_{1}$, moyennes sur toute la hauteur ;

Calcul 2 : calcul sur la cellule formée de deux compositions axiales. La bibliothèque évolution de la partie haute est créée à partir d’un calcul APOLLO à une température modérateur $T_2$ et une densité d’eau $N_{2}$, moyennes sur la moitié haute. Celle de la partie basse est créée à partir d’un calcul APOLLO à une température $T_3 < T_2$ et une densité d’eau $N_{3} > N_{2}$, moyennes sur la moitié basse.

Les trois calculs de bibliothèques sont faits à la même température combustible $T_{C}$, moyenne sur toute la hauteur.

Le tableau V indique les écarts obtenus sur la distribution axiale de puissance entre les calculs 1 et 2.

Nous constatons que ceux-ci sont faibles et, par conséquent, une seule température d’évolution (c’est-à-dire une seule bibliothèque évolution) suffit dans les calculs 3D avec contre-réactions.

5. Création des Neplins

En tenant compte des résultats obtenus et décrits dans les paragraphes précédents, les étapes nécessaires à la création des tables des sections efficaces à deux groupes dépendant de la température combustible, de la densité d’eau, du taux d’irradiation, de la densité de bore, de la concentration xénon, etc... sont les suivantes :

Calcul APOLLO MULTICELLULE sur l’assemblage dans les conditions nominales $T_{comb}$, $D_{H_2O}$ jusqu’à mi-évolution (8000 MWD/t)

condensation des sections efficaces des noyaux lourds et des produits de fission à 30 groupes

Calcul APOLLO MULTICELLULE à 30 groupes en évolution aux conditions nominales $T_{comb}$, $D_{H_2O}$

à chaque pas d’évolution

sortie des sections efficaces à 2 groupes

$E = f(\tau_k, T, D_{H_2O} \ldots)$

sortie des concentrations des noyaux lourds et des produits de fission $N_{1}(\tau_k)$
Tableau IV

Écart relatif des sections efficaces des 99 groupes de sections efficaces des 99 groupes d'absorption intégrées sur l'espace et l'énergie

<table>
<thead>
<tr>
<th>Burn-up MWJ/t</th>
<th>$k_{eff}$ 99 groupes</th>
<th>$k_{eff}$ 30 groupes</th>
<th>$\delta$ US5 %</th>
<th>$\delta$ Pu9 %</th>
<th>$\delta$ Pu40 %</th>
<th>$\delta$ Pu41 %</th>
</tr>
</thead>
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<td>0,97283</td>
<td>-0,28</td>
<td>0,09</td>
<td>0,24</td>
<td>0,05</td>
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<td>0,93909</td>
<td>0,93823</td>
<td>-0,35</td>
<td>0,11</td>
<td>0,36</td>
<td>0,03</td>
</tr>
</tbody>
</table>
### Tableau V

**Ecart sur la puissance entre le calcul "1 COMPO" et le calcul "2 COMPOS" $\frac{2-1}{2}$ %**

<table>
<thead>
<tr>
<th>Cote z en cm</th>
<th>1000 MWJ/t</th>
<th>5000 MWJ/t</th>
<th>10000 MWJ/t</th>
</tr>
</thead>
<tbody>
<tr>
<td>49,15</td>
<td>-0,21</td>
<td>-0,70</td>
<td>-1,00</td>
</tr>
<tr>
<td>67,44</td>
<td>-0,30</td>
<td>-0,40</td>
<td>-1,00</td>
</tr>
<tr>
<td>85,73</td>
<td>-0,10</td>
<td>-0,20</td>
<td>-1,12</td>
</tr>
<tr>
<td>104,02</td>
<td>+0</td>
<td>+0,09</td>
<td>-1,20</td>
</tr>
<tr>
<td>122,31</td>
<td>+0,08</td>
<td>+0,35</td>
<td>-1,30</td>
</tr>
<tr>
<td>140,60</td>
<td>+0,24</td>
<td>+0,50</td>
<td>-1,40</td>
</tr>
<tr>
<td>158,89</td>
<td>+0,30</td>
<td>+0,70</td>
<td>-1,22</td>
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<tr>
<td>177,18</td>
<td>+0,50</td>
<td>+0,80</td>
<td>-0,95</td>
</tr>
<tr>
<td>195,47</td>
<td>+0,50</td>
<td>+0,90</td>
<td>-0,50</td>
</tr>
<tr>
<td>213,76</td>
<td>+0,40</td>
<td>+0,80</td>
<td>+0,09</td>
</tr>
<tr>
<td>232,05</td>
<td>+0,40</td>
<td>+1,00</td>
<td>+1,40</td>
</tr>
<tr>
<td>250,34</td>
<td>+0,20</td>
<td>+0,90</td>
<td>+1,50</td>
</tr>
<tr>
<td>268,63</td>
<td>+0,08</td>
<td>+0,36</td>
<td>+1,70</td>
</tr>
<tr>
<td>286,92</td>
<td>-0,08</td>
<td>+0</td>
<td>+1,40</td>
</tr>
<tr>
<td>305,21</td>
<td>-0,30</td>
<td>-0,45</td>
<td>+1,20</td>
</tr>
<tr>
<td>323,50</td>
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<tr>
<td>341,79</td>
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<td>-1,20</td>
<td>+0,06</td>
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<tr>
<td>360,08</td>
<td>-0,80</td>
<td>-1,50</td>
<td>+0,04</td>
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<tr>
<td>378,37</td>
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<td>+0,01</td>
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<tr>
<td>396,66</td>
<td>-0,80</td>
<td>-1 60</td>
<td>-0,03</td>
</tr>
</tbody>
</table>

### Tableau VI

**Effet des contre-réactions sur la distribution radiale de puissance (Ecart en % avec-sans)**

<table>
<thead>
<tr>
<th>MWJ/t</th>
<th>150</th>
<th>13330</th>
</tr>
</thead>
<tbody>
<tr>
<td>-6,9</td>
<td>2,7</td>
<td>4,5</td>
</tr>
<tr>
<td>-3,7</td>
<td>1,8</td>
<td>1,7</td>
</tr>
<tr>
<td>-5,5</td>
<td>1,7</td>
<td>0,2</td>
</tr>
<tr>
<td>-4,1</td>
<td>0,2</td>
<td>-0,6</td>
</tr>
<tr>
<td>-3,9</td>
<td>-0,6</td>
<td>-1,7</td>
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<td>-1,7</td>
<td>-0,7</td>
</tr>
<tr>
<td>-2,7</td>
<td>1,2</td>
<td></td>
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<tr>
<td>-3,7</td>
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<td>0,5</td>
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<tr>
<td>-5,5</td>
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<td>-4,1</td>
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<td>-0,5</td>
</tr>
<tr>
<td>-2,7</td>
<td>1,2</td>
<td></td>
</tr>
</tbody>
</table>

- 85 -
Calculs APOLLO MULTICELLULE en reprise à 30 groupes

Lire les cartes \( N(x) \)

Faire varier \( T_c \) ou \( D_{Ho} \) ou les deux à la fois autour des points nominaux

Sortie des sections efficaces à 2 groupes

\[ S = f(x, T, D) \]

S'il on a \( N \) valeurs de \( x \), \( P \) valeurs de \( T \) et \( Q \) valeurs de \( D \), il faut effectuer \( N \times P \times Q \) calculs de flux par APOLLO MULTICELLULE à 30 groupes et par assemblage.

Ce schéma de calcul présente l'avantage de faire des calculs simples pour obtenir les sections efficaces et d'agrandir les tables, si cela est nécessaire, au cours du calcul.

Par contre, le nombre de calculs APOLLO est important (200 en général par assemblage), donc le prix pour la création des bibliothèques à contre-réactions est élevé.

Des améliorations de ce schéma sont possibles. Elles consisteraient à condenser dans APOLLO les sections efficaces en une bibliothèque à un nombre très réduit de groupes (4 groupes par exemple), de conserver cette bibliothèque dans le calcul de diffusion et de faire dans NEPTUNE pour chaque élément un calcul de spectre à chaque pas d'évolution pour obtenir les sections efficaces à 2 groupes tenant compte des conditions thermohydrauliques locales.

II/ CALCULS DE COEUR POUR LE CYCLE 1 PAR CRONOS /4/

Les calculs de coeur ont été faits à trois dimensions et avec prise en compte du couplage entre la neutronique et la thermohydraulique grâce aux modules TRIDENT et FLICA III du système NEPTUNE.

Les résultats présentés sont obtenus sur le suivi du 1er cycle d'un PWR de 900 MWe.

1. Effets des contre-réactions

Nous comparons les résultats de calculs à 3D sans contre-réaction par TRIDENT où les températures moyennes sont de 700 °C pour le combustible et de 304 °C pour l'eau, aux calculs à 3D avec contre-réactions par CRONOS.

a) Distributions axiales de puissance

En début de cycle, le calcul CRONOS engendre une distorsion de la distribution axiale de puissance vers le bas due à la densité de l'eau plus grande ici (figure 6). Le déséquilibre axial de puissance passe de 0,2 % pour le calcul TRIDENT (les réflecteurs inférieurs et supérieurs n'étant pas identiques) à - 5 % pour le calcul CRONOS à 150 MWJ/t.

De plus, le couplage neutronique thermohydraulique conduit à une distribution axiale de puissance plus aplatie due à la variation de la température combustible (figure 7).

En fin de cycle, la distribution axiale de puissance devient plus uniforme. Le déséquilibre axial n'est plus que de - 1,9 % (figure 8) à comparer à la valeur + 0,24 % obtenue par TRIDENT (figures 9 et 10).

La réduction du déséquilibre axial de puissance, en fin de cycle, est due en partie au déséquilibre de la distribution axiale du taux de combustion (figure 11) : le pic du taux d'irradiation est situé dans la partie inférieure du coeur où la densité de l'eau est la plus forte. Cela implique un équilibre de la distribution axiale de puissance de part et d'autre de la ligne médiane.
b) Distributions radiales de puissance

Le tableau VI permet d'analyser les modifications introduites sur la distribution radiale de puissance par la prise en compte des contre-réactions.

Au début du cycle, le calcul CRONOS donne une distribution radiale de puissance plus "aplatie"; un basculement sur les écarts de la distribution radiale de puissance est observée : écart de -7% sur les assemblages centraux et de +6,5% sur les assemblages périphériques.

À la fin du cycle, ce basculement a presque disparu : cela peut être dû à la différence des taux d'Irradiations obtenus entre les deux calculs et à une compensation entre les effets des contre-réactions (tableau VII et tableau VIII distribution radiale des températures combustibles et des densités d'eau).

2. Comparaison des résultats théoriques et des résultats mesurés

a) Réactivités

Le tableau IX montre les valeurs du facteur de multiplication $k_{eff}$ calculées par CRONOS où, à chaque pas d'évolution, nous imposons la valeur expérimentale de la concentration de bore.

Les différences entre ces valeurs et 1 représentent les erreurs du calcul.

La dérive de 600 pcm observée en cours d'évolution peut avoir plusieurs origines :
- la capture des produits de fission autres que le xénon et le samarium dont la concentration est bien calculée par CRONOS ;
- les propriétés nucléaires du Plutonium ;
- l'erreur systématique qui existe sur les mesures des taux d'Irradiation.

Celle qui nous paraît actuellement la plus vraisemblable (mais que nous n'avons pas encore complètement vérifiée) est l'insuffisance du formalisme MULTI-CELLULE pour le traitement de l'usure des poisons consommables.

b) Distributions radiales de puissance

Le tableau X présente les erreurs sur la distribution radiale de puissance par rapport à l'expérience en début de cycle. On observe dans la zone centrale un effet de damier (effet de 3%) qui peut être dû, soit à la théorie, soit aux erreurs des puissances expérimentales calculées à partir de mesures d'activités.

Par contre, le calcul CRONOS permet d'obtenir un bon accord sur les puissances expérimentales dans les assemblages périphériques.

En fin de cycle, la prédiction de la carte de puissance est correcte (tableau XI) malgré la dérive observée sur les valeurs de $k_{eff}$.

CONCLUSION

Ce travail nous semble avoir apporté la preuve que l'ingénieur dispose à l'heure actuelle d'un outil de calcul à la fois précis et fiable : précis parce que l'ensemble des aspects physiques est pris en compte ; fiable parce que la confrontation à l'expérience est satisfaisante notamment en ce qui concerne les distributions de puissance.

Cela ne signifie pas cependant que nous estimons que cet outil a atteint le terme de son développement. La légère dérive en réactivité que nous avons observée devra être analysée plus à fond. Par ailleurs, des simplifications du schéma de calcul sans perte appréciable de précisions - donc des réductions des coûts - nous paraissent encore réalisables.
### Tableau VII

**Distribution radiale de la température combustible moyennée sur toute la hauteur en °C**

<table>
<thead>
<tr>
<th></th>
<th>660</th>
<th>732</th>
<th>782</th>
<th>788</th>
<th>818</th>
<th>812</th>
<th>833</th>
<th>799</th>
</tr>
</thead>
<tbody>
<tr>
<td>605</td>
<td>696</td>
<td>798</td>
<td>770</td>
<td>830</td>
<td>778</td>
<td>832</td>
<td>755</td>
<td></td>
</tr>
<tr>
<td>556</td>
<td>751</td>
<td>763</td>
<td>803</td>
<td>805</td>
<td>830</td>
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<td></td>
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<tr>
<td>533</td>
<td>740</td>
<td>748</td>
<td>822</td>
<td>779</td>
<td>835</td>
<td>778</td>
<td></td>
<td></td>
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<td>736</td>
<td>783</td>
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<td>808</td>
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<td></td>
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<td>764</td>
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<td>827</td>
<td>776</td>
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<td>798</td>
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<td>788</td>
<td>762</td>
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<td></td>
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<tr>
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<td>691</td>
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<tr>
<td>567</td>
<td>666</td>
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<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **MWJ/t**
- **150**
- **13330**

### Tableau VIII

**Distribution radiale de la densité d'eau moyennée sur toute la hauteur du coeur en 10^23 noyaux/cm³**

<table>
<thead>
<tr>
<th></th>
<th>0,14212</th>
<th>0,14103</th>
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<th>0,14023</th>
<th>0,13378</th>
<th>0,13987</th>
<th>0,13358</th>
<th>0,13314</th>
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<td>0,14038</td>
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<td>0,13582</td>
<td>0,14174</td>
<td>0,13509</td>
<td>0,14113</td>
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<td>0,13469</td>
<td>0,14141</td>
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<td>0,14027</td>
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<td>0,13463</td>
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<td></td>
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<td></td>
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</tbody>
</table>

- **MWJ/t**
- **150**
- **13330**
Tableau IX
Valeurs des facteurs de multiplication calculés $k_{eff}$

<table>
<thead>
<tr>
<th>Burn-up MWJ/t</th>
<th>$k_{eff}$</th>
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</thead>
<tbody>
<tr>
<td>0*</td>
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<td>1000</td>
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<td>5000</td>
<td>0,994</td>
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<tr>
<td>10000</td>
<td>0,991</td>
</tr>
<tr>
<td>13300</td>
<td>0,990</td>
</tr>
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</table>

*sans xénon

Tableau X
Ecart en % Calcul-Expérience
sur la distribution radiale de puissance
début du cycle

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
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</thead>
<tbody>
<tr>
<td>-3,3</td>
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<td></td>
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</tr>
<tr>
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<td>-2,9</td>
<td>0,7</td>
<td>-2,0</td>
<td>1,7</td>
<td>-0,8</td>
<td>1,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-2,4</td>
<td>1,4</td>
<td>-1,2</td>
<td>1,9</td>
<td>-0,9</td>
<td></td>
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<td>-0,9</td>
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</tbody>
</table>

Tableau XI
Ecart en % Calcul-Expérience
sur la distribution radiale de puissance
fin de cycle

<table>
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<tr>
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<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
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<td>-1,6</td>
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<td>-0,8</td>
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<td>0,5</td>
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<td>0</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>0,7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Figure 1
Assemblage sans poison

Figure 2
Assemblage avec 8 poisons

Figure 3
Assemblage avec 12 poisons

- Tube d'Instrumentation
- Trou d'Eau
- Poison
Figure 4
Assemblage sans poison
Description du calcul à 6 cellules

1: Tube d'Instrumentation
2: Trous d'Eau

Figure 5
Assemblage avec poisons
Description du calcul à 8 cellules

1: Tube d'Instrumentation
2: Trous d'Eau
3: Poisons
Figure 6
Effet des contre-réactions thermohydrauliques sur la distribution axiale de puissance début du cycle 150 MWJ/t

Figure 7
Distribution axiale de la température combustible moyennée sur le cœur
Figure 8
Effet des contre-réactions thermohydrauliques sur la distribution axiale de puissance fin de cycle 13330 MWJ/t

---

Figure 9
Calcul sans contre-réaction à 150 (1) 5000 (2) 9812 (3) 13330 (4) MWJ/t
Figure 10
Calcul avec contre-réactions à 150(1) 5000 (2) 9812 (3) 13330 (4) MWJ/t

Figure 11
Effet des contre-réactions sur la distribution axiale des taux de combustion - fin de cycle 13330 MWJ/t
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Recognizing that, in most practical situations, the deviation of the XY flux-distributions at the various elevations of the core from those predicted by a synthesis solution are small, the core is modeled as a perturbation of the "base" reference situation calculated by the MERCATOR-XY nodal simulator. MERCATOR-Z operates on the macroscopic cross-sections, condensed in each Z plane, to solve the diffusion equation, in one dimension, in terms of XY averages of the flux at each Z level. The core model is pseudo 3-dimensional, to the extent that the cross-sections changes related to the various perturbing effects (water density, boron, xenon, Doppler and burn-up) are calculated for different compositions and in different axial regions of the core, and are condensed by means of the adjoint fluxes in order to account for the perturbation of the XY flux distributions. A distinctive feature is the solving of the diffusion problem simultaneously for direct and adjoint fluxes and for the importance distributions related to axial-offset, which are used in efficient digital controllers predicting critical boron concentration at the same time as rod positions satisfying imposed axial offset. The code also provides the axial bucklings to feed back into the XY simulator. Applications results on the Tihange reactor are presented.

1. INTRODUCTION

In most situations encountered in practical PWR core simulation, it is observed that the spatial flux distributions do not differ much from those resulting from simple multi-slices synthesis calculations. This was the starting point for modeling the core as a perturbation from its synthesis approximation. This simplified model aims at providing fast, yet accurate predictions of reactivity balances in static and Xe-transient situations, as well as an assessment of the power peak.

2. THE MODEL

The basic assumptions and features of the perturbation approach will be explained at best along a short description of the core model.

2.1. The reference, unperturbed base "0" of the core is that represent-
ed by the 2-groups diffusion, XY geometry, nodal simulator MERCATOR XY /1/.
A reduced representation of the base is formed, at each burn-up step, by the following results :

a. The set of base parameters: E0 (cycle exposure), TWO (average water tempera-
ture), PÆL0 (power), FÆG0 (average fluxes; G = 1/2 for fast/thermal flux).

b. The set SXÆG0 of flux-volume core averaged X-sections (G = 1/2 for fast/thermal
group, SX = SK for ÆX, SN for ÆY, SC for total group capture ÆC, SR for
removal ÆR, and SD for diffusion).
c. MERCATOR XY results are further condensed on compositions "C" grouping fuel assemblies of similar properties (for example, the successive batches of fuel). For each composition, the base file contains the composition distributions EOC (Exposure, O: base, Composition), FGOC (normalized fluxes), POC (normalized power), the composition radial bucklings BRGOC, and SXGOCV, the derivatives of SXG, calculated about the base 0 state of each composition C, with respect to the smoothly variable effects V (V = Exposure, DW: density of water, TU: temperature of fuel, θ:pron). These differential X-sections result from composition averaging by MERCATOR XY of the values supplied by LWR-WIMS /2/.

2.2. Any deviation \( \delta \) SXGC of a composition X-section from its base value is XY averaged by means of "statistical weights" WSKGOC:

\[
\delta \text{SXG} = \sum C \cdot \text{WSGOC} \cdot \delta \text{SXG} \tag{1}
\]

also calculated by MERCATOR XY from the condition that the averaging process keeps invariant the reactivity predicted by first order perturbation theory:

\[
\frac{\delta \text{SXG} \sum C \cdot \phi_1^{f} \phi_1^{a} \phi_2^{f} \phi_2^{a}}{2 \cdot \left( \phi_1^{f} \phi_2^{f} + \phi_1^{a} \phi_2^{a} \right)} = \frac{\delta \text{SXG} \cdot \text{FGO.FAKO}}{(\text{SM10.F10} + \text{SM20.F20}) \cdot \text{FA10}} \tag{2}
\]

The left member is the reactivity effect of \( \delta \) SXGC applied to the fuel assemblies \( \sum C \), calculated from the direct \( \phi_1^{f} \) and adjoint \( \phi_1^{a} \) fluxes; \( k \) is the number of the neutron balance equation in which SXG enters. The denominator is the total fission rate over the core, weighted by \( \phi_2^{f} \). The second member is the reactivity effect of \( \delta \) SXG in the point model of the base; FGO and FAKO are direct and adjoint fluxes of the base, calculated from the SXG set. WSKGOC is then simply the ratio \( \delta \text{SXG} / \delta \text{SXG} \) as taken from (2).

2.3. Smooth perturbations. The core is axially partitioned in broad regions "R" and the level VCR of the smoothly variable perturbations V (V = E, DW, Xe, BP, TU) are calculated in each partition CR of each composition. DWCR is calculated by enthalpy balance from current input parameters PREL, TW, from the volumetric flow rate QW, and with a simplified inter-composition mixing model. ECR is obtained by modulating the composition exposure increment \( \Delta \text{EOC} \) of the core burn-up step \( \Delta \text{EO} \) by the composition normalized power profile PCR (see later). The X-section deviations SXGCR associated to VCR are calculated from the base differential X-section:

\[
\text{SXGCR} = \text{SXGOCV} \cdot \text{VCR} \tag{3}
\]

The local flux FGCR is approximated by the synthesis (this is actually the main approximation of the model):

\[
\text{FGCR} = \text{FG} \cdot \text{FGOC} \cdot \text{FGR} \tag{4}
\]

where FG is the absolute flux, and FGR the normalized flux profile calculated (see 2.3.) on the axial model of the core.

Xe poisoning SC2XCR is calculated from local E- and DW- corrected X-sections and local fluxes FGCR. TUCR, entering into the Doppler effect, is taken from a simple model assuming that the mean fuel-to-water temperature drop is proportional to local power \( \text{POC.PCR} = \sum C \cdot \text{SKGCR.FG.FGCR} \). Because of the DW and E effects on the power X-section SKGCR, the power profile PCR is not necessarily the same in all compositions.

2.4. Sharp perturbations. The axially sharp perturbations introduced by the grids and control rods are applied directly on the axial representation of the core. The grids enter through fixed incremental X-sections SCFi defined on the fine diffusion i-mesh. The group bank GB of control rods is represented by a triplet (SC1GB, SC2GB, SRC1GB) of X-sections applied on the i-mesh (piston model) through mobile X-sections (SC1Mi, SC2Mi, SRC1Mi) depending on the group insertion steps into the core. The control rods triplets are effective X-sections adjusted for correctly reproducing SCZ, SRC (hence the flux ratio) and the eigenvalue when simulating the group introduction in MERCATOR XY. In addition, in order to mitigate the piston approximation, another set of profiles FGIC, PIC, BRGIC and statistical weights WSKGIC, calculated in a rodded MERCATOR XY is used for the rodded part of the axial model in order to better assess the perturbations in the presence of rods. Particularly the increased neutron leakage-to-rods effect on the water temperature coefficient is accounted for by rodded radial bucklings BRGIC which are larger than their base value BRGOC.
3. DIFFUSION PROBLEM

3.1. After XY averaging the smooth perturbations SXGVCR with the proper stat. weights WSKGNC (N = 0,1):

\[ SXGVR = \sum_C WSKGNC.SXGVCR, \]  

(5)

the base, smooth and sharp contributions are added together to form, on the i-mesh, the X-sections of the 2-group diffusion model:

\[ SXGi = SXGO + SXGFi + SXGHi + \sum_v SXGVR \]  

(6)

The axial reflectors are represented explicitly or, better, through logarithmic boundary conditions equivalent to transport albedos, like in MERCATOR XY.

3.2. The static diffusion problem is solved, on i-mesh, by a center-of-mesh finite-differences discretization. A purposely developed method solves the diffusion equations simultaneously for direct and adjoint fluxes, and uses an effective WIELANDT acceleration of the outer iterations.

An interesting feature of the code is obtaining, as a by-product of the critical diffusion problem, the importance distribution \( \Psi \) related to axial-offset \( A\Phi \). Let

\[ \kappa \phi = f \phi / \lambda \]  

(7)

be the 2-group matrix representation of the discretized diffusion equations. \( A\Phi \) is defined as a ratio of linear functionals of flux \( \phi \):

\[ A\Phi = \langle \mu \kappa, \phi \rangle / \langle \kappa, \phi \rangle \]  

(8)

where \( \kappa \) is the power operator and \( \mu = \pm 1 \) for i above or below the mid-plane of the core. Then \( \Psi \) is the solution of an adjoint non-homogeneous problem 3/\n
\[ \kappa^* \Psi = f^* \Psi / \lambda + (\mu - A\Phi) \kappa \]  

(9)

\( \Psi \) is obtained as the sum of a converging series \( \sum t \Psi^{(t)} \), the successive terms of which are calculated recursively from

\[ \kappa^* \Psi^{(t)} = (\mu - A\Phi) \kappa, \kappa^* \Psi^{(t+1)} = f^* \Psi^{(t)} / \lambda. \]

The inversion of \( \kappa^* \) makes use of the same factored, and WIELANDT-reduced matrix as for the critical problem, so that the series converges after a few terms. As a result, \( \Psi \) calculation takes only a marginally additional time.

3.3. The results of the critical diffusion problem are the direct and adjoint fluxes FGi and FAGi and the power Pi on the i-mesh. Conceptually these fluxes should be regarded as XY average of the fluxes in each Z plane. Region axial averages FGR are derived for synthesis purpose (4).

3.4. The adjoint fluxes FGAi enter into the calculation of i-wise statistical weights:

\[ WSKGI = FAKI.FGI / \sum_i (F1i.SN1i + F2i.SN2i) FA1i.\Delta Zi \]  

(10)

and region stat. weights WSKGR = \( \sum_{i,e} WSKGI. \Delta Zi \), which allow to evaluate any X-section change on the i-mesh (ex. : control rods) or on the CR partition in terms of reactivity:

\[ \delta \rho_{CR} = \delta SXGCR.WSKGNC.WSKGR.ASX \]  

(11)

where ASX = 1/\( \lambda \) for SX = SN, + 1 for SX = SR, and -1 for SX = SC.
These perturbation theory stat. weights are used for predicting critical boron or rod banks position, and all the reactivity coefficients. For example, the water temperature coefficient AMOTW is calculated by imposing 1K on TW, letting the thermo-hydraulic routine calculate the resulting density variation DWCR over the core, and integrating its reactivity effect by:

$$\text{AMOTW} = \sum_{x,c,r} \text{WSKGNC.WSKGR.SXGOC.DWCR.ASX}$$

(12)

All the X-sections are affected by the density, including the diffusion X-sections entering in (12) through terms SXGOC. BRGHC. This formulation neglects cross-effects of density change on Xe and fuel temperature distributions. The other reactivity coefficients AMOB (boron), AMOP (power), AMOT (fuel temperature) and AMOGB (control rods differential effectiveness) are obtained in the same manner.

3.5. $\psi$ distributions are used for predicting $\Delta \phi$ changes resulting from core perturbations by means of:

$$\delta \phi\nabla = \left[ \left< \delta \left( \mu \frac{1}{\alpha} \right) \phi, \psi \right> + \left< \left( \mu - \lambda \right) \delta \chi, \psi \right> \right]/\left< \chi, \psi \right>$$

(13)

where the second term gives the effect of $\delta \chi$ at constant $\phi$, and the first the perturbation theory correction due to $\delta \psi$.

$\Delta \phi$ and reactivity stat. weights are used in effective dual digital controllers allowing the prediction, after any core perturbation, of both critical boron and control bank position satisfying an imposed $\Delta \phi$.

4. MODES OF OPERATION

4.1. The code can operate in exposure mode or Xe-transient mode. In the first mode the exposure ECR is allowed to progress in each CR node but the Xe poisoning is calculated at equilibrium. In the second, ECR is frozen but Xe poisoning is calculated in transient condition for the successive input time-steps by solving analytically the I and Xe kinetic equation in each CR. In order to allow large burn-up or time-steps, the code uses a predictor-corrector method of solution.

4.2. For almost axially unstable conditions, great care must be taken in order to avoid excessive oscillations due to the feedback of physical effects on the flux distribution. The problem is taken care of by the classical under-correction procedure: if $\phi^{(n)}$ and $\phi^{(2)}$ are the last two iterates of the core distribution (fluxes or power), the physical effects are calculated from $\left< \left( \omega \left[ \phi^{(n-1)} \right] \left[ \phi^{(n)} \right] \right) \right.$, with $\omega$ empirically adjusted to minimize the number of feed-back iterations necessary to obtain converged consistent fluxes and physical effects distributions. For some problems, $\omega$ must be chosen as low as 0.3. This method, not fully satisfactory, could be improved by means of a modal analysis /4/ allowing to separate the transient mode. The second mode of the direct and adjoint problem have been purposely made available in the code.

5. EQUIVALENT AXIAL LEAKAGE CROSS-SECTION

5.1. It has been attempted to derive from the results of MERCATOR Z which corrections should be applied to the reference MERCATORY XY model in order to account for the axial effects on reactivity balance and XY distribution.

The reactivity equivalence principle is again used to evaluate the corrections: let SXGVR the deviation, from its base value, of any X-section SXG, due the effect V in node CR. The reactivity effect of V, integrated over the composition C is, according to (11):

$$\delta \phi_{V,C} = \sum_{x,r} \text{WSKGNC.WSKGOR.SXGCR.ASX}$$

(14)

but here, the region stat. weights WSKGOR may be calculated exactly from the direct flux of the axially uniform unperturbed base core, which is a known chopped cosine/tdal distribution, and the adjoint flux FAGi of the current perturbed core.
5.2. Let SLGOC be axially uniform increments to the composition group capture X-sections SCGOC of the base. SLGOC contribute to a reactivity change:

\[ \Delta \rho_{OC} = -(WS110C.WS110.SL10C + WS220C.WS220.SL20C) \]  \hspace{1cm} (15)

calculated from the unrodde base composition WS, and from the stat. weights WSGOC of the point model SXGO:

\[ WSGOC = FGO.FAKO / \left[ (SN10.F10 + SN20.F20).FA10 \right] \]  \hspace{1cm} (16)

5.3. The SLGOC accounting for the axial behaviour of V in composition C is then simply obtained by equalling the reactivity effects (14) and (15). Presently, such effective leakage X-sections are calculated only for the exposure ECR, which is the most composition-dependent effect. As only one equivalence relation is available, it has been selected to obtain SL20C by balancing separately the reactivity effect of SC2ECR, and SL10C by balancing the contribution of the other X-sections.

5.4. The contribution of the other effects, including axial leakage, are simply represented by constant axial bucklings BZG9 which force the neutron balance of the modified point model of the base:

\[
\begin{align*}
(SC10 + SL10 + SD10.BZ19) \quad F1 &= (SN10.F1 + SN20.F2)/\lambda \\
(SC20 + SL20 + SD20.BZ29) \quad F2 &= SR10.F1
\end{align*}
\]  \hspace{1cm} (17)

to the axial model results FG and \( \lambda \).SLG0 result from the averaging:

\[ SLG0 = \sum C WSGGOC.SLGOC. \]

6. APPLICATION RESULTS

Most of the experience with the code has been gained on following the Tihange reactor (WESTINGHOUSE-type PWR, 2650 MWth, 157 assemblies of 15 x 15 rods, 12 ft high, no partial-length rods). A few calculation results will be selected in order to assess the validity of the code or more exactly, of the LWR-WIMS-MERCATOR X-¥-MERCATOR Z chain.

6.1. Fresh core hot zero power (HZP) condition results are firstly selected to evaluate the model without feed-backs.

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Fig. 1 - Average axial profile for fresh core, HZP conditions.
Fig. 1 compares the predicted axial averaged power shape $P_i$ to the in-core measurement data. The selected i-meshing and R-partition are indicated. The grids fixed X-sections SCGFi are obtained by simply redistributing to the grids locations the axially averaged grid absorption X-sections calculated by LWR-WIMS. The axial reflectors are represented by logarithmic boundary conditions derived from a LWR-WIMS transport calculation of core-reflector interaction.

It is observed that the overall distribution is almost cosinusoidal and thus not very sensitive to reflector representation because the extrapolated length is small ($\sim 10 \text{ cm}$) with respect to core length. For purpose of comparison are also given $\lambda$ and power profiles for axially homogenized grids: it is observed that the flux depression into the grids is satisfactorily accounted for by non-axially self-shielded X-sections, and that the reactivity effect of explicit versus axially homogenized grids is 139 PCM.

6.2. The triplet "piston" representation of the control banks allow to reproduce correctly the shape of reactivity worth curves. The reactivity coefficients, obtained from perturbation theory are, within IPCM/°K the same as calculated by MERCATOR XY, and are also correctly (within 2 PCM/°K) predicted over the range of HZP test conditions.

6.3. Fig. 2 illustrates the use of the $A\Phi$ and criticality controllers. Starting from an unrodded condition, the first part of the problem shows an $A\Phi$ control within $\pm 1.5\%$ band around $-7.5\%$: the 36 steps insertion prediction by the controller is only 3 steps far from the correct insertion. The second part is a critical bank insertion search also terminated after two iterations.

![Critical Bank Insertion Control and $A\Phi$ Control](image)

Fig. 2 - Critical bank insertion control and $A\Phi$ control.

6.4. Fig. 3 simulates a Xe build-up test after shut-down from 50%, with criticality maintained by boron and control rods. Accurate simulation of core history prior to and during the test are mandatory for good simulation results: the results obtained when supposing equilibrium Xe as initial condition are likewise shown for comparison.
Fig. 3 - Poisoning evolution following shut-down.

Fig. 4 shows a simulation of a free Xe-oscillation test. The period and decay rate of the oscillation are satisfactorily predicted, but the amplitudes are underestimated; this may be attributed to the difficulty of restoring the exact actual core history prior to the test.

Fig. 4 - Simulation of free xenon oscillation test at cycle 1.
6.5. Fig. 5 gives, at nominal conditions, 12 steps control bank insertion, simulation results at beginning, middle, and end of first cycle. Contrarily to fresh HzP conditions, the results are here quite sensitive to the representation of core edges were exposure remains low and flux varies rapidly. Particularly, the diffusion meshing must be fine enough to follow the bump in thermal flux due to neutrons coming back to the core after slowing-down in reflector.

Except for a systematic over-prediction at core edges, the overall evolution of the power profiles over the cycle is correctly predicted. At first cycle, the shapes of in-core flux profiles in the various instrumented assemblies are pretty much the same, so that the flux synthesis assumption should not be bad.

Fig. 6 gives the prediction of critical boron and AΦ over the cycle 1.

---

Fig. 5 - Cycle 1 normalized axial profiles at BoC, MoC and EoC.

Fig. 6 - Cycle 1 boron concentration and axial off-set.
6.6. At the end of cycle 2, a 20 days stretch-out was performed.

Its simulation is a severe test imposed on the capability of the code to correctly perform a reactivity balance during this period when all the core parameters vary rapidly. The simulation, shown at fig. 7, was conducted in exposure mode, the measured relative power PREL, water temperature TW, and control bank position KGB being entered at the 3 exposure steps indicated, whilst AØ and critical boron are calculated by the code.

The AØ increase due to redistribution effects is well predicted; the indicated Xe-induced AØ oscillations are not simulated in exposure mode. The deviation of predicted critical boron remains constant (6 PPM) within about 2 PPM over the 15 days period whilst the reactivity released by temperature let-down was about 300 PPM.

![Graphs of RELATIVE POWER, WATER TEMPERATURE, BORON, and AXIAL OFF-SET](image)

Fig. 7 - Stretch-out simulation at end-of-cycle 2.

6.7. The behaviour of a typical reload core is now presented.

Fig. 8 gives, at beginning of cycle 3, the bunch of measured profiles (after intercalibration corrections) in the fresh assemblies, together with average of all profiles. Fig. 9 shows the same data for the one-year old fuel. Comparing the shape of individual profiles to the average one gives some feeling about the error linked to the flux synthesis assumption. In the present case, the error on Fq may be estimated to about 5%. Within the unrodded part of the core, where the peak generally occurs, the radial deformation of the XY flux map when moving axially is pretty smooth and depends primarily on local exposure and water density: perturbation theory could therefore be
extended to predict the XY deformation in terms of change of FGOC, considered (like AØ) as ratio of linear functionals of fluxes. The importance distribution associated with this ratio can be calculated, as for AØ, by a repetitive use of the same factored, and WIELANDT reduced matrix as used in the diffusion problem.

Fig. 8 - HFP, BOC 3 experimental U235 fission rate profiles in fresh assemblies

Fig. 9 - HFP, BOC 3 experimental U235 fission rate profiles in one year old assemblies.
Fig. 10 shows boron and AØ evolution over cycle 3, and Fig. 11 the axial profiles.

The equivalent leakage sections account correctly for the flattening of about 3 to 5% the XY power map resulting, a nominal condition, from the 3-D effects.

Fig. 10 - Boron concentration and axial-off-set during cycle 3.

Fig. 11 - Cycle 3. Normalized axial profiles at BOC, MOC and EOC.
6.8. Fig. 12 shows, at beginning of cycle 3, HZP, unrodded condition, the power profile, typically skewed towards the top. The calculated equivalent leakage X-sections are smaller than for nominal conditions because the central, high ECR part of the core is weighted by low adjoint flux, and at the top of the core, where the adjoint flux is high, the sinusoidal base flux is low. As few reliable low power level in-core maps are available, additional experience at HZP test conditions will be needed to assess the validity of the equivalent leakage X-sections model for these conditions.

![Graph showing HZP profile at beginning of cycle 3](image)

Fig. 12 - Unrodded, HZP profile at beginning of cycle 3.

6.9. Fig. 13 shows the simulation of a free Xe-oscillation test performed at beginning of cycle 3. The test conditions were cleaner than for the first cycle tests, and the prediction shows to be better.

![Graph showing free xenon oscillation test](image)

Fig. 13 - Simulation of free xenon oscillation test at BOC 3.
6.10 Finally, fig. 14 gives a typical end-of-cycle simulation of a load follow transient over 3 periods of load change. The target for this case was to minimize the boron variation (to reduce the effluents), with constraints on $A\theta$ and boron dilution rates. $F_z$ is equally indicated to illustrate the correlation between $A\theta$ and $F_z$. It is observed that the $A\theta$ constrain cannot be met during all the power recovery period.

Fig. 14 - Simulation of a load follow transient at end of cycle.
CONCLUSION

Designed as a low cost production code, MERCATOR Z results as a compromise between the conflicting requirements of performing reactivity balances in 3-D and avoiding true 3-D diffusion calculations. In spite of its simplified diffusion model it gives on the variety of core situations encountered in practice, good results in terms of reactivity balance, and an assessment of $F_q$ sufficient at design level.

Perturbation theory was systematically used to take profit of the valuable predictive information, obtained at marginal cost from the adjoint problem, to mitigate the synthesis approximation, and to design effective $A\Phi$ and criticality controllers which are very helpful in organizing the complex logics of the core simulation.

After a few years experience with the code, some areas of the model deserving improvement have been identified, for example: the handling of skin exposure effects, the treatment of physical and numerical instabilities by means of a nodal analysis, and the extension of perturbation theory for correcting the deviation from synthesis approximations.

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TWO-GROUP NODAL CALCULATIONS IN HEXAGONAL FUEL ASSEMBLY GEOMETRY

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The first year of operation of the Loviisa I reactor has been analyzed with the three-dimensional PWR-simulator HEXBU-3D, which is designed for the VVER-440 reactors. The program employs a real two-group nodal method to solve the diffusion equations in hexagonal fuel assembly geometry. The group fluxes are constructed from the asymptotic and transient spatial modes. Within nodes the former is approximated by third order polynomials and the latter by exponential functions. The method has been tested against two-dimensional fine-mesh calculations and against in-core measurements of the Loviisa I reactor. Though no tuning of input data was made the calculations agree well with measurements.

1. INTRODUCTION AND PROGRAM SUMMARY

The design of a fuel management code package for PWR-reactors began at the Technical Research Centre of Finland shortly after the start of construction of the first Finnish power reactor at Loviisa. The central part of the system is the three-dimensional PWR-simulator program HEXBU-3D/1/ which has been under continuous development for several years. The program is directly based on a similar two-dimensional program HEXBU/2/ which has been operational since 1974.

The main incentive for development of an own simulator program from the beginning were the special features of the core of the Novo-Voronesh type reactor VVER-440. Unlike other PWR-reactors the core consists of hexagonal fuel assemblies with shroud tubes and intervening water gaps as in BWR-reactors. Control rods consist of flux trap absorber assemblies connected to follower fuel assemblies, which are expelled from the core when the absorbers are inserted.

The goal of the program development has been the capability to calculate segmentwise average flux and power distributions in reasonable computer time with an accuracy comparable to fine-mesh finite-difference calculations in two neutron energy groups. Therefore HEXBU-3D performs a true two-group solution to the diffusion theory equations within the reactor core. In the nodal method of the program the axial segments of fuel assemblies are described by homogenized nodes having the shape of hexagonal prisms.

The two-group equations are treated within each node by analytical theory in a manner similar to that e.g. in references /3/ and /4/. The group fluxes are combined from two characteristic solutions, separable in space and energy, which are called the fundamental (or asymptotic) and transient modes of the solution. The spatial shapes of the two modes are approximated by third order polynomials and exponential functions within nodes.
A two level iteration technique is applied in the solution of the flux and power distributions. In inner iterations only the average flux values over nodes are considered and in outer iterations the internal flux shapes within nodes are improved. Such an iteration scheme has proved to be very efficient in both two- and three-dimensional calculations.

HEXBU-3D has a treatment of the feedback effects from Xenon-poisoning, fuel and moderator temperature and moderator density. Either the concentration of soluble boron in the moderator or effective multiplication factor can be directly iterated as the eigenvalue of the problem. Reflectors of the core and inserted control absorbers occupying full nodal cross sections are described by either of two types of boundary conditions, extrapolation distances or albedo matrices.

The water gaps between assemblies tend to isolate the assemblies neutronically from each other. Thus an indirect burnup calculation, where the isotopic burnup equations are solved in advance in cell calculations, is suitable for this type of reactor. HEXBU-3D integrates the nodal powers into nodal average fuel burnups and makes use of tabulated sets of burnup-dependent two-group data from cell calculations.

2. PRINCIPLES OF CALCULATION METHOD

2.1 The two-group flux model

Basic equations

The basic two-group equations solved in HEXBU-3D are within each node of the form

\[-D_1 \nabla^2 \phi_1(\vec{r}) + (\Sigma_{a1} + \Sigma_{12}) \phi_1(\vec{r}) = \frac{1}{k} [\nu \Sigma_{f1} \phi_1(\vec{r}) + \nu \Sigma_{f2} \phi_2(\vec{r})] \]

\[-D_2 \nabla^2 \phi_2(\vec{r}) + (\Sigma_{a2} + C_B \Sigma_{aB}) \phi_2(\vec{r}) = \Sigma_{12} \phi_1(\vec{r}), \]

where $C_B$ is the concentration and $\Sigma_{aB}$ the absorption cross section per unit concentration of boron in the moderator and other symbols have standard meanings. The boron absorption is shown explicitly, because instead of the effective multiplication factor the concentration $C_B$ can be (and in fact usually is) the criticality parameter or eigenvalue of the problem.

Analytical modal theory

For the benefit of the less familiar reader we review here the main features of the well-known analytical theory for finding the general solution to the coupled set of differential equations (1) with constant coefficients. Let us consider equations (1) as a matrix equation for the group fluxes:

\[
\begin{bmatrix}
-D_1 \nabla^2 + \Sigma_{a1} + \Sigma_{12} & \frac{1}{k} \nu \Sigma_{f1} \\
-\Sigma_{12} & -D_2 \nabla^2 + \Sigma_{a2} + C_B \Sigma_{aB}
\end{bmatrix}
\begin{bmatrix}
\phi_1(\vec{r}) \\
\phi_2(\vec{r})
\end{bmatrix}
= 0.
\]

(2)

We search for characteristic solutions to equation (2), separable in space and energy, of the form

\[
\begin{bmatrix}
\phi_1(\vec{r}) \\
\phi_2(\vec{r})
\end{bmatrix}
= f(\vec{r})
\begin{bmatrix}
\psi_1 \\
\psi_2
\end{bmatrix},
\]

(3)

where $f(\vec{r})$ is a common spatial mode for both groups and the constants $\psi_1$ and $\psi_2$ define a spatially constant energy spectrum. Equation (2) can have solutions of the form (3) provided that $f(\vec{r})$ satisfies the Helmholtz equation
Making use of the relation \( \nu^2 f(\mathbf{r}) = -B^2 f(\mathbf{r}) \) upon substitution of the trial solution (3) into equation (2) enables to eliminate \( f(\mathbf{r}) \) altogether, leaving the purely algebraic equation

\[
\begin{bmatrix}
(D_1 B^2 + \Sigma_{a1} + \Sigma_{12} - \frac{1}{k}\nu\Sigma_{f1}) & \left(-\frac{1}{k}\nu\Sigma_{f2}\right) \\
(-\Sigma_{12}) & (D_2 B^2 + \Sigma_{a2} + C_{B}\Sigma_{B})
\end{bmatrix}
\begin{bmatrix}
\varphi_1 \\
\varphi_2
\end{bmatrix}
= 0.
\]

(5)

This homogeneous set of equations for the constants \( \varphi_1 \) and \( \varphi_2 \) has a solution provided that \( B^2 \) is such that the determinant of the matrix vanishes. Separating the matrix into \( k \)-terms and the diagonal \( B^2 \)-terms we can represent equation (5) by the general matrix form

\[(\xi + B^2 D)\varphi = 0 \text{ or } (-\xi^{-1} D)\varphi = B^2 \varphi.\]  

(5')

Thus, formally, the characteristic bucklings \( B^2 \) are the eigenvalues and the characteristic spectra \( \varphi \) are the eigenvectors of a matrix \( D^{-1} \Sigma \) dependent on the material properties only - including the system \( k \) and \( C_B \).

The algebraic solution of the two-group system (5) will not be reviewed here. There are two characteristic bucklings, \( B_1 \) and \( B_{11} \), defining two spatial modes, \( f_1(\mathbf{r}) \) and \( f_{11}(\mathbf{r}) \), via the Helmholtz equation (4). Both modes are accompanied by characteristic spectra (flux ratios), e.g. \( R_1 \) and \( R_{11} \) with \( R = \varphi_2/\varphi_1 \).

The general solution to equation (2) is a linear combination of the separable solutions. Since \( f_1(\mathbf{r}) \) and \( f_{11}(\mathbf{r}) \) can in themselves contain an arbitrary constant, we can write without loss of generality

\[
\begin{bmatrix}
\phi_1(\mathbf{r}) \\
\phi_2(\mathbf{r})
\end{bmatrix}
= f_1(\mathbf{r}) \begin{bmatrix} 1 \\ \end{bmatrix} + f_{11}(\mathbf{r}) \begin{bmatrix} 1 \\ R_1 \\ R_{11}
\end{bmatrix} = f_1(\mathbf{r}) \begin{bmatrix} 1 \\ \end{bmatrix} + f_{11}(\mathbf{r}) \begin{bmatrix} 1 \\ R_1 \\ R_{11}
\end{bmatrix}
\]

(6)

A particular solution to the Helmholtz equation is determined e.g. by prescribing boundary values on the surface \( S \) of a closed volume. Now, if some arbitrary boundary values for the group fluxes are prescribed on \( S \), then unique boundary values for the spatial modes are determined by the algebraic set (6) with \( \mathbf{r} \) on \( S \), and hence unique particular solutions \( f_1(\mathbf{r}) \) and \( f_{11}(\mathbf{r}) \) are defined. This demonstrates the generality of the modal solution (6).

The mode \( f_1(\mathbf{r}) \), corresponding to an all-positive energy spectrum (positive \( R_1 \)), is termed the fundamental or asymptotic mode. The buckling \( B_1 \) is relatively small in magnitude and corresponds to the conventional material buckling - due credit being given to the system \( k \) and \( C_B \). In a light water reactor \( (L_1^2 \gg L_2^2) \) the buckling \( B_{11} \) is large and negative, roughly \( -1/L_2^2 \).

The mode \( f_{11}(\mathbf{r}) \) is a transient mode which deviates significantly from zero only near discontinuities in material properties, especially in \( \Sigma_{B} \). It is of opposite sign in the fast and thermal groups and its magnitude relative to the fundamental mode is greater in the thermal group than in the fast group by about a factor of 12 to 16. Yet the transient fast group countercurrent typically exceeds the transient thermal current in magnitude, representing strong local leakage of fast neutrons (see Figure 1).

Modelling of the spatial modes

Slow variations of the fundamental mode within modes suggest a polynomial approximation for \( f_1(\mathbf{r}) \). In HEXBU-3D this is assumed separable in the transverse and axial directions within each mode. Referring to the coordinate system of Figure 2 the fundamental mode is written as

\[
f_1(\mathbf{r}) = A f_{xy}(x_1, x_2, x_3) f_z(z)
\]

(7)
Figure 1. Two-group modal flux model of HEXBU-3D

Figure 2. Nodal coordinate systems
where A is an amplitude factor and \(x_1 x_2 x_3\) are coordinates with hexagonal symmetry in the transverse plane and \(x_1 x_2 x_3\) are Cartesian coordinates. The transverse and axial parts of the mode are approximated by symmetric third order polynomials.

\[
\begin{align*}
 f_{xy}(x_1, x_2, x_3) &= 1 + \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 \\
 &\quad + \beta_1 x_1^2 + \beta_2 x_2^2 + \beta_3 x_3^2 \\
 &\quad + \gamma_1 x_1^3 + \gamma_2 x_2^3 + \gamma_3 x_3^3 \\
 f_z(z) &= 1 + \alpha_4 z + \beta_4 z^2 + \gamma_4 z^3,
\end{align*}
\]  

(8a)  

\[ (8b) \]

where \(\alpha_i, \beta_i, \) and \(\gamma_i\) are coefficients to be determined. Insertion of (7) into the Helmholtz equation (4) leads to two similar equations with transverse and axial bucklings \(B_{xy}^2\) and \(B_z^2\) of the fundamental mode. These are determined iteratively during the calculation from the current flux shape and from the condition

\[ B_{xy}^2 + B_z^2 = B_1^2. \]

Obviously, the coordinates \(x_1, x_2\) and \(x_3\) are linearly dependent and we can impose an arbitrary condition on the linear term coefficients, e.g.

\[ \alpha_1 + \alpha_2 + \alpha_3 = 0. \]

This leaves only eight degrees of freedom in the expression for \(f_{xy}\). That is one degree less than a corresponding full third order polynomial would have in two dimensions, but the missing one degree of freedom in (8a) does not contribute to the solution of average values in nodes. Thus the approximation of the fundamental mode flux includes in effect 12 unknown parameters for each node.

The dimensions of the nodes (about 15 cm for the VVER-440 reactor) are considerably larger than the relaxation length of the transient mode. A suitable approximation is to describe the average behaviour of the transient at each of the eight surfaces of a node by the exponential solution of a one-dimensional situation in plane geometry. The required integral properties of the transient mode are then defined by eight parameters - the average amplitudes of the mode at the nodal surfaces.

The two-group flux model in HEXBU-3D contains altogether 20 parameters per node. In order to solve them an equal number of relations must be set up. A consistent choice for the model is the requirement of continuity of average flux and current across the eight nodal interfaces in both energy groups, which offers 16 relations per node. The remaining 4 relations arise from necessary conditions that are imposed on the coefficients of the fundamental mode to make the approximation (8) represent a general solution of the Helmholtz equation with fundamental mode buckling. Integrated residuals of the equation are required to vanish. Thus the original two-group problem is, in principle, reduced to a set of equations with 20 unknowns and 20 equations per node to be solved together with the problem eigenvalue.

2.2 Nodal iteration method

The two-level iteration scheme in HEXBU-3D consists of inner and outer iterations. The global flux distribution of the reactor core is adjusted in inner iterations with one unknown per node using nodal coupling coefficients based on approximately known flux shapes within nodes. During outer iterations the nodal flux shapes and hence the coupling coefficients are improved. The diffusion parameters are also recalculated at the same time to include the reactivity feedback effects due to actual flux and power distributions.

The continuous two-group diffusion equations (1) can be easily converted into formally exact nodal balance equations for average fluxes and currents by integration over the nodal volumes - consistent with the original model.
\[ \sum_{j=1}^{8} S_{ij} j_{ij}^{i+j} + V^{i}(\Sigma_{a1} + \Sigma_{12}^{i}) z_{ij} = \frac{1}{k} V^{i}(\nu_{f1}^{i} z_{ij}^{f1} + \nu_{f2}^{i} z_{ij}^{f2}) \]  

\[ \sum_{j=1}^{8} S_{ij} j_{ij}^{i+j} + V^{i}(\nu_{a1}^{i} + C b^{i}) z_{ij} = V_{12}^{i} z_{ij}^{1} . \]

\( z_{ij}^{f1} \) and \( z_{ij}^{f2} \) are the average flux in node \( i \) and the average net current density from node \( i \) into node \( j \) in energy group \( g \); \( V^{i} \) and \( S_{ij} \) are the volume of node \( i \) and the area of the interface between nodes \( i \) and \( j \).

The heart of the nodal iteration scheme then becomes the estimation and improvement of the internodal current densities - again consistent with the original model. We assume to know an approximate shape for the fundamental mode in two adjacent nodes, and in particular the averages of the functions and the normal derivatives at the interface. We further introduce a pure tilt term of the general fundamental mode solution into both nodes to account for a variable macrogradient between the nodes. Then, applying the complete average continuity conditions for the interface fluxes and current densities in both groups will ultimately yield a set of four equations containing the interface quantities - both fluxes and currents - and the fundamental mode amplitudes in the two nodes. Hence, all the interface quantities can be solved in terms of the fundamental mode amplitudes or, equivalently, their nodal averages. In particular, the current densities can be represented as

\[ j_{ij}^{g} = k_{1}^{ij} z_{ij}^{g} - k_{2}^{ij} z_{ij}^{g} ; \quad g = 1, 2 . \]  

Insertion of expressions (10) into equations (9) and adding them together yields the one group difference equations

\[ (\sum_{j=1}^{8} S_{ij} k_{ij}^{j}) f^{i}_{1} - (\sum_{j=1}^{8} (S_{ij} k_{ij}^{j} z_{ij}^{j}) + V^{i}(\Sigma_{a1}^{i} + C b^{i} z_{ij}^{1}) z_{ij}^{1} = \frac{1}{k} V^{i} \nu_{f1}^{i} z_{ij}^{f1} . \]

where \( k_{ij}^{j} = k_{1}^{ij} + k_{2}^{ij} \) and the cross sections bearing an asterisk are of the form

\[ \Sigma_{i}^{*} = \frac{\Sigma_{i}}{z_{ij}^{i}} + \frac{\Sigma_{i}^{f1}}{z_{ij}^{f1}} \]

The spectral effects are accounted for by recalculation of the cross sections (12) in each outer iteration. The coupling coefficients are derived during outer iterations from the approximate nodal flux shapes defined by the average values of the fundamental mode from the previous inner iteration. In practice the parameters of the flux model within nodes need not be explicitly calculated. The evaluation of the coupling coefficients is the most time-consuming part of the whole iteration and it takes roughly three quarters of the total running time.

For inner iterations equation (9) is further reduced to a simplified form

\[ (\sum_{j=1}^{8} k_{ij}^{j} + \Sigma_{a}^{i} + \lambda \Sigma_{a}^{i}) f^{i}_{1} = \sum_{j=1}^{8} k_{ij}^{j} f^{j} . \]

The formal cross sections \( \Sigma_{a} \) and \( \Sigma_{a}^{i} \) have different expressions depending on whether the criticality parameter is the boron concentration or the effective multiplication factor and the eigenvalue \( \lambda \) is equal to \( C_{b} \) or \( -1/k \), respectively. In the line over-relaxation iteration the nodes are swept along axial channels or one fuel assembly at a time using always the latest iterates on the right side of equation (13). The eigenvalue is evaluated from the total neutron balance in the reactor. Convergence is typically reached in 40-60 inner iterations and 4-6 outer iterations.
2.3 Calculation of burnup

Burnup calculations are performed in an implicit way i.e. the program makes use of tabulated sets of burnup-dependent cross sections evaluated by a cell burnup program. The calculation consists of successive iteration of the flux and power distributions and integration of nodal burnups between them. The integration is carried out by a semicorrector method which allows fairly long burnup steps to be taken without cumulating burnup errors.

At the beginning of a burnup step the power distribution is extrapolated node by node from the present and preceding distributions (if any) to the end of the step. Burnup increments of nodes are integrated assuming linear behaviour of the power during the time step. A new power distribution is then calculated using the estimated nodal burnups. Since obviously the result does not coincide with the extrapolated power distribution, the burnup increments of the step are corrected according to the calculated nodal powers. However, another power distribution is not calculated with the corrected burnups except optionally for the first step when extrapolation of powers is not possible.

As a test of the method the reactivity life time of the first core of the Loviisa I reactor was calculated with burnup steps of 50 and 100 days (6 and 3 steps, respectively). The difference turned out to be a fraction of a day of reactor operation and the assembly powers and burnups agreed within 1%. Thus the method offers a considerable saving in computer costs, because the corrected burnup integration adds a negligible contribution to the total running time.

3. CALCULATION RESULTS

3.1 Comparison with fine mesh calculations

HEXBU-3D has been tested against detailed two-dimensional calculation in the transverse plane. Real fine-mesh (one mesh point per thermal diffusion length) two-group calculations in three dimensions were not possible. The accuracy of the axial description of the flux has been studied by varying the heights of nodes in three-dimensional calculations. However, due to the assumption on the transient mode flux the heights cannot be reduced to less than a few thermal diffusion lengths.

The two-dimensional comparison was made with the multigroup diffusion theory program TRIGON /5/. The test problem was the initial core of the Loviisa I reactor containing fuel assemblies of three different enrichments. The problem had exactly the same formulation for both programs: homogenized fuel assemblies with the same two-group cross sections, side reflector described by extrapolation distances (8 cm in both energy groups) and no power-dependent feedback effects, because TRIGON does not treat them. The mesh spacing in the finite-difference calculation was 1.7 cm which should ensure a sufficiently accurate diffusion theory solution to the problem.

The results are shown in Figure 3 as percentage differences of average assembly powers between HEXBU-3D and TRIGON solutions for a 30° sector of the Loviisa I core. HEXBU-3D seems to overpredict slightly the powers near the periphery of the core because of a global tilt of about 2%. Although a flat power distribution is very sensitive to small changes in reactivity, the reason for the tilt is somewhat unclear. According to further calculations it corresponds to a reduction of 0.2 cm in extrapolation distances or 0.3% in production cross sections of the most reactive assemblies. If the tilt is removed the maximum difference in assembly powers will be less than 1% and especially in the central region of the core it will be as low as 0.2%.

A three-dimensional configuration similar to Figure 3 was used to test the axial model of the program. Axial asymmetry was created by partial insertion of one control assembly group and by treatment of thermo-hydraulic feedback effects. The problem was run with three different node heights of 25, 12.5 and 6.25 cm. As Figure 4 shows, the deviation between the average axial power distributions of the first and third cases is very small, less than 1% of the mean. The assembly powers of all cases agreed to 0.2% and the differences between the two lowest node heights practically vanished. Thus a node height
HEXBU-3D $k = 1.0050$
TRIGON $k = 1.0047$

Fuel enrichment

Relative assembly power by HEXBU-3D
Deviation from fine-mesh solution, %

Figure 3. Comparison of assemblywise power distribution calculated by HEXBU-3D with fine-mesh finite-difference solution.
Figure 4. Comparison of average axial power distributions calculated with different node heights.
Figure 5. Loading pattern of Loviisa-1 initial core for 60° sector.
of 25 cm or ten nodes per fuel assembly for the VVER-440 core gives an accuracy which is consistent with that for the transverse direction.

3.2 Comparison with in-core measurements

Comparisons with experimental data obtained from the in-core instrumentation of the Loviisa-1 reactor during the first cycle of operation are presented. The fuel loading pattern of the initial core is given in Figure 5. The configuration possesses, in fact, 30 degree symmetry. A wide range of fuel enrichments - 1.6, 2.4 and 3.6 percent - are employed. At several locations the lowest and highest enrichments are located adjacent to each other implying large transient mode fluxes arising from large differences in thermal absorption properties (approximately 1:1.5).

The in-core instrumentation system of the Loviisa-1 reactor consists of two extensive sensor systems. First, there are 210 core outlet thermocouples in the flow exit channels of fuel assemblies, which number 349 in total. These thermocouples enter the reactor vessel from the top. Secondly, there are 36 self-powered neutron detector assemblies, each containing four local 25 cm long rhodium detectors and one full core length vanadium detector. These detector assemblies are inserted into the central instrumentation thimbles of the hexagonal fuel assemblies. They also enter the reactor vessel from the top and include a core inlet thermocouple at their tip.

The two-group data used in the calculations reported here has been generated by the grand old METHUSELAH II cell burnup code /6/ with some minor modifications, including the METHUSELAH III library. The modifications pertain mainly to the specific geometric aspects of the VVER-440 lattice and some adjustments of data derived from classical "Yankee Core I" comparisons. Boundary conditions at different reflector and absorber interfaces have been calculated applying 1-dimensional geometry and typically an $S_4$ transport approximation. All data can be considered as unadjusted to the Loviisa-1 reactor.

The comparisons presented include the assemblywise power distributions and axial power distributions at the beginning and end of Cycle 1, as well as the critical boron concentration during the cycle.

Assemblywise power distributions

Figures 6 and 7 compare HEXBU-3D calculated assemblywise power distributions with measured power distributions based on the core outlet temperature measurements, assuming equal flow through the assemblies and constant core inlet temperature. In both cases the reactor power is about 90 % of the nominal 1375 MW. The core average burnup is about 1300 and 9400 MWD/MTU for the BOC1 and EOC1 cases, respectively. In the BOC1 case the regulating control rod group (locations 1 and 7) is 30 % inserted.

Each measured value has been averaged over symmetric locations and is thus supported by 4 to 10 independent measurements. The standard deviation of the individual measurements within a symmetry group is typically 2 % increasing to 5 % in the extreme peripheral low-power assemblies. Hence, the averages should have standard deviations from less than 1 % up to 2 %, respectively.

The deviations from measurements are typically less than 2 % with extreme peripheral deviations less than 5 %. The powers in the peripheral assemblies tend to be slightly overestimated. Power ratios of adjacent assemblies of differing enrichment are reasonably well predicted. Despite the changes that take place in the assemblywise power distribution during the cycle, the deviations at BOC1 and at EOC1 remain strikingly similar. This is also apparent in the overall statistics by enrichments:

<table>
<thead>
<tr>
<th>Enrich.</th>
<th>Average deviation, %</th>
<th>Number of measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.6 %</td>
<td>-1.0</td>
<td>106/105</td>
</tr>
<tr>
<td>2.4 %</td>
<td>-0.1</td>
<td>52/53</td>
</tr>
<tr>
<td>3.6 %</td>
<td>+2.4</td>
<td>50/50</td>
</tr>
</tbody>
</table>
LOVIISA-1
KXX 77-05-02 (BOC1)
HEXBU-3D
YQ30T (FLOMIX 05)

Location number in 60° sector
Relative assembly power by HEXBU-3D
Deviation from measurements, %

Figure 6. Comparison of assemblywise power distribution calculated by HEXBU-3D with measured distribution based on core outlet temperature measurements of Loviisa-1, beginning of cycle 1.
Figure 7. Comparison of assemblywise power distribution calculated by HEXBU-3D with measured distribution based on core outlet temperature measurements of Loviisa-1, end of cycle 1.
These deviations, although small, are statistically significant relative to the basic scatter of measurements within symmetry groups.

There is one crucial point about interpreting the core outlet temperature measurements that should be mentioned here. There exists some doubt as to whether the coolant at the outlet thermocouple is completely mixed or not. This is roughly equivalent to whether the thermocouple feels the complete transient mode power contribution or only a part of it. In the presented comparisons the thermocouple is assumed to feel half of the transient mode power, because this assumption markedly improves the agreement of the measured and calculated power ratios of adjacent fuel assemblies, especially where large interassembly transients occur. However, we do not have complete faith in this hypothesis. An alternative explanation would then have to considerably reduce the interassembly transients in the model without disturbing the fundamental mode solution and hence the good overall agreement.

Axial power distributions

Figures 8 and 9 give comparisons of axial power distributions calculated by HEXBU-3D with rhodium detector measurements for selected locations in the BOCl and EOCl cases. The rhodium detector signals from different elevations must be corrected prior to comparison for a number of effects, including fuel and detector burnup, cable background signal and individual sensitivity of the detector. Since the detector readings represent an average over the nodal height (25 cm), the comparisons are made with interpolated nodal values obtained from the HEXBU-3D results by third order interpolation for the individual detector elevations. Independent normalization of the measurements have been made at each location.

The selected locations cover different radial locations, proximity to control rods and different enrichments. The deviations from measurements are typically less than 2% in both cases despite the marked change in the distributions during the cycle.

Reactivity and cycle length

Figure 10 gives a comparison with measured data of the critical boron concentration calculated by HEXBU-3D in a simulation of the first operating cycle. The simulation was carried out in 12 steps characterized by reactor power level, regulating control rod group position and core inlet temperature. The typical step was about 1000 GWh or about 30 full power days. Shorter steps were used to cover the plant start-up phase.

Except for some deviations during the irregular start-up period, agreement between calculation and measurement is very good up to about 7000 GWh. Subsequent raising of the control rods seems to bring about a small discrepancy which persists to the end of the cycle. During the last step the reactor operating parameters are set to match the shutdown conditions. At 9400 GWh or 285 full power days 26 ppm of boron remain in the calculation. This is equivalent to an error of about +3.5% in the cycle energy.

3.3 Summary of comparisons

The comparison of HEXBU-3D with a fine-mesh solution and the internal check obtained by varying the axial node height within HEXBU-3D demonstrate that the code is solving the two-group diffusion problem with sufficiently high accuracy.

The comparisons with measured data for the first cycle of the Loviisa-1 reactor show that HEXBU-3D together with the unsophisticated METHUSELAH data is providing a good description of reality. An issue somewhat in doubt is the correct interpretation of the Loviisa-1 core outlet thermocouple readings, which is intimately connected with the degree of agreement between HEXBU-3D calculations and measurements.
REFERENCES

/1/ E. Kaloinen, R. Teräsvirta: "HEXBU-3D, a Three-Dimensional PWR-Simulator Program for Hexagonal Fuel Assemblies", to be published in report series of Nuclear Engineering Laboratory, Technical Research Centre of Finland.


Figure 8. Comparison of axial power distributions calculated by HEXBU-3D with in-core neutron detector measurements (Rh-SPND's) of Loviisa-1, beginning of cycle 1.
Figure 9. Comparison of axial power distributions calculated by HEXBU-3D with in-core neutron detector measurements (Rh-SPHD's) of Loviisa-1, end of cycle 1.
Figure 10. Comparison of boron concentration from HEXBU-3D with measured data for Loviisa-1, cycle 1.
DEVELOPMENT AND QUALIFICATION OF THE

3 D SYNTHESIS METHOD

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ABSTRACT

The synthesis method is currently used in the safety evaluations, for the prediction of the maximum axial power shape and the hot channel factor.

A generalized synthesis method developed in FRAMATOME is presented. It takes into account some 3D corrections, and gives a good agreement when compared to 3D diffusion calculations or measurements. This very cheap computational tool is therefore very useful, in addition to the real 3D calculations. It will be used in FRAMATOME's new Digital Protection System.
1. INTRODUCTION

Les Études de Pilotage et les Études de Capacité de Puissance nécessitent le calcul d'un très grand nombre de distributions de puissance tridimensionnelles, en condition normale et accidentelle. Compte tenu des différents cycles, instants dans le cycle, transitoires lents avec évolution du Xénon et transitoires rapides avec ou sans cinétique, le nombre de pas de calcul se chiffre en milliers. Ceci exclut l'usage de calculs 3D directement. Les calculs sont alors effectués en 1D axial et 2D radial. La méthode de synthèse permet d'obtenir, pour un coût très faible, la distribution 3D dont on extrait en général le facteur total de point chaud $F_0$, le facteur d'élévation d'enthalpie $F_AH$.

Cette méthode est également utilisée par FRAMATOME dans les Protections du CP3.

Une méthode de synthèse généralisée a été développée. Elle permet une bonne comparaison avec des distributions de puissance mesurées en réacteur et avec des distributions calculées par un code 3D. L'utilisation de certaines valeurs issues de calculs 3D, ou de mesures, est un des éléments importants.

2 - MÉTHODE DE SYNTÈSE

2.1. Notations

Il importe avant tout de bien définir les notations. Dans tous ce qui suit, on appellera :

$P(x,y,z)$ la distribution de puissance relative dans le cœur elle est normée à 1 $\frac{\int P(x,y,z) \, dv}{\int dv} = 1$

$F_z$ la distribution axiale de puissance moyenne

$\bar{P}(z) = \frac{\int_{x,y} P(x,y,z) \, dx \, dy}{\int_{x,y} dx \, dy}$

$P_r(x,y,z)$ la distribution radiale relative de puissance à la cote $z$ $P_r(x,y,z) = \frac{P(x,y,z)}{\bar{P}(z)}$

(il s'agit là d'une définition)

$F_Q$ le facteur de point chaud

$= \text{Max} \{P(x,y,z)\}$

$x.y.z$

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$Q(z)$  la distribution axiale de puissance maximale  

\[ = \max_{x,y} \left\{ \bar{P}(x,y,z) \right\} \]

$F_{xy}(z)$  le facteur radial de point chaud à la cote $z$  

\[ = \max_{x,y} \left\{ \bar{P}_z(x,y,z) \right\} \]

$P_{\Delta R}(x,y)$  la distribution radiale d'élavation d'enthalpie  

\[ = \frac{\int P(x,y,z) \, dz}{\int dz} \]

$F_{\Delta R}$  le facteur d'élavation d'enthalpie  

\[ = \max_{x,y} \left\{ P_{\Delta R}(x,y) \right\} \]

2.2.  **Hypothèses de la méthode de synthèse simplifiée :**

Nous avons, par définition :  

\[ P(x,y,z) = P_z(x,y,z) \times F(z) \]

On peut faire la constatation suivante, qui peut être appuyée sur des raisonnements théoriques et/ou sur des résultats de calculs 3D et mesures :  
Il y a généralement, dans un cœur type PWR, bonne séparation des variables $(x,y)$ et $z$. Ceci conduit au fait que les distributions radiales relatives de puissance sont sensiblement constantes à l'intérieur d'une même "tranche" du réacteur. La figure 1 illustre bien un cœur où existent deux tranches : la tranche sans barres et la tranche avec barres. On aura donc sensiblement :  

\[ P_z(x,y,z) = P_{z1}(x,y) \text{ pour } z < z_0 \]

\[ = P_{z2}(x,y) \text{ pour } z > z_0 \]

où $z_0$ est la cote de position des barres, que l'on appellera "interface" entre les tranches 1 et 2.

On constate de plus que les distributions radiales relatives à l'intérieur d'une même tranche sont sensiblement indifférentes aux variations de niveau de puissance, de niveau et de distribution de Xénon.

Ces constatations étant faites, elles autorisent le calcul des distributions radiales relatives de puissance par un code 2D XY ; on prendra toutefois soin d'ajouter des incertitudes pour tenir compte des approximations faites.

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De la même façon, la distribution axiale de puissance moyenne $\overline{P}(z)$ peut être calculée avec un code 3D. Cette hypothèse est valable dans les cas où il n'y a pas de dissymétrie radiale importante dans le cœur. Noter que l'on ne fait pas l'hypothèse que les distributions axiales relatives de puissance sont les mêmes dans chaque crayon ! Elles ne le sont d'ailleurs pas, comme le montre la figure 2.

Cette hypothèse est confirmée par des calculs 3D et par l'expérience acquise en centrale.

La méthode de synthèse est couramment utilisée pour calculer $Q(z)$. Les considérations précédentes conduisent à :

$$Q(z) = F_{xyi} \times \overline{P}(z)$$

où $F_{xyi}$ est le facteur radial constant applicable à la région $i$, la région $i$ étant déterminée pour la configuration des grappes existant à la cote $z$.

Cette méthode est illustrée dans la figure 3.
Figure 2: Taux de réaction mesuré dans différents canaux.
FIGURE 3 - ILLUSTRATION DE LA MÉTHODE DE SYNTHESE SIMPLIFIÉE et généralisée
CALCUL DE Q(z)
En fait, en regardant les choses de plus près, on s'aperçoit que les hypothèses faites ne sont pas strictement respectées, comme on le verra au paragraphe 2.3. Pour pallier cette déficience, l'utilisation de facteurs radiaux de conception est très utile.

L'utilisation de ces valeurs permet la réalisation de calculs génériques pour un type de centrale donnée. Il suffira alors de vérifier que, dans la réalité, $F_{xy1}(z)$ ne dépasse pas la valeur de conception utilisée dans les études.

2.3. Généralisation de la méthode de synthèse

Les hypothèses concernant les distributions radiales relatives de puissance ne sont pas valables dans les conditions suivantes :

- au voisinage des interfaces des tranches sur une zone que l'on appelle zone de transition,

- aux extrémités haute et basse du cœur (réflecteurs)

- dans la première moitié de chaque cycle autre que le cycle 1. Ce phénomène est dû à l'introduction des assemblages neufs, qui produisent des distributions radiales relatives de burnup différentes entre le haut, le milieu et le bas du cœur. Le cycle 1 n'est pas concerné. L'épuisement arrange sensiblement les choses pour les autres cycles.

La figure 4 montre des valeurs de $F_{xy}(z)$ pour différents cycles.

La figure 5 montre comment, dans le cas où il y a deux tranches, le $F_{xy}(z)$ passe de la forme $F_{xy1}(z)$ à $F_{xy2}(z)$ dans la zone de transition autour d'une interface.

Le premier problème peut être résolu par une méthode empirique, à l'aide d'une formule de transition ajustée sur l'expérience ou les calculs 3D.

Le deuxième problème peut être résolu à partir de calculs 3D existants pour chaque tranche, ou de mesures. En effet, les hypothèses d'insensibilité aux variations de niveau de puissance et d'empoisonnement Xénon étant toujours valables, on peut appliquer, pour chaque tranche, une correction :

$$P_{ri}(x,y,z) = P_{ri}^{2D}(x,y) \times e_i(x,y,z)$$
Figure 4 : Variation de $F_{xy}(z)$ en fonction de $z$ pour différents taux $xy$ d'épuisement et pour différents cycles (calculs 3D, coeur sans barres).
Figure 5: $F_{xy}(z)$ dans un cœur contenant un groupe partiellement inséré (calculs 3D)
Figure 6 : Calcul de $F_{xy}(z)$ dans la zone de transition.
Comparaison calcul 3D/formule empirique utilisée dans COSTAR.
On notera que cette méthode permet d'obtenir des valeurs sur le maillage fin utilisé en 2D, avec des calculs 3D effectués sur un maillage plus grossier.

On tiendra compte des incertitudes associées à la première série d'hypothèses en ajoutant éventuellement une correction pessimiste en fonction du niveau de puissance et un facteur maximal pour les oscillations radiales du Xénon.

2.4. Application - Le code COSTAR

Le code COSTAR est capable de traiter le problème dans toute sa généralité. Les informations utiles proviennent de calculs de diffusion à 1, 2 et 3 dimensions.

Il est utilisé en général pour calculer la distribution de puissance axiale maximale $Q(z)$ et/ou le facteur d'élévation d'enthalpie $\Delta H$. L'option 3D permet de traiter le problème assemblage par assemblage, y compris les points chauds de chaque assemblage.

3. COMPARAISON AVEC DES CALCULS 3D

Les calculs suivants ont été effectués successivement avec un code de diffusion aux différences finies et avec le code de synthèse COSTAR :

<table>
<thead>
<tr>
<th>CENTRALE</th>
<th>CYCLE</th>
<th>EPUISÉMENT</th>
<th>INSERTION GROUPE</th>
</tr>
</thead>
<tbody>
<tr>
<td>900 MW</td>
<td>1</td>
<td>Début de vie</td>
<td>19%</td>
</tr>
<tr>
<td>900 MW</td>
<td>1</td>
<td>Début de vie</td>
<td>55%</td>
</tr>
<tr>
<td>900 MW</td>
<td>1</td>
<td>Fin de cycle</td>
<td>55%</td>
</tr>
<tr>
<td>900 MW</td>
<td>3</td>
<td>Début de cycle</td>
<td>35%</td>
</tr>
</tbody>
</table>

Les figures 6 à 8 permettent de comparer les valeurs de $F_{xy}(z)$ calculées par le code 3D et par le code COSTAR dans les mêmes conditions, lorsqu'aucune incertitude n'est rajoutée au calcul de synthèse.
Figure 7 : Calcul du facteur radial en fonction de la cote.
Comparaison calcul 3D/calcul 2D/calcul de synthèse
COSTAR.
Figure 8 : Influence de l'option de traitement assemblage par assemblage dans le calcul de $F_{xy}(z)$ par le code de synthèse COSTAR.
La figure 9 montre la comparaison des distributions axiales de puissance maximale de point chaud en fonction de la cote.

Figure 9 : Calcul de distribution axiale de puissance maximale.
Comparaison calcul 3D/calcul de synthèse COSTAR.
La figure 10 permet de comparer les calculs des distributions d'élévation d'enthalpie par assemblage.

<table>
<thead>
<tr>
<th>1.022</th>
<th>1.026</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.089</td>
<td>1.017</td>
</tr>
<tr>
<td>1.112</td>
<td>1.021</td>
</tr>
<tr>
<td>0.995</td>
<td>1.085</td>
</tr>
<tr>
<td>1.004</td>
<td>1.111</td>
</tr>
<tr>
<td>1.147</td>
<td>1.046</td>
</tr>
<tr>
<td>1.137</td>
<td>1.047</td>
</tr>
<tr>
<td>1.068</td>
<td>1.156</td>
</tr>
<tr>
<td>1.065</td>
<td>1.172</td>
</tr>
<tr>
<td>1.137</td>
<td>1.056</td>
</tr>
<tr>
<td>1.149</td>
<td>1.048</td>
</tr>
<tr>
<td>0.932</td>
<td>1.052</td>
</tr>
<tr>
<td>0.946</td>
<td>1.050</td>
</tr>
<tr>
<td>0.780</td>
<td>0.666</td>
</tr>
<tr>
<td>0.775</td>
<td>0.643</td>
</tr>
</tbody>
</table>

Figure 10 : Calcul de l'élévation d'enthalpie moyenne par assemblage. Comparaison calcul 3D/calcul de synthèse COSTAR.
4. COMPARAISON AVEC DES MESURES

Les mesures en centrales FRAMATOME sont effectuées par l'instrumentation interne mobile. Les détecteurs sont des chambres à fission qui mesurent le flux dans le canal d'instrumentation, de façon continue. Ceci est effectué dans environ un assemblage sur trois. L'information est pré-traitée par le calculateur d'acquisition de données, qui réduit la précision de la mesure en réduisant le nombre de points de mesure à environ 60 sur la hauteur active. Ces informations sont ensuite traitées par un code de dépouillement des mesures, qui utilisera des distributions de puissance théoriques pour élaborer des valeurs de puissance "mesurées" en tous les points du cœur.

4.1. Problème de recalage des traces

Il est difficile de connaître avec précision une cote d'origine absolue commune aux différentes traces de flux. C'est pourquoi, on utilise actuellement la dépression de flux visible au droit d'une grille d'assemblage pour caler les traces de flux entre elles.

L'incertitude de positionnement axial d'une trace est alors de l'ordre de grandeur d'un pas de mesure, soit plusieurs centimètres. Un raisonnement simple permet de voir que cette incertitude se traduit par une incertitude importante sur la mesure du $F_{xy}$ (z) à toutes les cotes où il y a variation rapide du flux axialement. Ceci conduit à la création de pics radiaux n'existant pas, au niveau :

- du haut et du bas du cœur
- des grilles
- des extrémités des barres de contrôle

Les figures 11 à 13 illustrent ce phénomène. Ceci rend évidemment très difficile l'exploitation précise de ces résultats pour la qualification d'une méthode de calcul.

4.2. Qualification

Les coeurs PWR sont stables radialement. Les faibles effets de redistribution radiale due au Xénon sont pris en compte de façon conservative dans la méthode décrite.

Le véritable problème consiste à qualiﬁer l'utilisation du code ESPADON de calcul à une dimension axiale pour les cas de fonctionnement normaux et anormaux.
Figure 11 : Mesure du facteur radial en fonction de la note.
Figure 12 : Influence du calage des traces sur la mesure du facteur radial.
Figure 13 : Influence de la position affichée pour les barres sur le facteur radial mesuré.
Figure 14 : Efficacité différentielle d'un groupe - Comparaison mesure/calcul 1D ESPADON
Les essais physiques et les essais supplémentaires apportent des éléments positifs, au moins dans des cas pseudo-stationnaires.

La mesure d'efficacité différentielle de grappes de contrôle est un exemple montré figure 14.

Un suivi de charge en mode de pilotage à déséquilibre axial constant a été effectué sur une centrale et interprété avec le code ESPADON utilisé à FRANATOME. La figure 15 montre la comparaison entre la prédiction et la mesure. L'accord est bon. Il faut noter que cela ne peut être obtenu qu'avec l'utilisation d'un modèle à une dimension sophistiqué, incluant le traitement de tous les effets de contre-réaction, y compris sur les fuites transverses.

La figure 16 montre par ailleurs une comparaison entre un calcul de synthèse CYSSTAR et une mesure effectuée sur un réacteur.

5. APPLIATION DANS LES PROTECTIONS DU CP3

Les centrales du CP3 seront équipées d'un système de protection plus sophistiqué que les précédentes, afin de gagner des marges de fonctionnement.

Le principe est d'utiliser des détecteurs hors cœur multi-étages. Ceux-ci, convenablement calibrés par rapport à l'instrumentation mobile du cœur, élaboreront en permanence la forme axiale de puissance moyenne, à partir des courants mesurés dans chacune des sections. Ces informations sont traitées dans un micro-processeur.

La méthode de synthèse permet, moyennant la mesure en continu de la position des grappes, et la fourniture au micro-calculateur des facteurs radiaux fonction de la cote, de calculer les facteurs de point chaud Q (z), le facteur d'élevation d'enthalpie FAB comme illustré figure 17. Un algorithme permet alors de calculer le DNBR. Les incertitudes correspondantes sont, bien entendu, prises en compte, et ces informations servent à protéger le cœur contre la fusion, le LOCA, et l'ébullition nucléée.

6. CONCLUSION

La méthode de synthèse présentée ici est un outil de calcul présentant une bonne précision, et dont le temps de calcul est compatible avec les besoins des calculs de conception et les possibilités des micro-processeurs.

Elle apporte un complément utile aux calculs de diffusion 1D, 2D et 3D.
Figure 15 : Suivi de charge typique. Comparaison mesure/calcul 1D ESPADON.
Figure 16 : Comparaison du facteur radial mesuré avec le calcul de synthèse COSTAR.
PROTECTION CP3

\[ [P] \times [T] = [I] \]

Incore \hspace{1cm} \text{Transfer} \hspace{1cm} \text{Excore}

\[ Q(z) = \overline{P}(z) \times F_{xy}(z) \times PR \times FIQ \]

\[ F_{\Delta H} \leq \frac{1}{H} \int_{0}^{H} F_{xy}(z) \times \overline{P}(z) \, dz \times FIH \]

Algorithm : minimum DNBR

Surveillance : \( Q(z) < Q_{LOCA}(z) \)

Protection : \( Q(z) < Q_{FUSION} \)

\[ DNBR > DNBR \text{ limite} \]

Figure 17
THE APPLICATION OF HETEROGENEOUS THEORY TO PWR STUDIES

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ABSTRACT

A coarse mesh model based upon an heterogeneous formalism and the use of a space/energy kernel or Greens function calculated by Monte Carlo methods is described. Originally developed for pressure tube reactors the method is extended to PWR geometries. Comparisons with theoretical pin rating distributions and with theoretical and experimental estimates of assembly ratings for the Beznau reactor show the method to be a promising one in this application.

1. INTRODUCTION

The kernel method, which is described in this paper, is believed to be a novel variant of heterogeneous theory. It has been applied successfully to the problem of solving for rating distribution in a pressure tube reactor, and the theory is here extended to apply to the coarse mesh solution of light water reactors.

The basis of the method is the evaluation of a kernel describing the spatial distribution of the yield of fission neutrons in a regular array of rods, fuel clusters or assemblies as the case might be, with a fission source in one unit of the array. This Greens function can then be superimposed to described the spatial distribution of fission neutrons produced by a given distribution of sources, and hence permit a solution for the steady state eigenmode. Monte Carlo methods are used to generate the kernel in an 'exact' space/energy model problem, and refinements are introduced to approximate the effects of variation of fuel multiplication, of thermal absorption cross-section and, an extreme case of this, the treatment of reflectors.

The method has been investigated to give a preliminary indication of its performance in PWR application, but is not regarded as being fully developed or validated.

2. THE KERNEL METHOD

The method, which is a generalization of the formalism of Feinberg and Galanin /1/, can most simply be described by reference to the type of problem for which it was originally conceived, a regular lattice of relatively large, well spaced fuel assemblies typical of a pressure tube reactor system. For the purpose of our discussion, we may regard these assemblies as an array of large rods.

1. Typically half the neutrons born in a fuel element would be absorbed in the same element.
2. The elements were almost black to incoming thermal neutrons, so that once a neutron had crossed the pressure tube travelling inwards it had a high probability of ultimate absorption in the fuel element therein. The ultimate distribution of absorptions would therefore be relatively insensitive to changes in fuel absorption cross-section.

3. In the epithermal range – at least above the 1 eV resonance of Plutonium-240 – all fuel elements were closely similar, events being dominated by resonance absorption in Uranium-238, whose concentration would vary by only 2% or so with burnup.

It was therefore clear that almost all the neutron transport processes in the reactor involving neutrons born in one fuel element and absorbed in another would be rather closely modelled by superposition of solutions for the relatively simple case of a regular array of fuel elements with a source in one element, whilst the details of the thermal neutron behaviour could be approximated quite closely by a lattice cell calculation with only approximate boundary conditions to describe the interaction with fuel in neighbouring positions.

The problem of a regular lattice with source in a single element can easily be solved using Monte Carlo techniques with any desired degree of space and energy resolution. For the purpose of this description of the method we confine ourselves to a two-dimensional model and treat the fuel as line sources and sinks. The quantity scored is:

\[ K^f(r \rightarrow r') \]

the fission yield in an element at \( r' \) due to unit fission source in an element at \( r \). It is to be noted that this kernel includes very complicated neutron spectrum effects, particularly the fact that the neutrons travelling longer distances will be more thermalized and have a different effective multiplication. Thus a critical equation may be written in the form:

\[ \lambda S_j = \sum_i K^f(i \rightarrow j)S_i \]

where \( \lambda \) is the system eigenvalue

\( S_i \) is the fission source in element \( i \)

Because of the spectrum dependence included in \( K \) the corresponding buckling mode to give criticality (\( \lambda = 1 \)) will include correctly the change to a critical spectrum. The second spatial moment of \( K \) is, of course, the migration area, and it is in the calculation of neutron migration and streaming that the Monte Carlo technique has long been used in this form [2].

The extension to more general problems may be considered in two parts. A change in fission yield (or multiplication) with an unchanged absorption cross section is easily represented by an appropriate multiplier. This will be exact only if the new yield has the same energy dependence as the old one, but due to the observation that the most common changes arise in thermal multiplication conventional energy treatments give a good approximation. A change in the absorption cross-section may be modelled if necessary by the use of an additional kernel. For imagine that the original kernel was calculated for the highest cross-section to be encountered. Then a reduction in cross section will lead to a reduced number of absorption events. Let an appropriate fraction of the neutrons originally absorbed be restarted in the new system and tracked to their next fission. This second phase of distribution can then be allowed for as an additional kernel. We have noted that in many practical cases the distance travelled by such neutrons will be small, and it will therefore usually be a reasonable approximation to use one typical energy dependence of the restarted neutrons to define this kernel.
We thus obtain a more general critical equation in a two mode form:

\[
\lambda S_i = \frac{vE_f}{vE_f} \left\{ \lambda F_i S_i + \lambda \frac{\delta E_{ai}}{vE_f} k^{th}(i-j)S_i \right\}
\]

where \( \delta E_{ai} = T_a - E_{ai} \)

\( vE_f \) is the fission yield used in the Monte Carlo determination of kernels

\( vE_{fj} \) is the actual fission yield

The derivation of this equation is given in the Appendix. It will be seen that the approximation introduced in the treatment of changes in absorption cross-section, primarily that the energy dependence of the cross-section perturbation is the same for all fuel elements (and hence that the same thermal kernel can be used in all cases to permit summation of successive distributions) has something in common with conventional few group models. Because, however, the thermal kernel will normally be heavily diagonally dominant, the practical effect of the approximation is minimized.

It was possible to show that a tilt in the fission source distribution in a fuel channel had a small effect upon the solution, and so it was adequate to characterize events by a single parameter, total neutron yield, in each fuel element. The lattice calculation was used to relate this quantity to heat production. The neglect of this tilt, which is represented by a dipole source term in a conventional heterogeneous calculation, is not, however, equivalent to a monopole model. This is because the spatial transport around or through channels, including streaming effects, is included in the kernel by virtue of its being evaluated in the real geometry with finite size assemblies.

As is usual with heterogeneous representations, modelling of reflectors must be achieved by the use of dummy channels. A satisfactory base case is that of an absorbing but non-multiplying array of fuel elements in the reflector. A suitable choice of multiplication and cross-section perturbation may then be chosen for channels near to the core to give the required reflector saving.

The method proved to be rapid and of satisfactory accuracy in a 2-dimensional model of the 104 channel SGRWR reactor, and was easily implemented on the reactor mini-computer system.

3. APPLICATION TO PWR

The same formalism will clearly be applicable to a PWR considered as an array of individual pins. This would, however, be excessively laborious to solve, and we seek a simpler model. For a known distribution of fission source the integral equation can be collapsed in space.

Consider a PWR fuel assembly. By virtue of the batch fuel management system the multiplication of pins, and hence the fission source, is usually discontinuous at the boundaries of the assembly, whilst the absorption cross sections may only differ slightly and the flux is continuous.
FIG. 1. SUBDIVISION OF PWR CHANNEL TO ALLOW FOR NON-U NIFORM SOURCE DISTRIBUTION.

FIG. 2 SOURCE AND ABSORPTION DISTRIBUTION ALONG A LINE THROUGH POINTS A AND B

--- FISSION SOURCE DISTRIBUTION
--- ABSORPTION DISTRIBUTION

FIG. 3 SOURCE DISTRIBUTION FOR CORRECTION TERMS IN BOUNDARY REGIONS.
The lowest order representation possible would be to assume a flat fission source over the assembly, and in this case the formalism previously derived would remain appropriate, the kernels being determined either directly by Monte Carlo or by summation of pin kernels. But whereas for fuel cluster geometries the eventual distribution of neutrons is found to be insensitive to tilts in the source – the equivalent of dipole/dipole terms in conventional heterogeneous models – this will clearly not be the case in the PWR. The next simplest option is to permit a sub-division of an assembly as shown in Figure 1. This allows for a slope in the absorptions in the vicinity of the assembly boundaries, as shown in Figure 2, reflected in the source shape also shown in that figure. The model still has only one free parameter to describe each assembly (or mesh) region, but might be expected to give a rather better representation of the solution. It will be noted that this model has much in common with finite element methods or with methods for coarse mesh correction to diffusion theory, except that these are applied to the few group flux rather than to the fission source.

The tilt of thermal absorptions may be approximated in terms of the source in the central zone of the fuel, say \( Q \)

\[
\text{Tilt} = \alpha \left( \frac{Q_1}{\eta_1} - \frac{Q_4}{\eta_4} \right)
\]

where \( \alpha \) depends upon the size of the inner zone.

then

\[
\frac{S_1}{\eta_1} = \frac{Q_1}{\eta_1} + \alpha \sum_{k=1}^{4} \left( \frac{Q_k}{\eta_k} - \frac{Q_1}{\eta_1} \right)
\]

and the equations may be condensed to:

\[
S_j = \frac{\nu_E f_{ij}}{\nu_E f} \left\{ \sum_i K^f(i+j) S_i + \lambda \sum_i \frac{\delta_{ij}}{\nu_E f i} K^h (i+j) S_i + \sum_{k=1}^{4} \left( \frac{Q_k}{\eta_k} - \frac{Q_1}{\eta_1} \right) \right\}
\]

Again the kernels \( K^* \), which correspond to the source shape illustrated in Figure 3, may be deduced by integration of the basic pin-to-pin kernel. For a single mesh per assembly the kernels will be small for transfer across a whole assembly, and the equation will be effectively a nine-point one. From the representational standpoint the model is therefore of a similar complexity to that of two-group diffusion theory, but solution may be effected much more quickly because no inversion (or iteration) is required to obtain the next source iterate. For we have:

- Heterogeneous equation
  \[
s^{n+1} = A s^n
\]

- Diffusion equation
  \[
s^{n+1} = f^* B^{-1} s^n
\]

Similarly data preparation is simplified, an assembly being characterized by two of the three quantities:

\[
\frac{\nu_E f}{\nu_E f}, \ \frac{\delta_{ij}}{\nu_E f} \quad \text{and} \quad k \quad \text{(or } \eta \text{)}
\]
FIG. 4 RATING DISTRIBUTION IN CHEQUERBOARD LATTICE (EACH SQUARE CONTAINS FOUR FUEL PINS)
Variations in coolant density, enrichment, irradiation, Doppler, Xenon and boron concentration can all be approximated within this form, although it is possible to contemplate the computation of more than one kernel and interpolation to give a better representation of neutron transport if the accuracy of the model warrants this.

4. THEORETICAL TESTS ON THE METHOD

A simple theoretical test was performed to check that the model would perform satisfactorily even when the thermal absorption cross-section varied markedly between adjacent assemblies. In view of the derivation of the method it was considered that this would be a severe test.

An infinite chequerboard lattice of assemblies, each of 14 x 14 pins of new fuel and alternately 1.80\% and 2.78\% enrichment in Uranium-235 was calculated using diffusion theory and one mesh point per pin in six energy groups. Kernel calculations in unit cells of 2 x 2 and 14 x 14 pins were carried out and the rating distributions are compared in Figure 4.

The average assembly ratings obtained in the different approximations are shown in the Table below. It will be seen that the agreement is very good.

<table>
<thead>
<tr>
<th>Method</th>
<th>2.78%</th>
<th>1.80%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion Theory</td>
<td>1.102</td>
<td>0.898</td>
</tr>
<tr>
<td>Fine Mesh Kernel Method</td>
<td>1.105</td>
<td>0.895</td>
</tr>
<tr>
<td>Coarse Mesh Kernel Method</td>
<td>1.110</td>
<td>0.890</td>
</tr>
</tbody>
</table>

The fine mesh kernel model will be seen to give rating distributions very close to the fine mesh, few group diffusion theory result. Even in coarse mesh the assembly ratings are reproduced to within 0.5\% of the result for finer mesh. In this problem it will be seen that the flow of thermal neutrons is from the low rated to the high rated element, and thus in the opposite direction from the source difference. This is the most difficult case to model.

Figure 5 shows the results of a more detailed calculational comparison based on a simplified central zone of the Tihange reactor. The loading involves two enrichments, the higher of which contains burnable poisons. In this case each pin of the 15 x 15 array was represented explicitly in the kernel method. In this case the more highly absorbing cell has the lower reactivity and thus the lower pin rating. It will be seen the the maximum difference between the two calculations of pin rating is slightly in excess of 2\%. The position of this maximum difference, and next to a vacancy midway between two burnable poison pins may be significant; a similar effect can be seen at the interface between the cells two pitches away from such pins. It has not been established which result is to be preferred.

The results also serve to show that the kind of model for spatial source distribution envisaged in the earlier sections, and illustrated in Figure 1, should be a good representation of source distribution in an inner region assembly so long as the transition region covers the outermost two rows of pins.

The working hypothesis is that the coarse mesh source distribution computed by such a model could be used as source for a pin-by-pin computation to give local variation within an assembly.
FIG. 5  COMPARISON BETWEEN LWR-WIMS AND KERNEL METHOD CALCULATIONS OF PIN POWERS IN CHEQUERBOARD SUPERCELL FROM CENTRE ZONE OF TIHANGE 1 PWR.
5. COMPARISON WITH REACTOR OPERATIONAL DATA

The kernel method was used to calculate the third cycle of the Beznau 1 reactor which corresponded to burnup of 4300 MWD/Te. The computation was restricted to two dimensions. A simplified illustration of the fuel disposition is shown in Figure 6.

In order to represent the reflector a simple dummy multiplication factor was used in the reflector "assemblies". Its value was fitted to a one dimensional calculation.

![Fuel Distribution Diagram](image)

**FIG. 6** FUEL DISTRIBUTION IN BEZN AU 1, CYCLE 3
Figure 7 shows the results, with one 'mesh' per assembly and no allowance for source shape within the assembly. The theoretical comparison is with a full three dimensional diffusion theory calculation using the JOSHUA code and including thermal hydraulic feedback /3/. Given the degree of approximation used, the agreement is considered to be very promising.

The root mean square deviation between the kernel result and powers inferred from measurements is 2.5% compared to 1.3% for the 4 mesh per assembly JOSHUA calculation. The discrepancy is of the same order as observed difference between the ratings in supposedly symmetric positions in the core.

FIG. 7 NORMALISED RADIAL POWER MAP AT 4300 MWD/Te HA FOR BEZNAU 1, CYCLE 3 (OCTANT)
6. EXTENSION TO THREE DIMENSIONS

In order to assess the likely cost of a three dimensional kernel calculation a quadrant of the Beznau reactor was solved using one node per assembly and 16 axial meshes. This does not imply that a mesh representation would necessarily be the preferred axial representation.

The solution was not accelerated, but converged 4 times faster than the well established JOSHUA method using 4 meshes per assembly in the x-y plane and the same axial resolution. It is anticipated that the method will prove to be substantially faster than existing coarse mesh techniques when more fully developed.

7. CONCLUSIONS

Preliminary studies have suggested that the kernel model may prove to be a useful formalism for deducing a satisfactory coarse mesh representation of a PWR without recourse to the intermediate approximation of homogeneous diffusion theory. In very simple cases the method can be related to response function or partial current methods, but the particular form of space-energy linkage inherent in the method is considered to lead to improved internal consistency in this respect.

As a computational technique the method has proved to give encouraging results in two dimensions, where even the simplest application gives results for one node per assembly similar in accuracy to those obtained with 2 x 2 mesh diffusion theory. The capability to use the resultant source distribution to drive a consistent pin rating model for greater refinement may prove to be helpful.

Solution times are competitive even without acceleration, and in heterogeneous calculations the model has proved to be convenient for use on mini-computers.
APPENDIX

DERIVATION OF KERNEL EQUATION FOR A SYSTEM WITH VARYING ABSORPTION CROSS SECTION

It is assumed that a fission source kernel \( K_f^f \) has been obtained for a cell containing fuel which has the highest absorption cross section found in the system. Call this absorption cross section \( \Sigma_A^f \), and the fission yield cross section for this fuel \( \bar{\nu}^f \).

Now consider a fission source \( S_j \) in cell \( j \). The resulting fission yield in cell \( k \) is:

\[
\frac{\nu^f_k}{\bar{\nu}^f} K_f^{j-k} S_j ,
\]

but only if \( \Sigma_A = \bar{\Sigma}_A \) in all channels near to \( j \) and \( k \). If \( \Sigma_{A,k} < \bar{\Sigma}_A \) the kernel \( K_f^f \) will overestimate the absorptions in channel \( k \), and the excess neutrons must be restarted at the energy prior to their spurious absorption. The subsequent distribution of these restarted neutrons can also be described by a kernel \( K^\text{th}_{k} \), defined in the same way (and for the same material) as \( K_f^f \), except that the source neutrons have thermal energies.

The number of excess absorptions in cell \( k \) due to the fission source \( S_j \) is:

\[
\frac{\delta \Sigma_{A,k}}{\bar{\nu}^f} K_f^{j-k} S_j ,
\]

where

\[
\delta \Sigma_{A,k} = \bar{\Sigma}_A - \Sigma_{A,k} ,
\]

and the extra fission yield in cell \( j \) due to these restarted (second generation) neutrons is:

\[
\frac{\nu^f_j}{\bar{\nu}^f} K_f^{j-k} S_j \frac{\delta \Sigma_{A,k}}{\bar{\nu}^f} K^\text{th}_{k}(k \rightarrow l) .
\]

However, once again the number of absorptions in cell \( l \) has been overestimated, and a fraction of the neutrons must be restarted. It is assumed that the distribution of these third generation neutrons can also be described by \( K^\text{th}_{k} \), giving the following fission yield in cell \( m \):

\[
\frac{\nu^f_j}{\bar{\nu}^f} K_f^{j-k} S_j \frac{\delta \Sigma_{A,k}}{\bar{\nu}^f} K^\text{th}_{k}(k \rightarrow l) \frac{\delta \Sigma_{A,l}}{\bar{\nu}^f} K^\text{th}_{l}(l \rightarrow m) .
\]

This process can be repeated ad infinitum, so the fission yield in any cell due to a given source distribution must be expressed as an infinite series. Writing \( \delta \Sigma_k = \delta \Sigma_{A,k} / \bar{\nu}^f \), the eigenvalue equation is:
\[ \lambda s_p = \frac{\nu_{f,p}}{\nu_f} \left\{ \sum_j s_j k_f(j,p) + \sum_{j,k} s_j k_f(j-k) \delta_k k^{th}(k+p) + \ldots \right\} \]
\[ + \sum_{j,k,l} s_j k_f(j-k) \delta_k k^{th}(k+l) \delta_l k^{th}(l+p) + \ldots \}
\]

(A6)

Now writing this equation in matrix form, where:

\[ \hat{S} = \frac{\nu_f}{\nu_{f,p}} S_p, \quad F_{ij} = k_f(j-i), \quad T_{ij} = \delta_j k^{th}(j+i), \]

(A7)

gives:

\[ \lambda \hat{S} = (1 + T + T^2 + \ldots ) \delta_k F_{kj} S_j \]

(A8)

Multiplying both sides by \( (1-T) \) gives:

\[ \lambda (1 - T) \hat{S} = FS, \]

(A9)

\[ \lambda \hat{S} = FS + T \hat{S} \]

(A10)

Rewriting equation (A10) in the usual notation gives:

\[ \lambda s_j = \frac{\nu_{f,i}}{\nu_f} \left\{ \sum_{i} s_i k_f(i+j) + \sum_{i} \delta_{j,i} s_i k^{th}(i+j) \right\} \]

(A11)

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/3/ GIBSON, I H et al. The Performance of UK Coarse Mesh PWR Calculations in Comparison with Reactor Data. (this conference)
During the past few years substantial progress has been made in the development of efficient numerical methods for the solution of multidimensional diffusion equations. Some of these methods have also been extended to neutron transport and fluid dynamics problems. The finite element method originally developed on a physical basis for the analysis of problems in structural mechanics has emerged as an important tool in the study and design of nuclear reactor systems. Two papers of this session deal with the theory and application of a LWR calculation system based on FE methods for the global reactor solution. Very flexible 2-D and 3-D FE methods with iterative solution procedures have been implemented in the NEPTUNE system of reactor calculations and successfully applied to large power reactor problems. A. Kavenoky presents a comprehensive paper on the capabilities of NEPTUNE. P. Reuss gives an example of a realistic core follow study.

There is still potential to accelerate the FEM. A. Kavenoky demonstrates this by using a combination of acceleration methods. Kaplan's synthesis method is used among other techniques to obtain an initial flux guess, a procedure also successfully applied to the acceleration of finite difference methods.

FE methods are most efficient alike other coarse mesh methods in problems with large homogeneous regions. Yet smooth variations of cross-sections can also be accounted for, a property which is shared by FEM together with modern coarse mesh methods based on local flux expansions. This feature is essential for the application of coarse mesh methods to 3-D long-time depletion studies. It is equally important for the analysis of short-time reactor transients.

Results of FEM applied to mildly heterogeneous elements were not discussed at this meeting but have been published elsewhere. The FEM as implemented in the NEPTUNE systems is also well suited to include thermo-hydraulic feedback. This is clearly demonstrated by the presentation given by P. Reuss. The method has also been extended to the solution of space-time kinetics problems.

P. Siltanen's paper deals with a two-group nodal 3-D method in hexagonal geometry. Because of its good agreement of theoretical results and measurements it appears to be well suited for Nowo-Voronesh type reactors. The method seems to fulfill the requirements of being both accurate and computationally efficient. The method is similar to that used by M. Mélice in the MERCATOR-xy code. Mélice discusses an extension of this method to the pseudo 3-D systems MERCATOR-z in which perturbation theory is systematically used to avoid true 3-D calculations.
Another approximate solution for 3-D problems is presented by A. Darraud. As far as I know, synthesis methods have not been used much in LWR calculations. In a simplified or more generalized form synthesis methods might be useful in addition to and as a complement to true 3-D calculations. Darraud mentions an interesting application of this method to a digital protection system.

J. R. Askew presents some new ideas and encouraging first results to the solution of the global reactor problem and the calculation of individual pin powers. The method is an extension of a method originally proposed by Feinberg and Galanin to PWR geometries. Though the authors do not consider the method as being fully developed the quoted results show surprisingly good agreement with more conventional methods and experiments. The main advantage of this method seems to be, apart from the very high computational efficiency, that a coarse mesh representation of a PWR can be deduced without recourse to the intermediate approximation of homogeneous diffusion theory.

There is still scope and need for further development of coarse mesh methods and refinements of existing methods. Up to now the treatment of the core-reflector interface is one of the problems which does not seem to be adequately solved in PWR coarse-mesh calculations. The now widely adopted procedure of using constant albedos obtained by a 2-D fine mesh calculation may be sufficiently accurate in steady-state problems. It has yet to be verified in transient core analysis.
Session 3

Chairman - Président
Prof. A. HENRY
(United States)

Séance 3
IMPROVEMENT OF PARAMETERS FOR A
3-D REACTOR SIMULATOR WITH EXPERIMENTAL DATA

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Abstract:

A commercial available reactor core fuel management system (FMS) was used in the simulation and analysis of the behaviour of the Mühleberg boiling water reactor core. The results of core follow calculations were compared to experimental data such as TIP traces and gamma-scan distributions. As a result of these comparisons certain analytically derived parameters in the initially used parameter sets (which themselves partially are based on experimental data) were adjusted. The very good agreement between experiment and theory allows us to plan plantsupporting calculational activities in the field of reactor core fuel management.

1. Introduction

Reactor Fuel management /1/ covers all activities in managing nuclear fuel through the whole nuclear fuel cycle. A critical activity within is the so called "In-Core Fuel Management", covering all functions related to fuel utilization in a nuclear power reactor core, with respect to safe and economic operation of the reactor.

In-Core Fuel Management, the central technical activity in overall nuclear fuel cycle management, provides the long term fuel cycle planning, reload design, operation monitoring and guidance.

Nuclear fuel management incorporates a unique interrelationship among procurement, fuel design, reload design, core loading and the operation of the plant.

With its own In-Core Fuel Management activities, a power utility can
1. get a deeper understanding of the behavior of its reactor,
2. check the calculations carried out by the fuel supplier,
3. give active operational guidance and
4. do fuel management in its own responsibility
To perform In-Core Fuel Management functions, sophisticated computer models and reactor analysis techniques /2/ has to be applied.

The Bernische Kraftwerke AG (BKW) and the Kernkraftwerk Leibstadt AG (KKL) have jointly purchased the Fuel Management System (FMS) /3/ from Scancraft A/S, Norway.

In this paper we are reporting our experience in using FMS to follow the Mühleberg core through its first 5 cycles and we try to answer the principal question "What is a production code".

2. KKM - the BWR Plant of Bernische Kraftwerke AG

The Kernkraftwerk Mühleberg (KKM) is equipped with a GE-BWR class 4 type reactor rated at 997.2 MWe with a gross electrical output rating at 320 MWe (net). The core contains 240 assemblies. 57 cruciform control rods are used for reactivity control. First criticality was reached in 1971; normal power production was attained in 1972.

The initial core loading consisted of 228 active (7x7 type) and 12 dummy assemblies and was rated at 947.4 MWe. In addition to the control rods 104 boron stainless steel temporary control curtains were used for reactivity control. Cycle 1 operation can be divided into three periods:

- Cycle IA included fuel loading, initial heatup and testing followed by several months at full power. EOC 1B some reshuffling was performed in the core, four assemblies were replaced and 34 curtains were removed. At start of cycle 1C, four assemblies were replaced by four Gd containing bundles (7x7), some reshuffling was done and 20 additional curtains were removed. To reduce mechanical curtain-channel interaction, the bypass flow was reduced by plugging the corresponding holes in the lower grid plate. This caused boiling in the interchannels, which complicates the analysis of this operating period. As a result of these problems with the curtains, the cycle 1C operation consisted of a relatively short full power period using excess core flow and feed water temperature reduction, followed by a cooldown period. EOC 1C an accumulated exposure in terms of the initial core loading of about 11'100 Mwd/UE was attained.

- For cycle 2, the twelve dummy fuel assemblies in the core were removed and replaced with active fuel assemblies to expand the core size from 228 to 240 fuel assemblies. Also the 46 boron stainless steel temporary control curtains remaining in the core from Cycle 1C were removed for Cycle 2 operation. The bypass flow holes in the lower core plate that were plugged for Cycle 1C operation due to the channel-curtain interaction were unplugged for Cycle 2 operation. At the end of Cycle 1C, 106 initial core bundles were discharged, two initial core bundles discharged at the end of Cycle 1B were reinserted, eight fresh Gd containing 7x7 type bundles were loaded and 108 8x8 type (with Gd) reload bundles were loaded. At startup of Cycle 2 operation the core loading therefore consisted of 120 7x7 initial core bundles, 12 7x7 Gd containing and 108 8x8 reload bundles. Cycle 2 operation was interrupted after three weeks of operation due to shutdown for feedwater sparger replacement and a minor change in core configuration took place as a result of gamma scanning activities part way into the cycle. Four 8x8 type reload bundles and two initial core bundles were removed for gamma scan and were replaced by six initial core bundles discharged at the end of Cycle 1C. The loading of Gd containing fuel bundles into the core in Cycle 2 resulted in relatively low excess reactivities throughout the cycle.
The low excess reactivity remained fairly constant over the cycle due to the Gd burnout.

At the end of Cycle 2, 48 initial core bundles were discharged. The 4 for gamma scan purposes removed 8x8 bundles were reinserted, 4 initial core bundles discharged at the end of Cycle 1C were reinserted and 40 fresh 8x8 bundles were loaded. Core loading for Cycle 3 thus consisted of 80 7x7, 12 7x7 Gd-bearing and 148 8x8 bundles.

For Cycle 4 the thermal power rating was increased to 997.2 MWt from the previous 947.4 MWt to reflect the increase in core size in Cycle 2 from 228 to 240 fuel bundles. At the end of Cycle 3, all of the 80 initial core 7x7 bundles remaining in core were discharged and 80 8x8 bundles were loaded. Due to scheduled outages at some hydroelectric plants, the shutdown date was extended to accommodate the hydroplant outages.

The Cycle 5 core loading consisted of 4 7x7 and 236 8x8 type fuel bundles.

Except for the shutdown in Cycle 2 the reactor operation is characterized as continuous with no longer shutdowns, resulting in high capacity factors.

Excess core flow and bypassing the high-pressure feedwater heaters were utilized throughout the cycles for operating flexibility in maintaining full power and in extending full power cycle exposure capability.

3. Fuel Management System (FMS)

FMS /3,4,5,6,7/ has been employed for analyses carried out in this study. This software system enables a user to do a systematic approach to optimal fuel utilization. For fuel cycle and core management, the system consists of the four computer codes - RECORD, FALC, FCS-II and PRESTO. A schematic outline of the system and the FMS approach to optimal fuel loadings is given in Fig. 1.

![Diagram of Fuel Management System (FMS)](image)

**Fig. 1** The Fuel Management System FMS
The basic assumption of the FMS calculation procedure is the separability of the local nuclear calculations from the global core calculations. The local nuclear calculations are performed in a unit cell of the core, made up by the fuel assembly and associated water gaps, control rods, curtains, etc. The overall fuel cycle process is simulated for the various purposes with 0 to 3-dimensional core models.

The unit cell is analyzed with the two-dimensional burnup code RECORDER. Fuel pins, flow box, water gap and holes, control rods, burnable poison pins and curtains are explicitly represented and each fuel pin is subject to separate neutron multigroup spectrum calculations. All nuclear data required for the simulation of core performance are generated with RECORDER and stored in the data bank for use by the global core models.

To study the overall fuel cycle the reactor model is a three radial region core model, where twelve years of reactor operation are analyzed. The number of fuel assemblies to be loaded and shuffled between the regions at each reloading are being determined by the linearer program FALC, which provides an operation research model of the fuel cycle. FALC generates a solution which minimizes the levelized fuel cycle costs, subject to constraints of required reactivity at the end of each cycle in each region and the material balance requirements.

The feasibility of the solutions generated with FALC are examined with the multi-region model in FCS-II, and analyzed with one-dimensional calculations. The influences of the reactivity distribution on core reactivity power distribution may be determined at this level. Detailed analyses of the core loading and operating strategy for the subsequent cycle may be evaluated in three dimensions, using the nodal core simulator PRESTO. The most important task here is to demonstrate feasibility of the control system in providing an adequate power distribution control over the entire operating period. The core simulator PRESTO had been widely used in this work to carry out core follow calculations.

4. The γ-scanning experiment

With the γ-scan method /8/ relative EDC power distributions can be obtained from the measured 140Ba-activity-distributions. 140Ba (T1/2 = 12.8 d) is relatively quickly saturated, so that its local activity can be considered proportional to local power, if the reactor was operated for a certain time at a relatively high power level with a constant power distribution /9/. 140Ba was measured by means of the 1.536 MeV γ-line of its daughter product 140La. Comparisons between measured 140Ba-distributions and calculated EDC power distributions has to be performed very carefully. The constant power-assumption at the end of a cooldown operating period represents a rough guess and therefore our model was expanded in order to calculate 140Ba-distributions. Burnup distributions were measured by means of 137Cs (662 keV, T1/2 = 30 y) and 144Ce (2.186 MeV of its daughter product 144Pr, T1/2 = 248 d). Because of the relatively long half lives these isotopes are not near to their saturation during the examined insertion period of a fuel assembly in the reactor, so that local activity can be assumed to be proportional to local burnup.

At 24 axial positions (nodes) on all four edges of each scanned fuel assembly γ-spectra were taken with a Ge(Li)-detector-multichannel-analysersystem commonly used in γ-spectroscopy. The local activities were extracted from the measured γ-spectra by integrating over the appropriate γ-line. The measured activity yields were corrected for decay and the dead time of the data acquisition system. The activity distributions were approximated with a Fourier least square fit in order to get measured and
calculated values at the same axial position. From the four axial distributions (four edges) per fuel assembly the nodewise average was calculated and nodal activity ascertained. The error compared to the measurement of individual rods is small. The reproducibility of the measurement were within 2 % in all cases. The overall error was 1.5% to 3.5% /9/. The relative activity distributions were then directly compared with the corresponding relative distributions calculated by PRESTO.

Comparisons between the γ-scan results and the PRESTO calculations were done on the basis of axial and radial (plane by plane) 140Ba-distributions. 140Ba-distributions are more sensitive on parameter variations than the burnup distributions are (integrating effect).

5. Core follow calculations

The core performance of KKM through the first cycle has been simulated with FMS and compared with operational data /10/. The aim of the study was to provide a systematic review of core performance of KKM through the first three cycles and to determine the capability of FMS to reproduce operational data and, hence, its capability to predict the future behaviour of the KKM core.

The data bank has been generated, using the RECORD code, and for the treatment of Gadolinium fuel the code system THERMOS-GASPOL-RECORD has been used. These codes give the burnup dependency of the average two group assembly data for use in the global models. Coefficients describing the Xenon-Doppler effect and the effect of the absorber curtains and control rods in PRESTO are calculated in special RECORD-runs.

PRESTO was initialised by specifying data describing the core configuration and its hydraulic characteristics. Parameters for the boiling model and slip correlation are based on experimental data from the FRIIG loop. Boundary conditions for the reflectors were established by fine mesh calculation. A first core follow calculation in full core representation was performed in order to check the PRESTO results with TIP traces. The operating history was subdivided into 26 burnup steps, characterized by operating data such as core thermal power, total coolant flow rate, feed water enthalpy and control rod pattern, derived from the heat balance at a representative point in time during each burnup step. The spatial distributions of power density, void fraction and fuel exposure were calculated at beginning and end of each burnup step. A first fine tuning of the model has been performed in the subcooled boiling model and reflector parameters using TIP traces. However, the TIP traces turned out to be rather insensitive to these parameter variations /11/.

In general, FMS was flexible enough to treat the rather unusual operating history of the first cycle of KKM /10,11/. Analytically derived boundary conditions for the side and bottom reflector are not quite satisfactory. Therefore, at the end of Cycle 1C γ-scan results were used to check PRESTO results. The calculation of 140Ba-distributions turned out to be rather sensitive on variation of reflector parameters as well as parameters in the boiling model /11/.

As a result of the comparisons of the axial distributions for the scanned assemblies as well as the radial distributions, minor adjustments in the analytically derived boundary conditions of the bottom/top and side reflector and in the subcooled boiling model data were applied. These adjustments were done with the aid of a detailed parametric study supported by additional fine mesh calculations. The final core follow calculation for Cycle 1 was then performed using the improved parameters and a more detailed subdivision of the operating history. The results of the improved core follow calculations are shown in fig. 2.
Fig. 2 Comparison of relative $^{140}$Ba distributions measured with $\gamma$-scan and calculated by PRESTO before (left fig.) and after final fine tuning (right fig.)
During the whole Cycle 1 for example the assembly AM 78 was located nearby the core centre and the assembly AM 163 at the core boundary. PRESTO reproduces especially well the effects of coastdown operation (increased core flow, reduction of feed water temperature; in the lower core part: small bump in the AM 78 distribution). However, the relative activity distributions used in this work allow only for the fine tuning of parameters influencing the shape of the calculated distributions. The measurement of absolute activity distributions with \( \gamma \)-scan method is incomparable more difficult and lies often outside the possibilities of a utility.

Using the improved parameter set in PRESTO, the core follow calculations through the Cycles 2 to 5 were performed. At the end of the Cycles 4 and 5 additional \( \gamma \)-scan results are available. A preliminary comparison of calculated and measured \(^{140}\)Ba-distributions show a promising good agreement. The detailed analysis will be performed in the near future.

6. What is a Production Code

The simulation of the physical behaviour of a complicated system like a nuclear power reactor on a digital computer requires very large, sophisticated mathematical models. If computer models should be used as tools within nuclear fuel management activities, some specific aspects should be considered in the development of such codes. The following section describes some basic points.

- Who shall use the code?
  The design of a code is (or should be) dependent on the abilities and interests of its users and on the tasks that have to be accomplished by the code. As a general rule, only the bare minimum of quantities should be input, all other parameters should be assigned default values by the code. The average user will then use the standard default parameters, whereas the specialist can use parameters of his own choice. This approach also ensures that for all standard applications the procedures followed by the code-users are the same, and a comparison of results is done more easily.
  Examples: Determination of the mesh-layout in a nuclear lattice code should rather be done by the code than by the user. Parameters used in numerical methods (e.g. relaxation parameters) should be preset by the code.

- How shall quantities be given in input?
  During the development of a model on a digital computer, most efforts are usually put on the model itself, and quantities are very often input in a format most suitable for the computer. Comparatively little effort is spent for the input processor. For a user not familiar with the code, input becomes impractical or impossible.
  As a general rule, all input quantities should be given in macroscopic units that can directly be taken from the specifications of the problem to be solved. The code then converts the quantities to those being used internally.
  Examples: Water and steam densities: The user only specifies the temperature, the code determines water and steam densities and saturation pressure.
  Number densities: A code that requires the user to calculate number densities will never be used as a production code.
  Quantities referring to geometrical locations (control rods, fuel elements) should be input by the coordinates familiar to the user, perhaps with different optional coordinate references for different users.
A reactor simulator to be used by the reactor engineer on site has to use data provided by the process computer, and has to produce an output sheet similar to that which the process computer prints out.

. How should the input be organized?
Data input should be such that misinterpretation by the code is reduced to a minimum. Most errors occur when data have to be punched in specific columns on a card, and punched cards have to be sequenced in a given order. A good input routine has therefore the following features:

- free format (not position dependent)
- sequence of punched cards or card images
  arbitrary or almost arbitrary. Each card
  has therefore either an identifier (numeric or literal) specifying its type, or the
  input is in NAMELIST - format with individual assignments of values to variables.

. Restart options, data files, library files
Reactor Physics calculations are usually executed in a series of single calculations, each of which uses the results of the previous calculation and passes its results over to the next calculation (e.g. core follow, step through cycle). For a production code, these restart files contain all information needed to specify exactly the case that was run to produce the restart file, such as geometry, core loading and fuel type maps, power, void, core flow, neutron flux distributions, but also the cross section tables for each fuel type used for interpolation. The input routine is then set up in such a way that the restart file identifier is specified in the input, and subsequently all data are taken over from the restart file. The user then only specifies the data that differ from the data set on the restart file, and no other data and/or library files are needed.

The structure of the restart file must be independent of the parameters chosen in the case that produced the file, within some boundaries, such as problem size.

In nuclear lattice calculations, the libraries are not copied onto the restart file. The latter, however, should again contain all restart parameters.

. Output files to be used with other codes
Nuclear lattice physics could produce condensed few group cross sections and related parameters that are subsequently used as cross section libraries in core simulators. Usually this output file is being processed by an auxiliary code to extract the specified parameters for the simulator, but it also serves as a source of information for the program user. Its format should be such that extensions are readily incorporated without any need to modify the interface programs to other codes. It has been found that a format with coded card images and keywords to structure the data is extremely flexible and useful (12). The interface program then searches for the specified keywords and the corresponding data.
7. Conclusions

We have simulated the physical behaviour of the Mühleberg BWR through 5 operating cycles with the code package PMS. The agreement between measured and calculated power distributions is good, taking into account the uncertainties resulting from the incore instrumentation (TIP). Gamma scan measurements have been performed to compose bundlewise axial and radial end-of-cycle power-distributions (i.e. Ba-140). This model independent information allowed an additional fine tuning of some shape dependent parameters.

The quality of the results obtained from a simulator has to be checked with experimental data as often as possible. Only a carefully calibrated simulator enables a user to do efficient fuel management work.

In order to be a tool in nuclear fuel management, a production code has to have a flexible input, built-in standard default values, and a suitable file handling. More efforts have to go into this area of code development.

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CALCULATIONS WITH THE EIR LIGHT WATER REACTOR CODE SYSTEM

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ABSTRACT

A computer code system for core calculations in light water reactors has been developed during the last several years. Accuracy, computing speed and data management aspects of the nodal diffusion method used to determine the 3-dimensional flux distribution are discussed. The performance of the code system is demonstrated for a startup experiment of the Mühleberg boiling water reactor.

1. INTRODUCTION

At EIR a small group of scientists has worked on LWR calculations for about ten years now. The purpose of this work is to support the Swiss industry and utilities in their calculations of operating power reactors and to perform advanced fuel cycle studies. During the last few years criticality calculations for various fuel element storage pools have been performed. A study on the utilization of thorium in LWRs is in progress.

The first computer code system /1-2/ which had been developed was not sufficiently accurate for certain applications, e.g. for reactors containing a burnable poison in the fuel. An entirely new code system was then conceived. Its main components are the library program STOBOX, which generates multi-group cross sections from the ENDF/B data files, the fuel element homogenization program BOXER /3/ and the reactor program SILWER.

Three quarters of the SILWER computing time is spent by the flux calculation which is based on a nodal diffusion method with the quadratic transverse leakage approximation /4/. The two flux programs that are available in SILWER are compared in Section 2 of this paper. In NODLEG the convergence is accelerated by means of the conventional single-level coarse-mesh rebalancing method and lines and planes are used to transfer data between disk and core storage. MCRNOD contains a multi-level coarse-mesh rebalance method and organizes the data in the form of almost cubical blocks /5/.

Section 3 describes the first application of the entire code system to a startup experiment of the Mühleberg nuclear power station. When calculated results are compared with those of a more exact method or with measurements, a standard to judge the observed
deviations is useful. Table I lists predictive accuracies for some important reactor physics parameters which were established at an IAEA panel and which are valid for all types of power reactors /6-7/.

**Table I** Predictive Reactor Physics Accuracies

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Accuracy (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Target</td>
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<tr>
<td>Reactivity:</td>
<td></td>
</tr>
<tr>
<td>Initial life-time</td>
<td>0.2-0.5</td>
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<tr>
<td>Life-time</td>
<td>2-5</td>
</tr>
<tr>
<td>Power distribution:</td>
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</tr>
<tr>
<td>Axial</td>
<td>3-5</td>
</tr>
<tr>
<td>Burnup and isotopic composition</td>
<td>2</td>
</tr>
</tbody>
</table>

2. 3-DIMENSIONAL FLUX CALCULATION

2.1. Computer Properties

Before discussing data organization some pertinent computer properties will be introduced in this Section. Although the numbers given are correct only for the CDC 6400 computer used by EIR, the conclusions may also be valid for other machines.

The core memory capacity of our computer is 100 K words (1 K = 1000). The two diffusion programs of SILWER have a length of 20 K words so that the core space available for the flux and coefficient data is 80 K words.

An approximate formula for calculating the computing cost CT (sfr) is given by

$$CT = (0.36 + 0.48 \text{ CM}^2) \ CP + (0.27 + 0.24 \text{ CM}^2) \ IO,$$

where CM = 0.03 · core memory (K), CP = central processor time (sec) and IO = input-output time associated with data transfer (sec). The cost function depends strongly on the core memory size.

Fig. 1 shows that it is advantageous to keep the number of data transfers between disk and main storage small. The IO-time needed to transfer 1 million words is 16 sec.
2.2. Storage Requirement

The nodal diffusion method /4/ uses a Legendre polynomial expansion of order \( N = 0,1,2,3, \ldots \) to represent the spatial shape of the flux within a mesh. The number of flux moments that have to be stored per mesh and group is equal to \( MP = 1 + \text{Max.}(0,(N-2) \text{ MD}), \) where MD is the number of dimensions. In addition \( MP = 2 \cdot \text{MD} \) outgoing currents and MD net leakages have to be saved during the flux iterations. These \( MP + MF + MD \) quantities are hence called "flux data".

The new outgoing currents are calculated from the relation

\[
J_i = \sum_{k=1}^{MQ} E_{ik} Q_k + \sum_{j=1}^{MF} R_{ij} I_j,
\]

where \( MQ = 1 + \text{Max.}(0,(N-2) \text{ MD}) \) is the number of source moments \( Q \) per group. The \( MF \cdot MQ + MF \cdot MF \) nodal coefficients \( E \) and \( R \) are calculated before the flux iterations are performed. They are stored together with the cross sections, and these quantities will be called "coefficient data". The number of cross sections per mesh is \( 4 \cdot MG + MS \), where MG is the number of energy groups and MS the number of scattering terms different from zero.

The flux and the coefficient data are stored in separate blocks on disk. The flux quantities are read and written during the iterations, while the coefficients are read only. For a two-group fourth-order approximation in 3 dimensions 20 flux and 165 coefficient quantities are needed in each mesh.

The convergence is accelerated by means of coarse-mesh re-balanceing /5/ and asymptotic flux extrapolation /8/.

In the coarse-mesh rebalance method the group structure and the mesh grid are collapsed into a coarser representation. The
storage requirement per coarse mesh is \((5 + MF)\) MGC + MSC, where MGC and MSC are the number of groups and scattering terms in the coarse representation.

To perform the asymptotic extrapolation the flux quantities in the present and the previous outer iteration are needed.

2.3. Program NODLEG

In NODLEG the planes that are perpendicular to the x-axis form the flux blocks. The block whose flux quantities are being determined and its two neighbouring blocks reside in core at the same time. For the asymptotic extrapolation the old flux quantities are placed into one of the two neighbour blocks. The coefficients are stored as lines with varying z-index.

The coarse-mesh grid is defined by an input parameter which indicates the number of fine intervals within a coarse interval. NODLEG uses a one-group scheme and keeps the coarse-mesh data always in core. A rather tight convergence criterion of 0.1 times the input flux convergence parameter was found to be the optimum value for the coarse grid.

A BWR with a power around 1000 MWe contains in the order of 600 fuel elements. If the mesh width is equal to the fuel element diameter, the grid will contain about 30·30·25 meshes. For such large problems NODLEG fills almost the whole core memory so that the costs of the calculation will be high. Some reduction in the size can be obtained by using larger meshes in the coarse grid. However, this procedure causes a slower flux convergence.

Table II compares results for the 3-D IAEA LWR benchmark problem /9/ which were obtained with the finite difference diffusion program VENTURE /9/ and the nodal programs QUANDRY /10/, IQSBOX /11/ and NODLEG. The nodal programs used a mesh grid division of 9·9·19 nodes corresponding to one mesh per fuel assembly. The error caused by the flux calculation is one contribution to the total calculative error. Table II shows that the reactivity error is very small. The error in the assembly power distribution of the nodal method lies near the lower target limit (c.f. Table I). The NODLEG computing time is larger than that of the most advanced nodal programs.

<table>
<thead>
<tr>
<th>Program</th>
<th>Order of approx.</th>
<th>Error in keff (%)</th>
<th>Max. power error between assemblies (%)</th>
<th>Computer</th>
<th>CDC-6600 time(min)(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>VENTURE</td>
<td>1</td>
<td>-.007</td>
<td>2.1</td>
<td>IBM 360/195</td>
<td>700</td>
</tr>
<tr>
<td>QUANDRY</td>
<td>(\infty)</td>
<td>.001</td>
<td>0.7</td>
<td>IBM 370/168</td>
<td>0.7</td>
</tr>
<tr>
<td>IQSBOX</td>
<td>5</td>
<td>.008</td>
<td>0.9</td>
<td>CDC 6600</td>
<td>1</td>
</tr>
<tr>
<td>NODLEG</td>
<td>4</td>
<td>-.008</td>
<td>1.3</td>
<td>CDC 6400</td>
<td>1.7</td>
</tr>
<tr>
<td>NODLEG</td>
<td>5</td>
<td>.005</td>
<td>1.0</td>
<td>CDC 6400</td>
<td>2.1</td>
</tr>
</tbody>
</table>

\(a\) Obtained by assuming 1 min CDC 6600 = 0.5 min IBM 360/195 = 2/3 min IBM 370/168 = 4 min CDC 6400 /12,13/.
2.4. Program MCRNOD

According to the last Section shorter computing times and a variable size of the main storage are desirable. Recently, a multi-level coarse-mesh rebalance method and a flexible data organization were developed by Honeck at EIR /5/. The nodal method with Legendre polynomials was coupled with Honeck's method, and the resulting program was called MCRNOD.

Fig. 2 illustrates a 3-level mesh. The first level is the fine grid itself. In each of the following levels the interval number is reduced by a factor of 2 for each direction. Brandt /14/ provides a simple explanation for the effectiveness of the multi-level iterative strategy. Assume that a Fourier analysis is done on the error in the solution at a given level. The error would be a sum of components of different frequencies. The high frequency errors are associated with errors between a node and its nearest neighbours. Simple iteration is very effective at reducing high frequency errors. The low frequency errors are associated with errors between nodes widely separated in the mesh. Iteration on the coarse mesh is no more effective in reducing low frequency error than is iteration on the fine mesh, but it is much faster. Therefore, low frequency error can be reduced using fast coarse mesh iteration.

The rebalance factors for the fine-mesh solution become discontinuous because they are the product of the rebalance factors of the different levels. To smooth out these discontinuities coarse-mesh iterations can be performed in the first level before applying the corrections to the nodal equations. From different test cases an optimum value of one smoothing iteration was derived for the MCRNOD program.

The multi-level coarse-mesh method relies on performing only a few iterations at each level before moving on to the next coarser level. A simple and effective method was found to terminate iteration at one level. The rebalance factors, $\delta$, approach unity as the problem converges. The difference $\delta - 1$ is a measure of the size of the correction being applied to the next finer level. The iteration is terminated when the relative change in the maximum $\delta$ between successive iterations is less than some criterion $\varepsilon_\delta$, or
when the relative change in the maximum $\beta$ between successive iterations is less than some criterion $\varepsilon_\beta$. The $\varepsilon_\beta$ terminates the iteration during the early cycles while $\varepsilon_\beta$ terminates the iteration during later cycles. A rather large value of $\varepsilon_\beta = 0.1$ was found to be optimum for MCRNOD. For $\varepsilon_\beta$ the fine-mesh flux criterion is used.

The organization of data in main and disk storage is called the Data Cube approach. It cuts the data into roughly cubical units, the volume blocks. Surface blocks are used to couple the volume blocks together (c.f. Fig. 3).

Originally the volume blocks contained the flux and coefficient data. In MCRNOD a volume block is divided into a flux block and several coefficient blocks. Before moving on to the next volume block the outgoing currents and net leakages at the block boundary have to be placed into the corresponding surface blocks.

For a given main storage space first the number of volume blocks is minimized to minimize disk transfer. Then the volume of each block is maximized to make the surface-to-volume ratio as small as possible.

For the solution of the nodal and multi-level coarse-mesh equations the five following separate processes are executed (in brackets the associated disk transfers are mentioned):

1. Set Up the surface blocks prior to starting the iteration (read flux blocks).
2. Iterate the coarse-mesh equations (read and write flux blocks).
3. Update the outgoing currents and flux moments using the nodal equations (read coefficient and flux blocks and write flux blocks).
4. Edit the coarse-mesh equations into the next higher level (read and write flux blocks).
5. Correct the solution of a level using the results of the next higher level (read and write flux blocks).
In NODLEG only the data transfers of the steps 3 and 5 are performed. The Edit-process is done directly during the nodal calculation.

The asymptotic extrapolation procedure is performed for the average fluxes only in MCRNOD. The remaining flux quantities are multiplied by the ratio of the extrapolated to the unextrapolated average flux. This procedure is less effective than extrapolating each flux quantity separately, as is done in NODLEG.

The 3-D IAEA problem was calculated with MCRNOD and NODLEG with a 9.9.19 mesh division. NODLEG required a core memory size of 36 K words, while MCRNOD had a 44 K memory at its disposal. Table III shows the fine grid data organization.

### Table III Data Organization for 3-D IAEA Problem

<table>
<thead>
<tr>
<th>Program</th>
<th>Flux blocks&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Coefficient blocks</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>WN</td>
<td>NB</td>
</tr>
<tr>
<td>MCRNOD</td>
<td>40</td>
<td>9.5.7</td>
</tr>
<tr>
<td>NODLEG</td>
<td>20</td>
<td>1.9.19</td>
</tr>
</tbody>
</table>

<sup>a</sup>WN = words per node, NB = nodes per block, WB = words per block, B = number of blocks, W = total number of words.

MCRNOD needs 20 additional words per node for the coarse-mesh coefficients in level 1. NODLEG omits the dummy nodes in systems with irregular boundaries and considers diagonal symmetry for the coefficient transfers. This is the reason that the number of data that have to be transferred is smaller in NODLEG than in MCRNOD.

### Table IV Iteration Number and Computing Time for 3-D IAEA Problem<sup>a</sup>

<table>
<thead>
<tr>
<th>Program</th>
<th>Nr.of iterations</th>
<th>CP-time (min)</th>
<th>IO-time (min)</th>
<th>Relative cost</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Update C.M.</td>
<td>Coef. Update C.M.1 C.M.2-4 Total</td>
<td></td>
</tr>
<tr>
<td>MCRNOD</td>
<td>34</td>
<td>280</td>
<td>0.8</td>
<td>6.2</td>
</tr>
<tr>
<td>NODLEG</td>
<td>35</td>
<td>560</td>
<td>0.8</td>
<td>5.3</td>
</tr>
</tbody>
</table>

<sup>a</sup>5 degree symmetry, 4th order approximation, flux convergence criterion = 0.0001. C.M. = Coarse-mesh grids, C.M.1 = Coarse-mesh grid level 1, C.M.2-4 = Coarse-mesh grids levels 2-4. 2 fine intervals per coarse in NODLEG.

Table IV compares iteration numbers and computing times. With a less effective extrapolation procedure MCRNOD needs the same number of fine grid iterations as NODLEG. The number of iterations in the coarse grids is reduced by a factor of 2 by the multi-level rebalance method. However, CP- and IO-times and the computing cost of MCRNOD are considerably larger. Therefore, NODLEG is used at present for the routine calculations in SILVER.
3. KKM STARTUP EXPERIMENT

The BWR of the Mühleberg nuclear power station (=KKM=Kernkraftwerk Mühleberg) produces a rated power of 947 MWth or 320 MWe. A startup experiment was performed on April 10, 1972 with a thermal power of 418 MW at an average fuel burnup of 165 Mwd/tU. Axial fission rate distributions were measured with the TIP-system (=transverse in-core probe system). The TIP-detectors are miniature U-235 fueled ionization chambers. A radial power distribution was deduced by the process computer from these measurements. The experimental error of the TIP-curves and of the radial distribution is in the order of 10 % and errors up to 15 % may occur at the core-reflector boundary /15/.

The recalculation of the experiment with the EIR code system will now be described and possible sources for inaccuracies will be mentioned.

70-group cross sections were generated with ETOBOX from the ENDF/B-4 data file. The resonance parameters of U-238 were modified according to Tellier /16/ leading to a reduction of the resonance absorption. The corresponding reactivity increase amounts up to 1 % for LWR cells.

The BOXER fuel element calculations were performed for fuel temperatures of 520 and 720ºC, for volumetric void contents of 0, 40 and 70 % and for burnup values of 0, 100 and 400 Mwd/tU. The spectrum of an average fuel cell was used to condensate the cross-sections of the different materials to 6 energy groups. This group number is unsufficient for high void contents. An increase of 1.5 % in \( \kappa_{eff} \) was observed if 8 or 12 energy groups were used for a case with 70 % of void. For a 0-void element the corresponding increase is 0.2 %.

The fuel cells were homogenized in space for the 2-dimensional calculation of the element. A heterogeneous treatment of the fuel rod may increase the reactivity by 1-2 % for fuel elements containing burnable poison pins /17/. For the KKM fuel elements which contained burnable boron-steel curtains but no 9d-cells a smaller heterogeneity effect may be expected.

The BOXER control rod homogenization procedure underestimates the control rod reactivity worth. A value of 0.7 % is possible for the KKM startup experiment /18/. In fact, the power values of the KKM fuel elements containing control rods are generally overestimated by the calculation (c.f. Fig. 4).

The 2-D calculation was performed with a diffusion program using modified diffusion coefficients for heavily absorbing materials. Errors in the order of 1 % in reactivity can occur /19/.

The fuel elements were kept critical by means of a boundary-albedo search. A more realistic consideration of the actual environment of a fuel element can cause significant changes in the calculated reactor power distribution which may amount up to 10 % at the core boundary /20/.

The tables of the homogenized 2-group macroscopic group constants of the fuel elements were transformed into second order polynomial functions (cross section correlation) /21/. The average accuracy for the representation of the tables is 0.2 %, and larger errors may originate from the necessary interpolation.
The reactor program SILWER contains a BWR and a PWR thermo-
hydraulics program /22/. The Nabizadeh- and the Dix-model can be used
for the free parameters of the void-quality correlation. In a test
case which contained one single fuel element the Dix-model produced
a higher void content of 7 % and a reactivity reduction of 1 %.

The reactor calculation was performed in a quarter core
geometry with 10 x 10 x 26 meshes using reflective conditions on interior
boundaries. The reflectors were assumed to consist of pure water. A
fourth order flux approximation and the Nabizadeh model were used.

A first calculation was performed using the control rod
pattern and the power of the startup experiment at zero burnup. The
calculated $k_{eff}$-value was 1.031. Thus, control rod insertion was too
small, and the power was overestimated for certain nodes. Correspon-
dingly, their burnup will be too large leading to an overestimation of
the reactivity drop. One can learn that the operation history of the
reactor should be followed as closely as possible.

Then, the reactor was burnt to an average burnup of 165
MWD/tU with an intermediate flux-void calculation at 30 MWD/tU. At
165 MWD/tU the calculated eigenvalue was 0.993 which corresponds to
a reactivity loss of 3.8 %. From the results of the fuel element cal-
culations a maximum loss of 2.5 % is expected. This difference could
not yet be understood. The average void content at 165 MWD/tU was
19.9%.

![Fig. 4 KKN at 165 MWD/tU: Comparison of Measured and Calculated Radial Power Distribution](image_url)
Fig. 4 compares the calculated and measured power distributions in the fuel elements. The result of the old code system which used the FLARE-EIR program is also included. The SILWER results show a maximum deviation of 15% and a root mean square error of 5%.

Calculated and measured axial power distributions are illustrated in the Figs. 5 and 6. The average fission rate over the 12 TIP-positions was normalized to 100. The maximum relative error of the SILWER calculation is 30%, and the average error is 10%.

FIG. 5 TIP-CURVE NR. 1 FOR KKM AT 165 MWD/TU
The convergence criteria used were 0.003 for the power between void-flux iterations and 0.001 for the flux between outer iterations in NODLEG. According to the 1-element test case 4 to 6 flux iterations before a new void calculation is performed are the optimum value and 5 flux iterations were used for the startup experiment. Tsuiki \cite{23} also recommends a small flux-iteration number.

8 void-flux iterations were needed at 0-burnup for convergence, and the corresponding CP-time was 41 min. They are composed of 3 min for the thermohydraulics calculation, 6 min for cross section interpolation, 15 min for the nodal coefficients and 17 min for the flux iterations. For the same calculation the program FLARE-EIR took 2 min.

One burnup step requires 0.5 min of computing time. At the following two time-points (at 30 and 165 MWD/tU) the number of void-flux iterations was reduced to 5 and the corresponding CP-time is now 25=3+4+9+9 min.

4. CONCLUSIONS

The startup experiment that was performed at 165 MWD/tU in the Mühleberg boiling water reactor is a severe test for a core calculation code system. The results depend strongly on the burnup distribution and therefore on the actual operation history. The power level of 50 % of the rated value requires a greater accuracy from the control rod calculation and from the thermohydraulics correlations than the normal operating conditions.
The radial power distribution was recalculated almost within the experimental error with the EIR code system. In comparison to the old system an improvement can be observed in the fuel elements containing control rods and in the core boundary elements. The axial power distribution is underestimated in the lower part of the core and overestimated in the upper part. Possible causes for predictive inaccuracies which were identified in the paper are: The basic cross section data, the homogenization of the fuel elements, the cross section correlation and the 3-dimensional thermohydraulics and flux calculations.

The error of the TIP-measurements is larger than the predictive accuracy target. More reliable experimental results are available from the bundle gamma scan measurements which were performed at the end of the first KKM reactor cycle. The recalculation of these experiments is a task for the future.

SILWER needs an order of magnitude more computing time than the old FLARE-EIR program. This is the price that has to be paid for the increased accuracy of the flux calculation. Unfortunately, the multi-level coarse-mesh rebalance method does not lead to an increased computing speed for medium sized problems. However, a gain may be expected for large and slowly converging problems.

The Data Cube approach offers a flexible organization of data in disk and main storage with a free choice of the size of the core memory. In combination with the nodal method the possibility to omit the unnecessary data transfer of the dummy meshes for systems with irregular boundaries should be introduced.

ACKNOWLEDGEMENTS

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VALIDATION OF A FLARE TYPE BWR SIMULATOR

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Summary

Validation work is reported using information obtained at the 50 MWe BWR with natural circulation at Dodewaard. Using input from LWRWIMS and BORREL, eigenvalues for ten cycles have been calculated with actual control rod positions. Power distributions measured with incore instrumentation and gamma scanning are compared with calculated values. The information that exists on the thermal hydraulics is discussed. Good agreement is obtained, the eigenvalues deviate .005 and the radial power with less than 3%. A systematic discrepancy has been observed in the axial power distribution.

Introduction

KEMA uses extensively a FLARE/1/ type BWR simulator for the fuel management and optimization of the 50 MWe natural circulation BWR at Dodewaard (the Netherlands) /2/. The formulation is that of FLARE-JAERI /3/ with some improvements of FLARE-APDA /4/.

A number of options has been added by KEMA. The most important ones are the automatic calculation of the Haling distribution, the calculation during a cycle of critical control rod patterns with a best fit to the Haling power distribution and the effect of Gd-poisoning /5/.

Neutronics input

The neutron physics input for BWRSIM is obtained from LWRWIMS /6/.

This code is used with a 28 groups-library. First a rough flux distribution in 28 groups is calculated with multi-cell and multi-region collision probabilities. The cross sections for all materials (about 30) are then condensed to 6 groups using the collision probability flux distribution. A fine flux distribution in 6 groups is calculated from which the eigenvalue and the power distributions are derived.

In addition to the validation work performed at Winfrith /6/, we have compared the power distribution from LWRWIMS with our own experiments. For a number of cases, cold irradiations as well as power irradiations, we found general good agreement. A typical case is given in table I for a 2.8% enriched uranium element with a burnup of 7 MWD/kg. The standard deviation between experiment and calculation is 3% which is the experimental uncertainty. We have excluded the pin f6 which shows a large discrepancy due to the
### Table I  
**Burnup distribution of a 2.8% enriched uranium element**

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>Experiment calculated</th>
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</thead>
<tbody>
<tr>
<td>a</td>
<td>1.33</td>
<td>1.23</td>
<td>1.17</td>
<td>1.16</td>
<td>1.15</td>
<td>1.18</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.32</td>
<td>1.24</td>
<td>1.15</td>
<td>1.12</td>
<td>1.17</td>
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<td></td>
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<tr>
<td>b</td>
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<td></td>
<td></td>
<td></td>
<td>.92</td>
<td></td>
</tr>
</tbody>
</table>

### Table II  
**Burnup distribution with a control rod inserted**

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
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<tr>
<td>a</td>
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<tr>
<td>d</td>
<td>.93</td>
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<td>1.34</td>
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<tr>
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<td>1.03</td>
<td>1.18</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>e</td>
<td>.97</td>
<td>1.29</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>f</td>
<td></td>
<td>1.01</td>
<td>1.19</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

|   | 1.35|     |     |     |     |     |
| f |     | 1.39|     |     |     |     |
influence of a stainless steel instrument tube adjacent to that position.
In Table II the burnup distribution is given for the same element at a position where during the irradiation a control rod has been inserted. In this case the burnup distribution was derived from the power distribution calculated with a $S_n$ theory. The discrepancies here are larger, about 7% standard deviation, partly caused by the larger experimental uncertainty. The maximum deviations are near the water filled spacer capturing rod at the position C3. This may be improved by a better subdivision of materials in the cross section collapsing procedure.

Thermal hydraulic input

The thermal hydraulic input is obtained from the program a further development of the program VOIDFLOW /7/. For each channel a stress of the inlet velocity and steam quality is given in the first iteration. At each segment the energy input is calculated for a given power distribution. The void fraction is obtained from the quality increase and a steam slip correlation function from Machaterre /8/. The driving head is calculated from the void fractions and friction losses are determined using the two phase flow multiplier from Martinelli-Nelson /9/. In the downcomer special care is given in treating the carry over and the collapsing of the steam bubbles below the sparger. A new estimation on the inlet velocities can be obtained from the condition that the pressure differential of each channel and the downcomer should be the same. The calculations are then repeated until convergence is reached.

From an extensive set of BORREL calculations a simple correlation function has been derived of the inlet velocity as a function of channel power for use in BWRSIM. At the full power condition the inlet velocity varies only very little for all elements. The quality slip correlation has been transformed in a quality void relation.

Measurements with an instrumented fuel bundle equipped with a turbine flow meter in 1971 gave a flow which was 20% lower than calculated with BORREL. Velocity measurements in the downcomer using a temperature noise correlation technique show the same trend. Recently a set of measurements has been carried out using the neutron noise correlation technique. A twin detector was inserted in an instrument tube and the noise correlation was calculated for different time lags between the signals of both detectors. The maximum of the correlation function gives then the average time of the steam bubbles causing the detector fluctuations, to travel from one detector to the other. In figure 1 the velocity distribution is given together with the calculated steam and water velocities. The interpretation of these measurements is difficult as the noise measured by the detector is of a very local nature whereas the correlation functions in use predict average quantities. The self power neutron detector is influenced by steam bubbles that are in the region between the four corner rods of the neighbouring elements. Only steam bubbles that live longer than 100 ms will contribute to the correlation function. These will be, at the subcooled boiling level, larger than average bubbles that will rise more rapidly. Thus between .5 m and 1.0 m a higher velocity is measured. At larger void fractions there is a tendency of the voids to coalesce in the centre of the bundle /10/, which would leave only smaller voids at the corners of the elements and an apparent lower steam velocity is measured above 1.0 m.
Eigenvalue prediction

We have calculated with BWRSIM for the nine cycles completed thus far and the cycle that is not yet finished the eigenvalues as function of burnup (figure 2).

For the control rod positions time averaged values have been used, which give rise to anomalies for those cycles in which the control rod patterns varied. The discrepancies are of the order of .005 Δk/k with the exception of the first cycles and the beginning of the last cycles. During cycle 1a the reactor was operated with boron steel curtains in order to reduce the excess reactivity to an acceptable level. The effect of these curtains has obviously been calculated erroneously as can be seen from the change in eigenvalue between cycles 1a and 1b, when these curtains were removed.

An interesting fact is the reduction of reactivity level between cycles 5 and 6 that may be due to the removal of the zircaloy control rod followers or to the switchover from the 2.5% enriched uranium elements to the 2.8% enriched elements containing burnable poisons. The burnable poison gadolinium seems to be the cause of the variation in the eigenvalue during the early part of the cycles 5 to 10, as the discrepancy seems to disappear at the time we expect that most of the Gd has burned away. The cycle length can be predicted with a deviation of 10 days. Using a bias of k = .996, cycle 7 was 15 days too short, cycle 8 5 days and cycle 9 10 days too long. What is of course more of academic interest, as a near optimum stretchout period is employed. Variations in cycle length should therefore bear no economic penalty.

Power distribution using incore instrumentation

The standard power distribution measurements use U-235 fission chambers TIP that can be moved in a number of channels. Assembly power is then calculated by the program TIPPEL using a number of void and burnup dependent factors. This of course obscures the distinction between calculation and experiment. We prefer therefore, for validation purposes, to calculate the fission rate of the TIP detectors from the BWRSIM values. For this purpose we weight the power of the adjoining elements with 1/k_0. This method assumes that Σa is independent of burnup and void. It is remarkable that this simple to implement scheme is in agreement, within a few percent, with the method used by Gibson /6/ who compared the fission rate of the TIP detector to the average fission rate as calculated by LWRWIMS. For three burnups during cycle 9 we give measured and calculated distribution for the available channels in figure 3, 4 and 5. In figure 5 the average fission rates for each channel is given. The standard deviation between TIP (T) measurements and BWRSIM (B) calculations is .03. The deviations for the axial distributions are larger. At the peak power position they reach .15. For the time the peak is at the top (figure 3) or at the bottom (figure 4) the deviations are more pronounced than at EOC. We have not taken the space grids explicitly into account. The grids may cause heavy perturbations k_0 being about .1 lower for the 50 mm height of the grids. The grids are positioned in some instances at the maximum flux. The effect of the grids can clearly be seen at the experimental curves. An other possible explanation is the kernel used in the calculation of the power distribution of BWRSIM. The contribution of the element itself to the next generation power is negative, to compensate the larger contributions of the neighbours.
Gamma scans

By gamma scanning the radioactivity distribution of certain fission products can be determined. During the refuelling period, at the end of cycle nine, we were in the position to measure all the elements in an octant of the reactor. This gave representative information as the reactor is operated in octant symmetry. Various average power distributions may be obtained by looking at fission products with different half lives. La-140 (T½ = 12.7 d of the mother Ba-140) gives the power distribution during the stretchout period. Zr-95 (T½ = 65.5 d) during the last months of operation and Pr-144 (T½ = 284 d of the mother Ce-144) of the last cycle. A drawback is the fact that only the outer fuel pins contribute to the signal and that the yields of the fission products are dependent on the fissioning isotope. The first point is reduced somewhat in so far the power distribution across elements is fairly flat and for the second effect corrections are calculated. A small program ISOMIS has been written to calculate the averaged power distribution eq. 1

\[ P_i = \frac{I - \int P_i(t) e^{\lambda t} dt}{\sum_{i=1}^{\infty} \int P_i(t) e^{\lambda t} dt} \]

where I is the total number of segments and \( \lambda \) the decay constant of the isotope of interest.

In table III the measured radial radioactivity distribution GAMMA of La-140 is given together with values obtained from BWRSIM and the TIP interpretation programm TIPPEL. The agreement between GAMMA and BWRSIM is good, the standard deviation is .04 which is of the same magnitude as the experimental uncertainty. Deviations with TIPPEL are fairly large up to .2 due to the extrapolation scheme used in TIPPEL to obtain the power of the outer elements.

In table IV the distribution for Zr-95 is given. The standard deviation is .05 again of the same magnitude as the experiments. The Pr-144 distribution shows large deviations due to the poor statistics and the complication that contributions to the radioactivity of this isotope of various cycles have to be considered. In figure 5 the axial distributions of La-140 and in figure 7 of Zr-95 for a number of elements along one of the axes is given. The effect of the spacers can well be observed. Obvious is also an underprediction of the lowest and highest segments. The trend in the deviations is consistent with the one observed by the comparison with the core instrumentation. The standard deviation of the gamma measurements and the calculated distributions of .07 is clearly larger than the experimental uncertainty of .03.

Conclusions

The combination of BWRSIM with input from LWRWIMS and BORREL can calculate the full power eigenvalues of the Dodewaard BWR with an accuracy of .005. Cycle length can be predicted with an uncertainty of 10 days using an experimental bias of \( K_o = .996 \). Radial power distributions are predicted to within the experimental uncertainties. The axial power distributions show some systematic discrepancies. Improvements of the code are expected from a better treatment of the Gd-poisoning, of the modification of the power kernel to a collision probability kernel and of the explicit representation of the spacer grids.
Table III  La-140 activity distribution

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σ = 0.04

Table IV  Zr-95 activity distribution

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σ = 0.05
FIG 1 EXPERIMENTAL AND CALCULATED VELOCITIES  EOC 9
Fig 2  Calculated Multiplication with BWRSIM
Figure 3 Fission Distribution Measured by TIP Detector

BU-CORE 10,144 MWd/kg
Fig 4  Fission distribution measured by TIP detector
FIG. 5 FISSION DISTRIBUTION MEASURED BY TIP DETECTOR
FIG. 7  AXIAL ACTIVITY DISTRIBUTION OF Zr-95
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A method has been developed to optimally determine the adjustable parameters of FLARE-type simulator to best fit the operating data on power distribution. The steepest gradient method is adopted for the optimization. This method has also been applied to modify the void-quality relation model by introducing an adjustable parameter. To overcome a problem of dependency of the critical eigenvalue on operating conditions, an adaptive learning algorithm has been developed to determine the critical eigenvalue from the observed operating history.

I. INTRODUCTION

The coarse-mesh program FLARE (1) is one of the most practical core simulators for in-core fuel management and core control planning, because of its short computer-time and small memory requirement. A drawback of FLARE-type simulator is that it requires a priori preparation of adjustable parameters (albedo and mixing factors of nodal coupling kernels), and the accuracy of calculated power distribution significantly depends on these parameters.

To overcome this drawback, it is desirable to develop a systematic tuning method of the FLARE parameters. A method has been developed to optimally determine the adjustable parameters of FLARE-type simulators to best fit the operating data on power distributions, and the accuracy of the FLARE is examined using the traversing in-core probe (TIP) data of an operating plant (2). The application of the parameter optimization technique has been extended to modify the void-quality relation by introducing an adjustable parameter to reduce the error in the calculated TIP readings.

The critical eigenvalue is required to predict power level, core flow rate and control rod pattern during reactor start-up, control rod swap and load following operations. It is also used to predict core cycle length. The critical eigenvalue should be unity in an ideal simulator, however, in the actual cases, it depends on the operating condition due to the incompleteness of the core simulator. Therefore, it is desirable to develop an adaptive learning algorithm to determine the critical eigenvalue from the observed operating history, and in this paper a method for this purpose is proposed.

Generally speaking, it is a right way to develop a precise core simulators without adjustable parameters, because they are able to predict core performance without any a priori knowledge of operating data. However, for some specified purposes, such as in-core fuel management and power maneuvering planning, FLARE-type simulator, with proper model adjustment techniques, is to be an economical and practical tool for core simulation.
Fig. 1 Measured and calculated TIP readings at 1.85 GWD/t
II. PARAMETER OPTIMIZATION FOR POWER DISTRIBUTION CALCULATION

II.1 FLARE Model

A brief outline of the FLARE model is presented. The neutron balance equation is

\[ S_\ell = \left( \frac{\beta_{10K}}{\lambda} \right) \left( \sum_\mathbb{M} W_{\mathbb{M}\ell} S_{\mathbb{M}} + \left\{ 1 - (b - \alpha_{\ell}) h_{\ell} \right\} S_\ell \right), \tag{1} \]

where
- \( \lambda \) = eigenvalue
- \( S_\ell, k_{\ell}, c_\ell \) = neutron source, multiplication factor, and albedo of spatial node \( \ell \), respectively
- \( W_{\mathbb{M}\ell} \) = nodal coupling kernels or probability that a neutron born at node \( \mathbb{M} \) is absorbed at node \( \ell \).

The summation \( \sum_\mathbb{M} \) is over the six nearest neighbors.

The multiplication factor, \( k_{\ell M} \), is given by a regression formula of the void fraction, power density, xenon number density, fuel exposure, and control rod fraction at node \( \ell \) for each fuel type. The kernel, \( W_{\mathbb{M}\ell} \), is given by

\[ W_{\mathbb{M}\ell} = \left( 1 - \frac{\beta}{\bar{\beta}} \right) \frac{(h_{\ell M}^+)^2}{2\delta_{\ell M}} + \frac{q}{\delta_{\ell M}} \frac{M_{\mathbb{M}M}}{\partial_{\ell M}^+, \partial_{\ell M}^+}, \tag{2} \]

where \( \delta_{\ell M}^+ \) is the node interval and \( h_{\ell M}^+ \) is the neutron migration area, which is also given by a regression formula of void fraction and control rod fraction. The kernel, \( W_{\mathbb{M}\ell} \), is composed of transport and diffusion components, and the mixing factor, \( \frac{q}{\bar{\beta}} \), is an input parameter.

Therefore, there are six input parameters: vertical mixing factor \( \frac{q}{\bar{\beta}} \), horizontal mixing factor \( \frac{q}{\bar{\beta}} \), core top albedo \( \alpha_{T} \), bottom albedo \( \alpha_{B} \), horizontal albedo with one external surface \( \alpha_{1} \), and that with two \( \alpha_{2} \).

II.2 Parameter Optimization

The performance index, representing the FLARE accuracy on power distribution, is defined as

\[ J = \frac{1}{K \times J} \sum_{j=1}^{K} \sum_{i=1}^{J} \left( \frac{T_{o}_{i}^{j} - T_{m}_{i}^{j}}{T_{m}_{i}^{j}} \right)^2, \tag{3} \]

where \( T_{o}_{i}^{j} \) and \( T_{m}_{i}^{j} \) are the measured and calculated TIP readings of TIP No. \( j \) and axial node No. \( i \), respectively. The TIP readings are normalized as the average is unity. The number \( J \) is 31 for a 784MWe BWR, which is employed as an example in this study, and \( K \) is 24.

The parameter adjustment is a nonlinear optimization problem:

\[ \text{Controlling variables} \quad \frac{\partial J}{\partial \alpha_{i}} \quad \text{parameters} \quad \frac{\partial J}{\partial \alpha_{i}} \quad \text{minimum} \]

The steepest gradient method is adopted to optimize the parameters. That is, the \( j \)-th parameter \( \alpha_{i} \) is revised, step by step, as

\[ \alpha_{i}^{j+1} = \alpha_{i}^{j} - c \left( \frac{\partial J}{\partial \alpha_{i}} \right)^{j}, \tag{4} \]

where the suffix \( i \) is the step count, \( c \left( \frac{\partial J}{\partial \alpha_{i}} \right)^{j} \) is the gradient at the point of the \( j \)-th step, and \( c \) is calculated properly to minimize the number of the steps required for convergence. The Fibonacci search technique is employed to calculate \( c \).

II.3 Results and Discussions

The parameter adjustment method has been applied to simulate the first cycle core of a 784 MWe BWR-4 type reactor, and the accuracy of FLARE code has been evaluated.

In Fig. 1, shown are examples of TIP readings at 2 strings: one from core center and the other from core peripheral region. The cycle exposure is 1.85 Gwd/\( \text{t} \), and the thermal power is the rated. In this figure, the solid lines are the measured TIP readings, and the broken lines (A) are the calculated results by FLARE using 6 parameters (albedos and kernel mixing factors) optimized by the steepest gradient method. The root-mean-square error (RMSE) in TIP readings, defined by Eq. (5) is 6.3%, which is not at all small enough to predict core performance for in-core fuel management and power maneuvering planning.

\[ \text{RMSE} = \sqrt{\frac{\sum_{j=1}^{K} x_{j}^{100}}{\%}}. \tag{5} \]

One of sources of the error could be attributed to the ambiguity of the model of void-quality relation. To reduce the error in the calculated TIP readings, an adjustable parameter is introduced in void calculation model. An example of void-quality relation is shown in Fig. 2, and the parameter introduced here is the magnification of void fraction \( \beta \). RMSE could be reduced to 3.6% by optimize the parameter.
Fig. 2 Optimization of void-parameter

<table>
<thead>
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<th>Case No.</th>
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<th>2</th>
<th>3</th>
<th>4</th>
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<td>Exposure</td>
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<td>2.38 GWD/t</td>
<td></td>
<td></td>
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<tr>
<td>Control rod sequence</td>
<td></td>
<td>B₂</td>
<td></td>
<td>A₁</td>
</tr>
<tr>
<td>FLARE parameters</td>
<td></td>
<td>Optimized at 1.85 GWD/t</td>
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<td></td>
</tr>
<tr>
<td>void-parameters</td>
<td>Initial guess</td>
<td>Optimized</td>
<td>Same as Case 2</td>
<td>Optimized</td>
</tr>
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<td></td>
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<td>1.06</td>
<td>1.06</td>
<td>1.05</td>
</tr>
<tr>
<td>RMSE in TIP</td>
<td>6.28%</td>
<td>3.61%</td>
<td>3.67%</td>
<td>3.66%</td>
</tr>
</tbody>
</table>

RMSE (Root-mean-square error) is defined by Eq. (5).
\( \beta \) (optimum \( \beta = 1.06 \)), and the calculated TIP readings are shown in Fig. 1 by broken lines (B).

Figure 3 shows TIP readings at cycle exposure 2.38 GWD/t and thermal power 99% of the rated, where the six FLARE parameters and void-parameter \( \beta \), used in FLARE calculation, and those optimized at cycle exposure 1.85 GWD/t. RMSE in TIP readings is 3.67%. The void-parameter \( \beta \) was tentatively optimized from the measured TIP readings at this exposure, and the result (\( \beta = 1.05 \), RMSE = 3.66%), which is almost equal to that at 1.85 GWD/t, shows that the parameters optimized at 1.85 GWD/t can be used to simulate the core at 2.38 GWD/t.

Results of FLARE simulation are summarized in Table I. RMSE in TIP readings could be reduced to less than 4%, by introducing a parameter in void calculation model and applying the parameter adjustment technique. The results also show that the parameters optimized at a time can be used to predict core performance in the near future.

III. ADAPTIVE LEARNING OF CRITICAL EIGENVALUE

III.1 Method of Adaptive Learning

Figure 4 shows an example of variation of critical eigenvalue calculated by a core simulator during reactor start-up operation. It is indispensable to know, in advance, the dependency of critical eigenvalue on operating conditions for power maneuvering planning. It is also required to get information on exposure-dependency of critical eigenvalue to predict core cycle length.

In this paper, an adaptive learning for power maneuvering planning is to be presented. The method is also applied to overcome the problem of exposure-dependency of the eigenvalue.

Basic idea of the method is that the critical eigenvalue \( \lambda_c \) is expressed by a quadratic equation of thermal power \( P \), core flow rate \( F \) and core average xenon density \( X_e \);

\[
\lambda_c = a_0 + a_1P + a_2F + a_3X_e + a_4P^2 + a_5F^2 + a_6X_e^2 + a_7PF + a_8FX_e + a_9X_eP,
\]

(6)

and the coefficients are determined by the least square method using the past operating data. The simultaneous equations to determine the coefficients \( a_i, i = 0, 1, \ldots, 9 \), by least square method are,

\[
\begin{bmatrix}
\langle 1 \cdot 1 \rangle & \langle P \cdot 1 \rangle & \langle F \cdot 1 \rangle \\
\langle 1 \cdot P \rangle & \langle P \cdot P \rangle & \langle F \cdot P \rangle \\
\langle 1 \cdot F \rangle & \langle P \cdot F \rangle & \langle F \cdot F \rangle \\
\vdots & \vdots & \vdots \\
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
a_2 \\
\vdots \\
\end{bmatrix} =
\begin{bmatrix}
\langle 1 \cdot \lambda_c \rangle \\
\langle P \cdot \lambda_c \rangle \\
\langle F \cdot \lambda_c \rangle \\
\vdots \\
\end{bmatrix},
\]

(7)

where

\[
\begin{align*}
\langle 1 \cdot 1 \rangle &= \sum_{n=1}^{m} 1 \cdot 1 \\
\langle P \cdot F \rangle &= \sum_{n=1}^{m} P^n F^n \\
\end{align*}
\]

\( m \) : data sampling no.,

\( m \) : number of samplings.

In the proposed method, the coefficients are revised adaptively according to the accumulation of operating data. The accumulation of data is controlled in two ways.

(a) Operating data are generally maldistributed, especially around the rated power and the rated flow rate. To get the fitting coefficients, which gives reasonably good results for whole operating condition, a weighting control of data accumulation has been introduced. That is, as shown in Fig. 5, the operating region is divided into 18 subregions by the division lines \( L_i \), \( L_j \), \ldots, \( L_k \), on power, flow rate and xenon density, and apparent number of data at each subregion is controlled to be equal to the weighting factor given in advance.

(b) The contribution of new data is more important than those of old data, or weight of older data should be diminished gradually. For this purpose, data accumulation is done by \( \langle P \cdot F \rangle \) is employed as an example),

- 213 -
Fig. 3  Measured and calculated TIP readings at 2.38 GWd/t  
(Using the parameters optimized at 1.85 GWd/t)
\[ \langle P, F \rangle = \gamma \langle P, F \rangle_{\text{previous sampling}} + \langle P, F \rangle_{\text{new data}} \]  

where \( \gamma \) is a constant between 0 and 1.

III.2 Results and Discussions

An example of results of eigenvalue fitting is shown in Fig. 4, where the broken lines are fitted \( \lambda_c \) and the power level predicted by criticality search using the fitted \( \lambda_c \). The maximum error in the predicted power level is about 4% in this case.

The method presented in this paper has been successfully applied to on-line prediction of power-flow trajectory during reactor start-up and control rod swap, as well as the off-line control rod programming.

IV. CONCLUSION

A method has been developed to optimally and automatically determine the adjustable parameters of FLARE-type simulator to best fit the operating data on power distribution. The method has also been applied to modify the void-quality relation by introducing an adjustable parameter in the void calculation model.

An adoptive learning method has been proposed to determine the critical eigenvalue, which is necessary to predict core performance, by using the past operating history efficiently.

These proposed methods of automatic accuracy assurance of FLARE code will be effective tools to use FLARE-type core simulators. However, the discrepancy still exists between the measurements and calculations, and more efforts are still necessary to improve the way of tuning of the model, as well as to revise its physical models based on theoretical grounds.

ACKNOWLEDGMENTS

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Fig. 4 Results of critical eigenvalue fitting and power level search

$X_e < 92\% \quad X_e > 92\% \quad \text{[normalized by the rated]}$

Fig. 5 Region specification for data accumulation and an example of power-up trajectory
1. Introduction

In BWR-cores gadolinia poisoning together with control rods is used for controlling excess reactivity and power shaping, thus keeping shutdown margin and power peaking within design limits and optimizing cycle exposure and fuel burnup. To verify that any core design with gadolinia poisoned bundles will meet the above defined requirements, normally detailed 3D-calculations with any standard code /1,2,3/ have to be performed by a stepwise burn to the end of cycle and with appropriate rod patterns selected at each exposure step. More simple methods, usually based on Haling calculations /4/ are commonly used for the design of reload cores. But for new design, especially for initial cores with gadolinia the Haling method alone will not lead to sufficient results.

Therefore we present a new design procedure for a multi-enriched initial core which led to a loading pattern with optimized gadolinia distribution and low power peaking.

2. Procedure for Evaluating an Optimum Gadolinia Design

For optimization of the gadolinia design together with the control rod pattern, the state of highest excess core reactivity is taken as the limiting exposure point. Most of the calculations are performed at that state, because in general for hot cases the power peaking factors and for cold cases the shutdown margins reach their maxima and minima, respectively. The objectives for optimization calculations at that exposure point will be discussed later. In order to prove if the optimized gadolinia design meets all the performance criteria, a three step initial cycle analysis with optimized control rod patterns and exposure accumulation is performed. The four break points are: beginning of cycle, the two states of maximum and of half maximum reactivity and end of cycle.

The excess core reactivity and the power mismatch factors between the different core regions and bundle-types throughout the cycle are obtained by back-stepping the target exposure distribution (Haling case) to other points in the cycle, followed by power calculations without control rods.

3. Application to an Initial Core with Multi-Enrichment Loading Pattern

An optimum gadolinia design is demonstrated for an initial core with four differently enriched bundle-types based on a scatter reload equilibrium cycle /5/. In multi-enriched cores the power mismatch between different enriched bundle-types is an additional contribution to power peaking. On the other side this contribution can be minimized with an appropriate gadolinia design by selecting carefully a well-matched number and concentration of gadolinia rods in the different enriched bundle-types. It is apparent that the optimization of gadolinia design becomes more important for multi-enriched cores.
Fig. 1: Behaviour of Core Excess Reactivity and Power Mismatch Factor in Four-Bundle-Cell Throughout the First Cycle

Fig. 2: Behaviour of Power Peaking Factor Throughout the First Cycle
The following two objectives will be helpful by approaching the optimal power flattening:

- It is desirable to keep the excess reactivity during the first half cycle within the relatively small band between 0.03 and 0.04 (Fig. 1). Too many control rods increase power peaking by high mismatch factors between controlled and uncontrolled cells. While on the other hand an insufficient number of control rods will not give enough flexibility for power shaping.

- The power mismatch between multi-enriched different bundle-types should be kept small in states with high control fraction. In Fig. 1 this power mismatch passes its minimum value at the maximum excess reactivity and reaches its maximum value at the end of cycle, where all control rods are withdrawn.

These objectives are well met with proper different gadolinia poisonings up to $3 \times 6 \%$ Gd$_2$O$_3$ in the bundle-type with the highest averaged enrichment.

Compared to a homogeneous initial core design, the axial power peaks in each bundle of a four bundle cell with different enrichments and gadolinia poisonings have different axial positions, which results in a flattened core-averaged axial power shape. This is a kind of axial power shaping without any distributed fuel or gadolinia poisoning in axial direction. Low gadolinia poisoning with maximum concentrations of $2 \%$ Gd$_2$O$_3$ are used for bundle-types in the peripheral core region in order to compensate the reactivity loss due to high leakage. The resulting flattened radial power is maintained in the cycle period with high control rod density in the core. This radial gadolinia distribution is also important for the cycle length, because the leakage and the gadolinia residual in the core are reduced at the end of cycle.

4. Power Peaking Behaviour throughout the First Cycle

The power peaking factors throughout the first cycle are affected by several parameters. As mentioned earlier, the power mismatches between bundle-types with different enrichments and different control states are optimized together with the Gd-poisoning at the cycle state of maximum excess reactivity in order to achieve power peaking factors as low as possible. A further parameter which affects the power peaking factors - mainly later near the end of cycle - is the control rod history. This is built up because of different burnups between controlled and uncontrolled bundles, and it becomes effective after the control rods are withdrawn. Fig. 2 demonstrates the influence of the control rods on the total peaking factor (Pq) throughout the first cycle. Most of the control rods are withdrawn at full power operation and the control fraction is about 15% at maximum, that means less than a quarter of all control rods are gradually inserted in core.

In order to get nearly a total compensation of the control rod history effect, the control rod pattern has to change infinitely by participation of all possible four different rod patterns. Only in this unpracticable case the total power peaking factor reaches with curve (1) the Haling target value. The other extreme case is a control rod program with no change of pattern sequence which results in an enhanced power peaking towards the end of the cycle caused by maximum influence of control rod history (2).

With regard to the availability of the reactor and the values of the total power peaking factors already reached at states without noticeable control rod history, the curve (3) is an optimized case with nearly constant lowest possible total power peaking all over the cycle.
References

/1/ D.L. Fischer, J.M. Harriman and M.J. Stedwell, "FLARE, A Three-Dimensional Boiling Water Reactor Simulator", GEAP-4598 (July 1964)


It seems to me that the few comments I have apply to most of the papers presented at the meeting as well as to those in the third session. Thus I shall make them in a general vein.

First of all it appears that the older analysis methods of performing unit cell computations for spectra followed by few group finite difference global computations are being replaced by schemes in which spectrum calculations are performed on an assembly basis and higher order coarse mesh or nodal methods are used for the global problem. As a consequence the spectra for particular fuel cells depends on the environment of the cell. In addition the global calculations run much more quickly so that three dimensional analysis has become fairly standard.

My second observation is that comparisons of the various design methods with experiment have been very encouraging. However it is not clear how much of this agreement is due to cancellation of errors or arbitrary adjustment of parameters.

This leads to my final point: I believe that the weak spot in the overall calculational model is the assembly calculation that leads to few-group-equivalent homogenized parameters to be used in the global calculations. Since, if the ratio of assembly averaged reaction rates to each other and to assembly leakage rates is known, global calculations can now be made to yield exact core eigenvalue and assembly powers, the problem becomes one of determining these rates as accurately as possible. It is a particularly difficult problem when depletion and thermal hydraulic feedback effects have to be accounted for, and it is possible that, to resolve it, it may be necessary to iterate between the global and the assembly calculations.

This focus on the assembly problem as being the matter of greatest concern in the overall calculational model may not be generally recognized since most calculational methods do not make use of a global model capable of reproducing completely correct average assembly properties even if they were known exactly beforehand. Thus some error arises from the global calculation as well as from the assembly spectrum calculations. I believe it would be useful to perform more benchmark type analyses to determine the relative sizes of these two sources of error and if errors in the global part of the calculation are significant to adopt global calculational procedures that avoid them.
Session 4

Chairman - Président
Dr. M. MELIÇE
(Belgium)

Séance 4
United States utility industry utilization of three-dimensional core simulations for LWR analysis is covered in detail. The nodal methods available for applications have three levels of sophistication, each with its own logical areas of application. Special considerations and implementation for BWR and PWR models are also discussed. Two special applications are then used to demonstrate particular selection considerations. Finally, benchmark comparisons are discussed in terms of advantages and difficulties.

Introduction

The purpose of this paper is to discuss the ways nodal methods are being utilized by the utility industry in the United States for LWR analysis. Although particular computer codes and nodal methods will be mentioned as examples, the thrust will be rather to illustrate the various levels of methods which have been developed, the requirements of practical implementation of these methods and the needs for future development. We will also discuss particular applications of the methods and then the types of benchmarking which need to be carried out in order to assess the adequacy of the overall calculational capabilities. Again while some particular benchmark results will be presented, the point here is to only examine the basic approach.

Levels of Nodal Methods

The author has found it convenient to separate the current status of nodal methods in terms of three levels of sophistication. In many respects these methods form the heart of the core simulators. Given the effective neutronic properties (i.e., cross sections) of each nodal region, these methods form the solution basis for the calculation of reactor power and flux distributions.

1. Flare Method

The first level of method is best described as the Flare Method because of its initial usage in the FLARE/1/Computer code. The EPRI-Node B (BWR)/2/ and EPRI-Node P (PWR)/2/ codes distributed by EPRI are based on the same method and are currently widely used in the United States. Other versions of the method are also in use worldwide. Originally heuristically derived, the method is almost always utilized in a single energy group formulation where only nodal K_x and H^2 values are needed at any state point. The method has several adjustable parameters including a form of albedo at reflector interfaces. These parameters are generally modified as the result of comparisons with either reactor data or more accurate calculations in reduced dimensions. While this method has known limitations and inaccuracies, there is much experience in its application and results are often quite acceptable and encouraging.
There should however be a great concern about usage in cases where no calculational or operational comparisons are available.

2. One-and-a-Half Group Methods

A large variety of methods have been developed which fall into this classification. Among them are the TRILUX/3/, PRESTO/4/, CETRA/5/ and ROCS/6/ methods and their various computer implementations. Although difficult to define this class of model exactly, the nodal equations generally involve the determination of coupling parameters between nodes which relate surface currents to nodal fluxes. To make this determination some basic approximations need to be made. Generally these occur in the assumptions of separability and of shape details of the flux within nodes. Application is generally made to an equivalent average group source calculation with later corrections for spectral gradients between assemblies or at the reflector interfaces. Albedos are almost always utilized for the reflector but success has been achieved in many cases with analytical calculations of the albedo values. Less dependence is made on experimental or calculational adjustments but normalizations are applied by some users.

3. Improved Nodal Methods

The improved nodal methods are the result of extensive efforts to develop more accurate nodal methods based on formal mathematical approaches. In general they integrate the 3-D fluxes over two transverse directions and then develop a treatment for the shapes of the transverse leakages across the node. This treatment becomes the clearly identified approximation of the improved methods.

Most implementations of the methods have been made in two-groups although multi-group extensions are almost always possible. It should be emphasized that these are "true" two-group calculations and not corrections to basically one-group solutions. Although not explicitly solved for in the iterative calculations, it is possible using these methods to reconstruct the flux-details within the node. This may be an important feature that will be discussed later.

When the reactor nodal properties are known, these methods have generally shown an ability to provide values of criticality, nodal powers and nodal fluxes that are very close to those obtained from finite difference solutions carried out on a very fine spatial mesh. The quoted running times of the methods are impressively small and computer time costs should not be a detriment to their use. When utilized in real reactor cases, the methods appear however to have increased memory requirements compared to the Flare and 1½ group methods. Implementation would then require more concern with memory management and input-output optimization. In most cases, the reflectors are treated explicitly rather than by albedos.

The choice between these methods must be determined by the developer and later by the individual user based on a variety of considerations. Some applications will require very rapid calculations but can afford some relaxation of accuracy. Likewise, if normalization measurements or calculations are available less inherent accuracy of the nodal method itself is necessary. Often availability of engineering and modeling features, such as those discussed in a later section, count as importantly as the nodal method itself in making
the choice. Comparisons of accuracy and computer resource requirements are also complicated by such differences. For this reason EPRI had included a variety of $1_{\frac{1}{2}}$ group methods and the Plare algorithm in the SIMULATE/7 nodal code which we have made available to a large number of utility and other users. We are also considering implementing one or more of the improved nodal algorithms during the next year. In this manner, the extensive engineering and modeling framework of the code can be applied over a range of nodal sophistication and need not be redeveloped in a new context.

Special Considerations

BWR analysis is complicated by many factors including the high degree of assembly heterogeneity. The large water gaps, the blade control rod, the burnable absorbers and the enrichment distribution complicate the calculation of power distributions within the bundle and also the calculation of equivalent homogenized parameters for use in nodal analysis. Several studies/5,6/ for example have shown that if standard flux weighted cross sections are calculated, the use of the $1_{\frac{1}{2}}$ group methods in the radial plane give better agreement with multi-group, explicit, heterogenous, fine-mesh calculations than either two-group, improved nodal methods or even two-group, homogenized finite difference calculations. The reason for this discrepancy (illustrated in Figure 1) is that the water gaps effectively isolate the assemblies as shown by the comparison of fast-to-thermal flux ratios in Figure 2. The fuel in the left hand assembly and the control rod in the far left water gap do not see the spectrum of the right hand assembly. However, as shown in Figure 3, when nodes are homogenized the spectral gradient extends further into the assembly and the fuel and control material are effectively moved next to the adjacent assembly. Thus the inherent $1_{\frac{1}{2}}$ group approximation, that the fast-to-thermal flux ratio is independent of adjacent nodes, is quite accurate in the radial plane and the better $1_{\frac{1}{2}}$ group methods appear preferable to the two-group methods. It is also possible to extend the $1_{\frac{1}{2}}$ group methods to include improved treatments of blade heterogeneities. All together it appears that these methods can be quite accurate for BWR analysis. Thus, the widespread use of the improved nodal methods for BWR analysis will await the implementation of improved heterogeneity treatments such as the work initiated by Koebke/9/7. The eventual payoff is probably mainly in the areas of increased confidence in results, less dependence on normalizations, and the ability to include the effect of core flux tilts on pin power distributions.

For PWRs, the situation is quite different. The assemblies are much more heavily coupled and inter-assembly spectral and spatial effects must be taken into account in order to obtain adequate pin power and exposure distributions. For these reasons, PWR analysis makes heavy usage of multi-group, two-dimensional, finite difference calculations with each pin explicitly represented. Microscopic depletion is maintained through each cycle. Nodal calculations are also utilized in order to include three-dimensional and thermal-hydraulic effects. However, since the explicit two-dimensional calculations are available, detailed normalization is possible and the requirements for inherent accuracy of the nodal technique is reduced. The improved nodal methods could offer real benefits if they could replace the explicit, finite difference calculations. In addition to the nodal solutions, this would require: the reconstruction of the flux within the node; the use of separately calculated, assembly, heterogenous pin power and, the microscopic depletion of the core. Following the depletion, new nodal parameters would have to be calculated including both design and burnup induced heterogeneities. While some work has been done in this direction, further implementation, wider experience and more comparisons with the explicit depletion calculations are required before this potential advancement can be utilized.
Figure 1 -- BWR Checkerboard Test Problem, Fine Mesh and Nodal Comparisons
Figure 2 -- Fast-to-Thermal Flux Ratio Distribution for Heterogeneous Calculations.
Figure 3 -- Fast-to-Thermal Flux Ratio Distribution for Homogeneous Calculations
Implementation

While the nodal method is the heart of the core simulator, there are other components which may be just as important in providing an adequate capability for reactor analysis. These components include the ability to model the important thermal-hydraulic conditions in the reactor, the ability to model the effect of local conditions on neutronic parameters and the ability to track history effects and their influence on neutronic parameters. In addition, efficient application requires engineering features to allow the user to easily carry out the many types of calculations which are necessary in a power reactor analysis program.

The basic thermal-hydraulic conditions modeled in many nodal calculations are coolant density (including voiding in a BWR) coolant temperature, and fuel temperature. Sophisticated calculations are not usually required since the important element is only the effect on neutronic properties. Once these local conditions are known the code must also be able to model the effect of these conditions on cross sections or reactivity. The history effects which are important include void history, control rod history, burnable absorber history, exposure and relatively short lived fission products such as Xenon and Samarium. The code input and internal logic must allow for the user to model all of these influences in an efficient but accurate manner. Capabilities range from multi-parameter parametric fits to multi-dimension tables with internal interpolation algorithms. There are many cases where the failure of a core simulator to adequately predict the reactor state has been caused more by inadequate treatment of these effects in that situation than by the adequacy of the nodal method itself.

The utility user also desires many engineering features in core simulator to ease its use. A subset of these features include automated reload shuffling, problem expansion from partial to full core, easy restart and branch calculations, prediction of in-core instrumentation responses, control rod withdrawal sequence definition and input and output in terms of standard plant parameters. Input data checking, graphics and summary output can also be important.

Applications

In order to illustrate the variety of nodal applications, this section will provide two specific applications. The first is as the basis for a safety evaluation methodology and the second is an on-line usage in a reactor plant for assessing and predicting fuel and safety limits. They illustrate the varying requirements on nodal codes and methods which may promote different selections by the same user in different cases.

This first case is a modeling procedure/10/ which is currently being developed to provide utilities with the capability required for detailed BWR fuel management, core following, and transient analysis capability. Most components have been completed with some additional work now under way. This system is illustrated in Figure 4. Each code provides the bulk of the input required for the next calculation in the sequence. Feedback effects are included by carrying out explicit branch calculations in the lattice physics codes. Cross-section or reactivity variations are then modeled in the full reactor representations.

CASMO/11/or CPM/12/provide sophisticated multigroup, transport, lattice physics capabilities which have proved to be very convenient for BWR analysis. Both calculate two-group macroscopic cross sections homogenized over the assembly and include explicit treatments of isotopic depletion. The current BWR model calls for carrying out complete burnup calculations at three void
Figure 4 -- BWR Analysis System
levels (generally 0, 40 and 70%). Branch calculations are then used to determine the influence of Doppler, control rod and instantaneous void on the two-groups cross sections. The effect of control rod history can be included in an additional depletion calculation at 0% void along with the appropriate branch calculations.

The NORG code reads the lattice physics output files and generates the nodal representation for the 3-D nodal code SIMULATE. COLLAPSE utilizes both SIMULATE input and output to provide consistent two-group neutronic input for the 1-D capability contained in RETRAN/13. RETRAN is then used for studying system transients including the effects of thermal-hydraulic feedback on the model.

In many ways SIMULATE is the central component of the system which relates the core physics to the transient analysis. It was chosen because of its ability to accurately model the same feedback effects desired in the transient analysis and because of its ability to adequately predict core power distributions. Overall the procedure should provide the user with an efficient automated capability for detailed off-line analysis.

The second application is the Power Shape Monitoring System (PSMS)/14/(Figure 5) which is an on-line analysis system currently implemented for BWRs. The codes operate on an essentially dedicated mini-computer at the reactor site. This computer has access to selected process computer data such as state-point characteristics and in-core detector responses. In this case the purpose of the core simulator is to rapidly provide power distribution data to the reactor engineer based on either current plant conditions or on a proposed reactor maneuver. In the core follow mode, measured changes in core conditions automatically trigger the core simulator to update the calculated reactor power. Calculations can be triggered on a time scale ranging from every few minutes when a maneuver is taking place to every few hours when only the Xenon distributions is changing. Core exposure is updated daily. In the predictive mode the reactor engineer can manually trigger the code to analyze a series of conditions which may occur a few minutes or a few weeks from the current time. In either mode, the nodal results can be used to either predict fuel failures from power changes or to assess safety limits.

For this application the nodal code selected was the Flare based code EPRI-Node B because of its overall speed, its low memory and low input-output requirements. The code can be normalized to either in-core measurements or to another simulator run off-line. Optimization of the code and its convergence characteristics was extremely important in its system implementation. Currently, typical 1/4 core calculations take about five minutes while smaller core sections can be analyzed for local condition changes (including small control rod motions) in a much shorter time. Interactive color graphics output is very important to allow for rapid interpretation of the results. A prototype system is currently on-line at the Oyster Creek BWR located in New Jersey. As can be guessed, the core simulator in this system is being applied to cases where there is very little experience in its use. Its ability to predict reactivity and power distributions both in normal high power and in low power, highly controlled situations is being critically assessed. However, particularly in off-normal conditions, the code results can be quite sensitive to the process computer values for the core state-point characteristics. Uncertainties in reactor power and in coolant flows may affect the ability to draw definitive conclusions. We do expect to shortly make some model improvements possibly including a basic change in the Flare algorithm itself.
Nodal Methods Benchmarking

Nodal methods have generally been tested in two ways. Both are necessary and useful but both also have their pitfalls.

The first type test is generally against accurate finite difference methods. Often "benchmark" problems are utilized where the local cross sections are uniquely specified and reference solutions are provided. While they provide a good basis for assessment these tests must be used with care. In many cases the "benchmark" problems are rather extreme and thus introduce situations which a production code was not designed to accurately handle. On the other hand, because of the accurate reference solutions available, one can lose sight of the desired accuracy of the nodal methods when considered in terms of the knowledge of the local conditions and homogenized effective cross sections in an operating reactor.

The other class of testing is against operating reactor data. In this case one is generally comparing predictions with real measurements of on-line instrumentation. Since on-line accuracy is often not as good as desired, EPRI has sponsored several large sets of gamma-scan data (for determining power distributions) and parallel sets of design and operating data from the same cores.

One must remember in comparisons with operating data that one is never testing just the nodal method. The comparisons, whether good or bad, are a result of a combination of the nodal algorithm, the lattice physics, the feedback and history modeling and the thermal-hydraulic model. Figures 6, 7, 8 and 9 show typical comparisons of nodal calculations with measured gamma-scan data from one BWR core. The comparisons show too much peaking at the top of the core where many control blades are located. This phenomenon could be the result of many difficulties including poor lattice physics and rod worth calculations, improper nodal calculations in steep gradients or near control rods or inaccuracies in the void model. In this case we believe it is the latter since purely thermal hydraulic benchmarks indicate that the void model in the simulator is presently predicting too few voids in the core. Obviously, as a result of this work a new void model will soon be introduced in the simulator.

Conclusions

In utility reactor analysis three-dimensional core simulators play a key role in fuel management, operational decisions and increasingly in safety analysis. Development of these simulators has generally been a process of assessing compromises between computer resource requirements and calculational accuracy. In the end, the success of the process is judged by the ability to adequately predict the behavior of operating reactors. Adequacy however must always be judged in terms of the requirements of the intended application.

References


12/ See reference /2/.


14/ Power Shape Monitoring System, EPRI Research Project RP-895.
Figure 8 -- Gamma Scan Power Comparison: Shallow Control
APPLICATIONS OF FMS - RECORD/PRESTO FOR ANALYSIS AND SIMULATION OF OPERATING LWR CORES

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ABSTRACT:

The RECORD and PRESTO Codes of FMS provide an integrated system for efficient analysis and 3-D simulation of LWR cores. The features of the two programs are briefly described in this paper. References for the underlying theory are provided. Examples of program verification by analysis of measured data from a number of operating power reactors are given. Xe-dynamics core-follow results are also presented. The application of such programs for fuel management and core-follow for operating guidance is discussed.

1. INTRODUCTION

Accurate predictions of core power distributions in operating power reactors involves adequate representation in 3-dimensions of integrated hydraulics and neutronics models, together with a system of generating required reactor physics data. When judging the adequacy and efficiency of calculational methods for predicting reactor performance in practical core-follow studies, it is of importance for a User to take into consideration both the efficiency of the simulator itself, as well as the adequacy of the reactor physics data on which the simulator relies and how efficiently this data can be generated.

This paper will describe some of the experiences accumulated through many years in applying the RECORD/PRESTO codes of FMS /1/ to the simulation of Light Water Reactor cores. FMS (Fuel Management System) is an integrated modular code system developed for efficient and accurate fuel management and core performance calculations in Light Water Reactors. The enlarged system, the basic units of which are shown in Figure 1, enables reactor simulations to be done at different levels of detail and spatial representation, and also includes 1 to 3-dimensional dynamics codes for transient analysis, and codes for fuel performance studies.

2. FEATURES OF RECORD AND PRESTO

For the overall reactor simulation, the basic codes of FMS are the RECORD and PRESTO codes. In this context, the RECORD code can be considered as the data generation unit of FMS, supplying the necessary reactor physics data to the PRESTO code, which performs the overall 3-dimensional simulation of a LWR core. The two codes are linked through a databank generated by RECORD, and subsequently activated by PRESTO.

The RECORD code performs reactor physics calculations on BWR and PWR fuel assemblies. It is a fast production code for calculation of neutron spectrum, group data and reactivity as function of fuel burnup in LWR fuel assemblies. With individual treatment of each fuel pin, the code calculates reaction rates, power and burnup distributions in two dimensions, taking into account most features
which arise in present-day LWR designs. Such features include variable fuel enrichments, burnable poison (gadolinium pins), burnable absorber (boron) shim rods, control absorbers (either cruciform rods or cluster control rods), soluble poison, voids, and other heterogeneities which may arise. Also of importance are flexible restart options, which enable straight-forward generation of group data at low power conditions, and the calculation of differential effects during burnup, such as control rod effects and influence of moderator density variations.

RECORD condenses the detailed calculations to give the few-group data and coefficients required by PRESTO and other macroscopic codes of FNS. These data are stored in a databank as function of fuel burnup, average void and other operating data for each fuel type in a given core.

The PRESTO code performs 3-dimensional calculations of power and fuel burnup distributions in BWR and PWR cores. Reactor operation may be simulated (predicted) for the following reactor states:

- Steady-state operation - zero to full power range
- Steady-state burnup calculation, including Haling option
- Transient state, Xe-dynamics calculation
- Cold, critical state
- Cold, subcritical state, shutdown margin calculation

Thermal-hydraulic feedback is accounted for in both BWR and PWR calculation. The reflector is treated by boundary conditions, based on results from a fine mesh, 2-group diffusion code, linked to PRESTO. In-core instrumentation readings (i.e., TIP system and LEAFM's) may be predicted and compared with actual readings. The calculation includes evaluation of the simulated reactor state against a number of User-specific operating limits.

The neutronic model of PRESTO is based on an approximation to 2-group diffusion theory, using a mesh spacing equal to the assembly pitch (BWR), or half the assembly pitch (PWR).

A central mesh point finite difference formulation is used for the fast flux ($\phi$) equation:

$$a_{ii} \phi_i - \sum_{6j} a_{ij} \phi_j = \bar{\sigma}_i \cdot \phi_i \cdot k^3$$  \hspace{1cm} (1)

where

$$a_{ij} = \frac{2D_{ij}}{D_{i} + D_{j}}$$ \hspace{1cm} (2)

$$a_{ii} = \sum_{6j} a_{ij}$$ \hspace{1cm} (3)

$\bar{\sigma}_i$ is a function of the 2-group macroscopic cross-sections for a cubical unit cell (node), and the fast to thermal flux ratio within the cell. $k$ is the mesh width (node width). The following mathematical approximation is introduced:

$$\frac{2D_{ij}}{D_{i} + D_{j}} = \sqrt{\frac{\sigma^-}{\sigma^-}} \cdot \sqrt{\frac{\sigma^+}{\sigma^+}}$$ \hspace{1cm} (4)

This reduces Eq.(1) to the form of a nodal coupling equation:

$$\psi_i = \sum_{6j} \psi_j \cdot \frac{D_{ij}}{p_i} k^2 \cdot \bar{\sigma}_i$$ \hspace{1cm} (5)

with

$$\psi_i = \phi_i \cdot \sqrt{\bar{\sigma}_i}$$ \hspace{1cm} (6)

and
\[ p_i = \frac{1}{V_i} \sum_{j} \frac{V_j}{6} \phi_{ij} \]  

By expressing the cell average flux in terms of the mesh point flux, \( \phi_i \), and the flux on the six interfaces to the nearest neighboring cells, \( \phi_{ij} \), one obtains:

\[ \overline{\phi}_i = a \phi_i + \frac{1-a}{6} \sum_{j} \phi_{ij} \]  

a has been determined by calibrating PRESTO 4-bundle calculations against 4-bundle RECORD calculations. Some examples of comparisons of PRESTO and RECORD (2-D) 4-bundle calculations are shown in Figure 2. A more complete description of the theoretical method underlying PRESTO is given in [2].

The basic 2-group macroscopic cross-sections and diffusion coefficients are calculated by RECORD for each fuel assembly type and transferred to PRESTO in the form of polynomials in exposure (E), void (a) and exposure-weighted void (\( a_E \)) for BWR's and in exposure and soluble boron content for PWR's. These are further modified in PRESTO, accounting for the following effects:

- Presence of control rod, including effect of absorber depletion
- Control rod history
- Local Doppler feedback
- Local equilibrium or transient Xe concentration
- Moderator density and density history are accounted for in PWR calculations

Burnable poison systems, such as temporary boron sheets (curtains), axially zoned gadolinium, boron-based shim rods, may be treated.

The thermal-hydraulics model of PRESTO calculates the channelwise coolant distribution and the axial steam void distribution within each channel of a BWR. The model is an approximation to that developed for the RAMONA codes, which have been calibrated directly against experimental loop data (FRIGG) on measured void profiles, over a wide range of operating conditions [3].

The PWR thermal hydraulics model, which is basically equal to the BWR model, calculates the axial coolant density profile for subchannels corresponding to the x-y nodes of the nuclear model.

Fuel assemblies are labeled independently of the reference coordinate system, allowing easy simulation of fuel shuffling, discharge of fuel, reinsertion of fuel from previous cycles, etc.

Fuel burnup calculation includes separate tracking of two fission product isotopes for \( \gamma \)-scanning prediction. The output data files generated by PRESTO may be used as input data to the fuel performance (PCI prediction) model FOSHO, and as initial condition data for the 3-D reactor transient analysis code, RAMONA-III, as shown in Figure 1.

A good balance between calculational sophistication and performance efficiency is an essential design criterion for Utility-oriented code systems like FMS. The system efficiency should be viewed both in terms of computer requirements and manhours needed to prepare input data and digest the output. Some typical parameters, describing the efficiency of RECORD and PRESTO, are given in Table I.

3. EXAMPLES OF SYSTEM VERIFICATION

3.1. Comparison of Code Results

A total of more than 20 BWR and PWR operating cycles have been analyzed. Various core and fuel designs, such as fuel with Gd as burnable poison, fuel with boron absorber rods (shim rods), cores controlled partially with absorber curtains
FIGURE 1. Main Programs of Fuel Management System - FMS.

FIGURE 2. Comparison of PRESTO 4-Bundle Power Distribution with RECORD/MD-2 5-Group Calculation with Explicit Pin and Water Gap Representations.
### TABLE I. RMS System Efficiency Parameters.

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>RECORD</th>
<th>PRESTO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Central Memory (CM) required</td>
<td>115 000₈</td>
<td>220 000₈ - 6 000 NODES</td>
</tr>
<tr>
<td></td>
<td></td>
<td>260 000₈ - 14 400 NODES</td>
</tr>
<tr>
<td>Typical CPU-run time*</td>
<td>8 x 8 Assembly,</td>
<td>1/4-core 800 MWe BWR, steady-state converged</td>
</tr>
<tr>
<td></td>
<td>burnup 0 - 35 000 MWD/TU</td>
<td>solution</td>
</tr>
<tr>
<td></td>
<td>250 sec per void value</td>
<td>(130 x 24 nodes) : 100 sec.</td>
</tr>
<tr>
<td>Time required for a new User to prepare</td>
<td>1 - 2 days</td>
<td>3 - 4 days</td>
</tr>
<tr>
<td>and de-bug input (example)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*CDC CYBER-74 Computer

### TABLE II. Summary of Calculated $k_{eff}$-values for Critical Lattices and Critical Core Configurations.

<table>
<thead>
<tr>
<th>No. (Cases) Points</th>
<th>Cold, Critical Lattice Measurements</th>
<th>Cold Critical Power Reactor States</th>
<th>Hot Operating, Core-Follow Calculations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Points</td>
<td>26 UO₂</td>
<td>10</td>
<td>128</td>
</tr>
<tr>
<td></td>
<td>30 UO₂ -PuO₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$k_{eff}$</td>
<td>$1.0008 \pm 0.0045$</td>
<td>$1.0026 \pm 0.0054$</td>
<td>$1.0009 \pm 0.0062$</td>
</tr>
<tr>
<td></td>
<td>$1.0071 \pm 0.0046$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### TABLE III. Examples of Calculated $k_{eff}$-values for Different Reactor Cycles.

<table>
<thead>
<tr>
<th>REACTOR</th>
<th>CYCLE</th>
<th>TYPE</th>
<th>CORE AVERAGE BURNUP (MWD/TU)</th>
<th>YEAR OF ANALYSIS</th>
<th>AVERAGE $k_{eff}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>BOC</td>
<td>BOC</td>
<td></td>
</tr>
<tr>
<td>Mühleberg</td>
<td>1</td>
<td>BWR</td>
<td>0</td>
<td>12 000</td>
<td>1974</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>&quot;</td>
<td>4 960</td>
<td>10 960</td>
<td>1975</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>&quot;</td>
<td>7 660</td>
<td>12 950</td>
<td>1977</td>
</tr>
<tr>
<td>Quad Cities</td>
<td>1</td>
<td>&quot;</td>
<td>0</td>
<td>10 700</td>
<td>1976</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>&quot;</td>
<td>8 410</td>
<td>9 950</td>
<td>1976</td>
</tr>
<tr>
<td>Santa Maria de Garona</td>
<td>7</td>
<td>&quot;</td>
<td>10 900</td>
<td>14 300</td>
<td>1978</td>
</tr>
<tr>
<td>Brunsblütel</td>
<td>1*</td>
<td>&quot;</td>
<td>0</td>
<td>8 000</td>
<td>1979</td>
</tr>
<tr>
<td>Beaver Valley</td>
<td>1</td>
<td>PWR</td>
<td>0</td>
<td>11 600</td>
<td>1979</td>
</tr>
</tbody>
</table>

*First Cycle not yet completed.
and different control rod types, have been analyzed. Average values of $k_{\text{eff}}$, as calculated for cold critical lattices, cold power reactor cores and hot operating power reactors, are shown in Table II. A summary of calculated hot, operating $k_{\text{eff}}$-values for a selection of cycles analyzed is shown in Table III.

Verification of power distributions, as calculated by PRESTO, has been performed as follows:

- by comparison with fine-mesh benchmark results /4/;
- by calculating axial fission chamber (TIP) traces and comparing with measured data /5/, /6/;
- by calculating the end-of-cycle (EOC) Ba-140 distribution and comparing with measured La-140 $\gamma$-scans /7/;
- by comparing calculated nodal power distributions with process computer results based on in-core instrumentation readings /6/;
- by calculating the EOC burnup distribution and comparing with measured Cs-137 $\gamma$-scans /8/.

Out of these, we consider TIP-comparisons and $\gamma$-scanning comparisons as the most accurate and reliable methods. However, experimental uncertainties and difficulties in relating the measured quantity to power produced in the fuel, puts a limit to the accuracy of the verification.

Examples of TIP-comparisons for two BWR's are shown in Figures 3 and 4. A PWR TIP comparison is shown in Figure 5. Comparisons of PRESTO power distributions with process computer results for a BWR and a PWR are shown in Figures 6 and 7, respectively.

A comparison of calculated and measured Ba-140 axial distributions for two selected fuel assemblies of the MÜhleberg Reactor (EOC-1), are shown in Figure 8, /7/.

Figure 9 shows a comparison of PRESTO calculated burnup distribution with $\gamma$-scan and process computer results /8/. The $\gamma$-scan comparisons are mostly within the experimental uncertainty, as indicated in Figure 8.

A quantitative statement on the calculational accuracy, based on TIP-comparisons, is difficult to make due to unknown experimental uncertainties, unexplained observed asymmetries and effects not explicitly accounted for in the calculation, such as localized neutron absorption in spacer grids, etc. In many cases, however, standard deviations as low as 8\% - 9\% are obtained when the sample consists of all available TIP locations (strings), each subdivided into 24 axial points.

For individual string TIP comparisons showing "perfect" shape agreement, standard deviations are typically 5\% - 7\%. This is therefore considered as the ultimate accuracy obtainable by TIP comparisons. Considering all available data, we find that the present PMS system is capable of calculating BWR and PWR power distributions with an accuracy comparable to that of present power distribution measuring systems.

4. ADVANCED APPLICATIONS

Traditionally, 3-D simulators have been applied to fuel management type calculations. The present trend is to extend the area of application to include near real time core-follow for the purpose of reactor operating guidance. Such calculations require:

- fast calculation
- capability for reliable prediction in the range from zero to full power
- interactive input of key parameters
- condensed output of key results
FIGURE 3. Example of Comparison of Calculated (PRESTO) and Measured TIP-Traces in a Small BWR.
FIGURE 4. Example Comparison of Calculated (PRESTO) and Measured TIP-Traces in a Large BWR.
An RMS version designed for use from an interactive terminal at the plant site is presently underway.

RECORD/PRESTO have been successfully applied to perform the following tasks:

- Reactor startup planning, arriving at an efficient startup procedure subject to local power ramp rate limitations. The Xe-dynamics mode of simulation was used, following the reactor power level from 0% to 100%, as shown in Figure 10. The maximum rate of change of local power was calculated as a function of time and checked against a given limit, as shown in the upper part of Figure 10. In the example shown, the limit was exceeded due to control rod withdrawals at the 65% power level. This could have been improved by iterating the calculation.

- Detailed analysis of control rod pattern exchange maneuvers (BWR) have been performed to study the degree of pellet-clad interaction and the associated cladding failure probability caused by control rod movements at intermediate power levels.

- Xe-transient core-follow calculations have been performed. An example of comparison of measured and calculated TIP-traces versus time through a BWR Xe-transient is shown in Figure 11. The first time points shown (1400 hrs) concern the reactor state at full power immediately after a two-hour operating period at low power. The next two time points (1700 hrs and 2040 hrs) show how the axial power swings back to the typical bottom-peaked distribution which, in this case, corresponds to the steady-state distribution. Very good agreement is obtained by following this Xe-induced power distribution swing with PRESTO.

These results are examples demonstrating the feasibility of the RECORD/ PRESTO system as a useful tool for reactor operating guidance, as well as traditional fuel management calculation.

FIGURE 5. Example of Comparison of Calculated (PRESTO) and Measured TIP-Traces in a PWR.
FIGURE 6. Comparison of Core Average Axial Power Distribution of a BWR, as Calculated by PRESTO with Process Computer Results.
FIGURE 7. Comparison of Calculated Assembly Power Distribution in a PWR with Process Computer Power Distribution Inferred from In-Core Instrumentation.

FIGURE 8. Comparison of Calculated and Measured Ba-140 Axial Distributions.
FIGURE 9. Relative, Assemblywise Burnup Distribution at EOC-1 of KKM, as Measured by γ-Scanning and Per Cent Deviation of PRESTO Calculation and Process Computer Results.
FIGURE 10. Reactor Startup Simulation using PRESTO.
FIGURE 11. TIP Comparison for Xe-Transient Core-Follow Calculation.
REFERENCES:


NODAL EXPANSION METHOD FOR THE ANALYSIS OF SPACE-TIME EFFECTS IN LWRs

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Abstract

The nodal expansion method (NEM) has been developed for the numerical solution of the transient few-group neutron diffusion equation in Cartesian geometry. Results of mathematical benchmark problems and comparison between computations and experimental data indicate that the method is accurate in a coarse mesh grid. The free-fall insertion of a control rod into an off-center assembly of a large PWR operating at 80 % of rated power has been simulated. The resulting transient flux distribution is strongly influenced by thermo-hydraulic feedback effects and delayed neutron holdback. The calculated flux distribution and coolant outlet temperature change agree well with the measurements.

INTRODUCTION

During the past few years substantial progress has been made in the development of efficient numerical methods for the solution of multidimensional diffusion equations /1, 2, 3, 4/. Great effort has also been spent towards the development of advanced computer programs capable of describing the neutronics and thermo-hydraulics of nuclear reactors /5, 6, 7, 8/. Increased accuracy demands and licensing requirements to analyze off-nominal core conditions led KWU to develop the space-time kinetics code IQSBOX. The code is based on the nodal expansion method (NEM) for the solution of the neutronic part of the problem and capable of using different models to account for thermo-hydraulic feedback effects. A modified version of the well known fluid dynamics code FRANCESCA /9/ is presently used for the analysis of BWRs. For coupled calculations of PWRs a simple closed channel model is being used and an improved version of COBRA-IIIC /10/ is being evaluated. In the first part of this paper the code's neutronic model will be described and some numerical results will be discussed which demonstrate the accuracy and computational efficiency of NEM.

In the second part of the paper results from a simulation of experiments, using IQSBOX, will be compared with measurements. At KWU it was felt desirable to perform transient measurements which would provide data for reliable nuclear methods development. To meet this requirement a series of transient experiments was carried out at the KKU PWR nuclear power station. One experiment which emphasizes 3-D effects is the rapid insertion of a single rod. Therefore a full core analysis of a single rod drop at 80 % power will be discussed in detail.
1.1 Basic Equations

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

\[
\frac{1}{V_g} \frac{\partial \varphi_g (\hat{r}, t)}{\partial t} + \nabla \hat{j}_g(\hat{r}, t)
\]

\[
+ (\Sigma_{ag}(\hat{r}, t) + \sum_{g=1}^{G} \Sigma_{gg}(\hat{r}, t)) \quad \varphi_g(\hat{r}, t)
\]

\[
= \sum_{g=1}^{G} (\Sigma_{gg}(\hat{r}, t)) + \frac{1}{\lambda} \sum_{j=1}^{J} (1 - \beta_j^j) \chi_{pg}^j \nabla \Sigma_{fg}(\hat{r}, t)) \varphi_g(\hat{r}, t)
\]

\[
+ \sum_{i=1}^{I} \chi_{dg}^i \lambda_i C_i(\hat{r}, t) + \chi_{eg} S_{ext}(\hat{r}, t) \tag{1.1a}
\]

\[
\hat{j}_g(\hat{r}, t) + D_g(\hat{r}, t) \nabla \varphi_g(\hat{r}, t) = 0 \tag{1.1b}
\]

\[
\frac{\partial C_i}{\partial t}(\hat{r}, t) + \lambda_i C_i(\hat{r}, t) = \frac{1}{\lambda} \sum_{g=1}^{G} \sum_{j=1}^{J} \beta_j^j \psi_{fg}^j \varphi_g(\hat{r}, t) \tag{1.2}
\]

The notation is fairly standard and in accordance with previous usage /1/.

A particular class of nodal methods is characterized by spatial coupling being expressed in terms of interface currents. Formally exact nodal equations of this type can be obtained by integrating (1.1a) and (1.2) over the volume

\[
V^m = a_x^m a_y^m a_z^m
\]

and (1.1b) over the six surfaces of box $m$. That leads to
\[
\frac{1}{V_g} \frac{d \phi_g^m}{dt} + \sum_{u=x,y,z} \frac{1}{a_u^m} \left[ (j_{gul}^- + j_{gur}^+) - (j_{gul}^+ + j_{gur}^-) \right] \\
+ (\Sigma_{ag}^m + \sum_{g=1}^G \Sigma_{gg}^m) \phi_g^m \\
= \sum_{g=1}^G (\Sigma_{gg}^{m^*} + \frac{1}{\lambda} \sum_{j=1}^J (1 - \beta_i^j) \chi_{pg}^j v \Sigma_{fg}^{im} \phi_g^m) \\
+ \sum_{i=1}^I \chi_{dg}^i \lambda_i C_i^m + \chi_{eg} S_{ext}^m \\

D_g^m \frac{\partial \psi_{gu}^m}{\partial u} \bigg|_s + (j_{gus}^+ - j_{gul}^-) = 0 \tag{1.3b} \\
\{ s = l, r; j, u = x, y, z \}
\]

\[
\frac{d C_i^m}{dt} + \lambda_i C_i^m = \frac{1}{\lambda} \sum_{g=1}^G \sum_{j=1}^J \beta_i^j v \Sigma_{fg}^{im} \phi_g^m \\
\tag{1.4}
\]

Apparently, \( \psi_{gus}^m (s = l, r) \) are average surface fluxes defined by

\[
\psi_{gus}^m = \frac{1}{A_u^m} \int_0^{a_u^m} \int_0^{a_w^m} \varphi_g(\vec{r}, t) \ dv \ dw
\]

With the average flux \( \overline{\psi}_g^m \) known from (1.3a) the neutron flux can be expanded into a quadratic polynomial

\[
\psi_{gu}^m (u) = \phi_g^m h_0 + \frac{\psi_{gur}^m - \psi_{gul}^m}{2} h_1(u) + \\
+ (\phi_g^m - \frac{\psi_{gur}^m + \psi_{gul}^m}{2}) h_2(u) \tag{1.5}
\]

- 259 -
\[ h_0 = 1 \]
\[ h_1 = 2u - 1 \]
\[ h_2 = 6u(1 - u) - 1 \quad (0 \leq u \leq 1) \]

Using the diffusion theory expression
\[ \psi_{gus} = 2 \left( j_{gus}^+ + j_{gus}^- \right) \]

and inserting the expansion (1.5) into Fick's law (1.3b) the resulting set of nodal equations can be solved iteratively. Coupling to adjacent boxes is achieved by requiring the partial currents to be continuous across element interfaces. Equ's (1.3 - 1.5) represent the basic variant of NEM.

Unfortunately, the simple basic variant of NEM is not sufficiently accurate for large meshes. Although the maximum error of NEM in this approximation is intolerable for large mesh sizes it converges to the exact solution of the diffusion equation for finer meshes.

1.2 Higher-Order Approximation

To improve the accuracy of NEM the expansion (1.5) has to be extended to include higher-order expansion functions. Integral and boundary conditions are already satisfied by the first three expansion functions. Useful expansion functions of third and fourth order are

\[ h_3(u) = 6u(1 - u)(2u - 1) \]
\[ h_4(u) = 6u(1 - u)(5u^2 - 5u + 1) \]
\[ (0 \leq u \leq 1) \]

The generalized expansion now reads
\[ \varphi(x, y, z, t) = \sum_{i,j,k}^{i+j+k=4} a_{ijk}(t) h_i(x) h_j(y) h_k(z) \quad (1.6) \]

As discussed above the first three coefficients of expansion (1.6) are determined by the nodal balance equations and continuity conditions. The higher-order coefficients can be determined by requiring that (1.6) solves the equivalent 1-D diffusion equation
\[ \frac{1}{V_g} \frac{\partial \psi_{gu}^m}{\partial t} - \frac{\partial}{\partial u} D_g^m \frac{\partial}{\partial u} \psi_{gu}^m + (\Sigma_{agu}^m + \sum_{g'=g}^G \Sigma_{g'gu}^m) \psi_{gu}^m \]

\[ = \sum_{g'=g}^G \Sigma_{g'gu}^m \psi_{gu}^m + \frac{1}{\lambda} \sum_{g'=g}^G \sum_{j=1}^J (1 - \beta_j^G) \chi_{pg}^j \psi_{fgu}^m \]

\[ + \sum_{i=1}^I \chi_{dg}^i \lambda_i \xi_{iu}^m - D_g^m L_{gu}^m + \chi_{eg} S_{ext}^m \]  

(1.7)

in a weighted residual sense.

Eq. (1.7) is again obtained by a formal integration process. The index \(u\) at the cross sections indicates a possible spatial dependency.

\[ \Sigma_{gu}^m \psi_{gu}^m = \frac{1}{A_u^m} \int_0^a \int_0^a \Sigma_g^m(\vec{r}) \varphi_g(\vec{r},t) \, dv \, dw \]  

(1.8)

If \( \Sigma_{gu}^m \) is constant inside the box, no assumption about the flux shape has to be made. In case of heterogeneous boxes an approximation of (1.6) can be used in (1.6).

The term \( D_g^m L_{gu}^m \) denotes the transverse leakage.

\[ D_g^m L_{gu}^m = -\frac{1}{A_u^m} \int_0^a \int_0^a (\frac{\partial}{\partial v} D_g^m \frac{\partial}{\partial v} + \frac{\partial}{\partial w} D_g^m \frac{\partial}{\partial w}) \varphi_g(\vec{r},t) \, dv \, dw \]

An approximation of \( L_{gu}^m \) can be obtained by using leakage information from adjacent boxes. A parabolic representation of \( L_{gu}^m \) has proven to be sufficiently accurate /2/.

\[ L_{gu}^m = \overline{L_g^m} + \frac{L_{1gu}^m - L_{0gu}^m}{2} h_1 + (\overline{L_g^m} - \frac{L_{1gu}^m + L_{0gu}^m}{2}) h_2 \]

Here \( L_{gu}^m \) designates the known average value of the leakage term which is given by a linear combination of partial currents. The boundary values \( L_{0gu}^m \) and \( L_{1gu}^m \) can be derived from continuity conditions. This procedure is equivalent to the determination of cross terms in the expansion (1.6).
\( \zeta_{iu}^m \) in (1.7) represents the solution of the partially integrated precursor equation.

\[
\frac{\partial \zeta_{iu}^m}{\partial t} = -\lambda_i \zeta_{iu}^m + \frac{1}{\lambda} \sum_{g=1}^{G} \sum_{j=1}^{J} \beta_i^j \nu \Sigma_{fgu}^m \psi_{gu}^m
\]

These equations could also be solved by weighted residual techniques. Investigations have shown that it suffices to set

\[
\zeta_{iu}^m = \frac{\sum_{g=1}^{G} \sum_{j=1}^{J} \beta_i^j \nu \Sigma_{fgu}^m \psi_{gu}^m}{\sum_{g=1}^{G} \sum_{j=1}^{J} \beta_i^j \nu \Sigma_{fgu}^m \phi_{g'}^m} \cdot C_{iu}^m
\]

Finally, the time derivative is approximated by

\[
\frac{1}{V_g} \frac{\partial \psi_{gu}^m}{\partial t} = \frac{1}{V_g} \cdot \frac{1}{\phi_g^m} \cdot \frac{d \phi_g^m}{dt} \cdot \psi_{gu}^m
\]

Third- and fourth-order coefficients of the expansion (1.6) are obtained by solving the WR-scheme

\[
\int_{0}^{u} \frac{d u}{\alpha_u} w_i \left( \frac{1}{V_g} \frac{1}{\phi_g^m} \frac{d \phi_g^m}{d t} + \Sigma_{agu}^m + \sum_{g=1}^{G} \Sigma_{ggu}^m \right) \psi_{gu}^m
\]

\[
- \frac{d}{d u} D_g^m \frac{d}{d u} \psi_{gu}^m + D_g^m L_{gu}^m - \sum_{i=1}^{I} \chi_{dg} \lambda_i \zeta_{iu}^m
\]

(1.9)

\[
- \sum_{g=1}^{G} (\Sigma_{ggu}^m + \frac{1}{\lambda} \sum_{j=1}^{J} (1 - \beta_i^j) \chi_{pg}^j \nu \Sigma_{fgu}^m) \psi_{gu}^m = 0
\]

As weight functions the following set of functions has been chosen for reasons of computational accuracy and efficiency

\[
w_0 = h_0 = 1
\]

\[
w_1 = h_1 = 2u-1
\]

\[
w_2 = h_2 = 6u (1-u)-1
\]
In the terminology of WR-methods this procedure is known as moments weighting. Other weighting schemes are possible /2/.

The final form of the nodal balance equations is given by

\[
\frac{1}{V_g} \frac{d \phi_g^m}{dt} = (\Sigma_{ag} - \Sigma_{g+g}^m + \Sigma_{g+g}^m) \phi_g^m + \sum_{u=x,y,z} \frac{2 C_{1gu}}{a_{1gu}^m} \phi_g^m
\]

\[
= \sum_{g+g}^G \Sigma_{g+g}^m \phi_g^m + \frac{1}{\lambda} \sum_{g'=1}^G \sum_{j=1}^J (1 - \beta_j^j) \chi_{pg}^j \Sigma_{f+g'}^m \phi_g^m
\]

\[
+ \sum_{u=x,y,z} \frac{1}{a_{1gu}^m} [(1 - C_{2gu}^m - C_{3gu}^m) (j_{g1u}^m + j_{gur}^m) - 2 C_{1gu}^m a_{3gu}^m]
\]

\[
+ \sum_{i=1}^I \chi_{dg}^i \lambda_i^i C_{g1}^m + \chi_{ge} S_{ext}^m
\]

and

\[
j_{g1u}^m = C_{1gu}^m (\phi_g^m + a_{4gu}^m) + C_{2gu}^m j_{g1u}^m + C_{3gu}^m j_{gur}^m - C_{4gu}^m a_{3gu}^m
\]

\[
j_{gur}^m = C_{1gu}^m (\phi_g^m + a_{4gu}^m) + C_{3gu}^m j_{gul}^m + C_{2gu}^m j_{gur}^m - C_{4gu}^m a_{3gu}^m
\]

where the \(C_{igu}\) are rational functions of \(D_{g}^m/a_{u}^m\) and \(a_{3gu}^m\) and \(a_{4gu}^m\) denote 3rd and 4th order expansion coefficients.

\((u = x,y,z); (g = 1,\ldots,G)\)

Boundary conditions may be chosen in the form

\[
j_g^{in} = A_g j_g^{out}
\]

where \(A_g\) is an albedo constant.

2

SOLUTION TECHNIQUES

The set of equations (1.9), (1.10a, b) is solved for each box as an inhomogeneous boundary value problem. The order of solution is completely arbitrary since the incoming currents are given as the outgoing currents of adjacent boxes. The first step in the solution process is to determine expansion coefficients (1.6) from last known values of fluxes and partial currents /2/. The old expansion coefficients are used to transform (1.9) into an easily solvable lower triangular matrix system and, in case of heterogeneous nodes, to evaluate integrals containing space-dependent cross sections. The nodal balance equations (1.10a, b) can then be solved by a conventional fission source iteration process.
Coarse mesh rebalancing and asymptotic extrapolation are used to accelerate convergence of the iterative solution process.

By using a fully implicit time-differencing scheme the solution procedure for the time dependent problem is basically the same as for a static source problem. Truncation errors due to temporal differencing are reduced by the well known frequency transformation technique /11/

\[ \phi_g(t) = \exp(\Omega t) \varphi_g(t) \]

where \( \Omega \) is a diagonal matrix of free parameters. The choice of \( \Omega \) is a delicate matter. Usually these parameters are derived from the past time behaviour of the transient solution.

As long as the rate of change of \( \phi_g(t) \) is smooth, this extrapolation procedure works satisfactorily. However, when rapid changes occur relatively small time steps must be chosen to retain accuracy. In such cases it is preferable to estimate the frequencies during the iterative solution process itself. The elements of the matrix \( \Omega \) for the time interval \( t_0 \leq t \leq t_0 + \Delta t = t_1 \) can be computed pointwise by

\[ \Omega^m = \frac{1}{\Delta t} \ln \frac{\sum_{g=1}^{G} w_g \phi^m_g(t_1)}{\sum_{g=1}^{G} w_g \phi^m_g(t_0)} \]  

(2.1)

where \( \sum_{g=1}^{G} w_g \phi^m_g(t_1) \) is a weighted sum of the group fluxes.

The calculation of \( \Omega^m \) can generally be stopped after a few iterations. The time derivative in (1.9) and (1.10a) may be replaced by

\[ \frac{1}{V_g} \frac{d \phi_g^m}{dt} = \frac{1}{V_g \Delta t} \left[ (\Omega^m \Delta t + 1) \phi_g^m(t_1) - \Omega^m \Delta t \phi_g^m(t_0) \right] \]

The solution of the precursor equations (1.4) is approximated by

\[ C_i^m(t_1) = C_i^m(t_0) e^{-\lambda_i \Delta t} + \sum_{g=1}^{G} \sum_{j=1}^{J} \beta_{ij} \nu \Sigma_{f_g}^{m} \phi_{g}^m(t_1) \]

\[ \times \frac{1 - e^{-(\lambda_i + \Omega^m) \Delta t}}{\lambda_i + \Omega^m} \]  

(2.2)

Experience has shown that the discussed solution procedure is numerically stable for all reasonable problems.

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NUMERICAL RESULTS

The method described above is the basis of the neutronic module of the computer program IQSBOX. It provides an effective means of analyzing multidimensional reactor transients accurately and at reasonable computing costs. The results obtained for various steady state /12, 13/ and transient /14/ benchmark problems demonstrate the accuracy and computational efficiency of NEM. An important feature of NEM is that mild heterogeneities caused by control rods partially inserted into nodes can be treated. Experience has shown that this property is essential for the application of coarse-mesh methods to static and transient problems. In this way 3-D calculations with only a small number of axial nodes can be performed without sacrificing too much accuracy.

A formulation of the representation of control rods is used in IQSBOX which requires no additional storage. The relevant NEM equations remain formally unchanged. This was accomplished by including the calculation of effective homogenized cross sections and source terms of the weighted balance equations in the iterative solution process. The number of iterations does not change by this procedure and consequently the computing time does not rise appreciably. On the other hand, the gain in accuracy is substantial, especially in difficult problems like the LRA-BWR benchmark /14/ (s. Figure 1).

The nodal expansion method is not restricted to two-group problems. The results obtained for a 4-group LMFBR benchmark problem indicate that NEM retains its attractive features, also being both fast and accurate for multigroup problems. Table I shows a comparison of the eigenvalues obtained with conventional finite difference diffusion codes and NEMBOX, the 4-group version of IQSBOX. Close agreement between the results of finite difference codes extrapolated to zero mesh size and the NEMBOX solutions is observed. Further results of IQSBOX which show that NEM converges towards the exact solution of the diffusion equation with finer mesh size are published in supplement 2 of the Argonne Code-Center Benchmark problem book (ANL-7416). A direct comparison between measured and calculated stationary flux distributions may be found in /13/. In the following sections an analysis of a single rod drop experiment is presented as an example for the performance of NEM in transient problems.

Table I: Values of keff for 2-D LMFBR Benchmark Problem /15/

<table>
<thead>
<tr>
<th>Model</th>
<th>Mesh size cm</th>
<th>CITATION /16/</th>
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<th>NEMBOX</th>
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<td>&quot;rods in&quot;</td>
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<td>1.104610</td>
<td>1.10998</td>
</tr>
<tr>
<td></td>
<td>2.7</td>
<td>1.111857</td>
<td>1.108409</td>
<td></td>
</tr>
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Fig. 1 3-D LRA BENCHMARK Problem: Normalized Power Distribution
EXPERIMENTAL VALIDATION

4.1 Short Description of Measurements

At KU the need was recognized to perform transient measurements in order to obtain sufficient data for validating reliably nuclear method development. To meet this requirement a series of transient experiments was carried out at the KU nuclear power station in the first quarter of the first fuel cycle. One of these experiments - an eccentric single rod drop after about 70 full power days at 80 % nominal power - will be discussed here in detail.

KU is a large PWR power plant with an electrical power output of 1300 MW. Its core contains 193 fuel elements with an active height of 390 cm. Fig. 2 shows the cross section of the core. The drop rod position of the experiment considered here is B10 near the lower right edge. The figure also indicates the positions of the 6 fuel elements instrumented with 6 self-powered, compensated $\eta,\beta$ -detectors each. These are 007, K09, H03, H13, F07 and B09, the last one lying next to the position of the falling control rod. The axial positions of the detectors are equal for all 6 fuel elements. Three detectors at a time are gathered around the mid plane of the upper and lower half of the core, as shown in Fig. 3. The absorbing medium in the detectors are cobalt wires with a length of 21 cm, and a diameter of 2 mm.

The fuel elements of the KU core have a square cross-section with 16 x 16 positions : 236 fuel rods and 20 guide tubes for control rod fingers, aeroball system and $\eta,\beta$-detectors as shown in Fig. 4.

During every transient experiment 64 measured quantities were fed into a data acquisition system at intervals of 40 ms by analogous measuring channels and stored on a digital tape. Among these are 30 $\eta,\beta$-detector signals - half of the uppermost and lowest detectors are not processed - and the outlet temperatures of the 6 instrumented fuel elements. Binary signals indicating the release of control rods and their arrival at the bottom are recorded, too. In this way all essential data of transients up to 8 min are stored on one tape for further processing by computer programs.

The recorded original detector currents cannot be compared immediately with corresponding calculated activations. They have to be corrected because of the finite time constant of the data measuring and acquisition system. Assuming the transfer function to be a simple exponential with time constant $\tau$ the relation of the undistorted function $F(t)$ and the distorted one $F^*(t)$ is given by

$$F(t) = F^*(t) + \tau \frac{dF^*(t)}{dt}$$

$\tau$ is measurable, its value is 27.1 ms for the incore detector channels. The derivative of $F^*$ is calculated by a least-square-fit of the measured activations $F^*$ in the surrounding of every time point. This correction effects noticeably only the activation curves of the detectors in the position B09 next to the dropping rod in B10. The measured curves of all other detectors remain almost unaltered by this correction because of their very small derivatives.
Fig. 2 Cross Section of KKU Core with Positions of n,β-Detectors and Aeroball System
Before starting ambitious time-dependent calculations care should be taken to check the static reactor model /18/. We felt the number of data from incore detectors not to be sufficient for this purpose. Therefore we used the data of the last aeroball shot before the transient in addition to these measurements. The D2-control rod bank was inserted by 70 cm during the transient and 56 cm during the aeroball shot. The insertion depth of all other control rods was 17 cm in both cases.

For convenient comparison with calculated values the data of the aeroball shot were interpolated in the surrounding of every incore detector and integrated over its height. Since there are 24 fuel elements instrumented by aeroball system (see Fig. 2) we obtained in this way 144 values for comparison with static calculations. This number is - together with the 36 values of the incore detectors - certainly a sufficient basis for a comparison.

The time-dependent position of the dropped rod is of particular importance for the considered transient. It is measured by the current in the lower end switch coil induced by the jack cog-rail of the falling control rod. The cogs of the rail give rise to a sinusoidal curve with rapidly decreasing periods until the control rod enters the shock-absorber. The position of the control rod end is obtained by counting the periods of the induced current up to the moment in question and multiplying this number with the constant distance of 1 cm between two cogs.

For the stationary state the resolution of the detector signals is limited by the analog-digital-transformer of the data acquisition system to a value of about 0.2 % of the average signal at full power. The corresponding value of the thermocouples is 0.25 K. At transient measurements this resolution deteriorates by superimposed noise by a factor of about 2. This does not include errors like zero displacement or poor compensation of the detectors.

The total error of the aeroball measurements amounts to about 1 %. The uncertainty in the position of dropping rods is about ± 5 cm.

4.2 Performance of Theoretical Calculations

The previously described rod injection into the fuel element B10 of the KKK core was simulated by means of the computer code IQSBOX mentioned in section 3. The cross-section of the core was subdivided into as many boxes or nodes of equal size as it contains fuel elements. In axial direction 16 planes were used as shown in Fig. 3. The mesh spacings were chosen to accommodate different material compositions - as axial reflectors, fuel element sections with and without burnable poison rods - and the position of the detectors.

Macroscopic cross sections for every box and their derivatives with respect to thermal-hydraulic parameters were transferred from the depletion code MEDIUM-2 /13/ to IQSBOX. The microscopic cross section data needed by MEDIUM on its side were computed by the cell spectral code FASER /13/, an advanced combination of THERMOS and 54-group-MUFT.
Fig. 3 Axial Position of $\alpha$, $\beta$-Detectors
Fig. 4 Cross Section of a KKU Fuel Element
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**Fig. 5** Difference between Calculated and Measured Activations in % of Average Value
On the outer boundary of the core albedos were used by IGSBOX calculated with a fine-mesh subdivision of the xy-plane taking explicitly into account the structure of the out-of-core region. These albedo values were used for all axial layers and were kept constant during the transient calculation. These assumptions are probably a somewhat crude approximation.

The core averaged values of the decay constants and the relative percentages of the 6 groups of delayed neutrons were calculated according to the burnup distribution within the core. These values were also kept constant during the calculation.

The transient calculations used the exponential transformation option. The time steps were automatically selected according to the relative changes in local neutron fluxes and fuel temperatures. The maximum flux change was limited to 12 % and the maximum difference in fuel temperature to 10 K between successive time steps. Small time steps of about 25 ms had only to be used during the period of rapid insertion of the control rod which ended at 2.2 seconds. Thereafter the time steps were gradually increased up to an upper limit of 1 s. The transient was followed up to a total time of 15 seconds in order to obtain the change in the outlet temperature of fuel element B09.

IGSBOX yields for both energy groups the mean fluxes in all boxes and the mean in- and out-currents through the six surfaces of every box. The average box fluxes are in general not sufficient for a direct comparison with measured local activations at least not in the neighbourhood of a dropping control rod. Therefore local flux values at the positions of the detectors or aeroball lances were calculated by means of a high-order interpolation method /19/ using the information available from the nodal calculation. This was done in time steps of 100 ms up to the end of the rod insertion period and for a few later time points.

These local fluxes were integrated over the height of the detectors and then used to calculate the average activations of detectors and aeroball system. The 2-group capture cross sections of the Co-wires in the detectors and of V in the aeroballs were obtained by means of the zero-dimensional spectral code GGC-4 /20/ and the one-dimensional $S_N$-code DTF IV /21/.

4.3 Results

In Fig. 5 and 6 are compared the measured and calculated activations of the steady state before the rod drop. Because of rotational symmetry in Fig. 5 only one quadrant of the core is shown. All measured values from the outside of this region are projected to the corresponding homologous positions inside. The figure shows the difference of calculated and measured activations averaged over the particular fuel elements. If there are two numbers in a square the upper one refers to the aeroball system, the lower one to the n,β-detectors, otherwise only the aeroball measurement is given. For both groups of devices the corresponding mean values of measured and calculated activations are normalized to one.

The calculated distribution is somewhat too flat. The maximum deviation of 5.7 % of the mean value occurs in a corner box at the core boundary. This indicates that probably the treat-
Fig. 6 Axial Distribution of Activations in Position B 09
ment of the reflector is the origin of this bias. The average square deviation is 3.0 % for the aeroball system and 2.2 % for the \(n,\beta\)-detectors. The deviations are small enough to regard the calculated steady state flux distribution sufficiently accurate as starting point for the transient calculations.

In Fig. 6 the calculated axial and the measured detector and aeroball activations are given in order to convey an idea of the axial flux shape in the core. The figure demonstrates that the pronounced flux tilt to the lower core half - brought about by control rods and coolant temperature rise - is reproduced fairly well by IQSBOX. In our calculations the influence of the grid-spacers was not taken into account. It is clearly visible, however, in the aeroball measurements.

The results of the time-dependent flux calculations are represented in Fig. 7 and 8. Fig. 7 shows the measured and calculated activations of some detectors lying rather far away from the dropping rod in B10. All values are normalized to one for the beginning of the transient in order to emphasize the time-dependence. In most cases only the curves of the uppermost (lower curve) and lowest detectors (upper curve) are drawn for reasons of clarity. Those of the position K09 are omitted because they would nearly coincide with the corresponding values of position H03.

These curves result mainly from the global effect of power reduction superimposed on local flux perturbations at the positions of the detectors. Since all calculated curves agree very well with the measured values - the largest difference is about 1 % for the lower detectors in F07 - IQSBOX is obviously able to reproduce correctly the total power decrease and the local effects of the dropping rod at remote core regions.

The change in activations next to the dropping rod - in the fuel element B09 - is given in Fig. 8. Again all curves are normalized to one at the beginning. The curves from the left side to the right correspond to the sequence of detectors from top to bottom. The detector signals demonstrate the time-dependent influence of the dropping rod. The gap between the two groups of curves corresponds to the distance between the upper and lower triplet of detectors.

The calculated and measured curves agree fairly well for the upper detectors of both groups. The maximum error is about 2 % of the initial value. The other four curves show larger discrepancies increasing up to 5 % of the initial values.

The reason for this bias at the end of the transient is not clearly understood until now. There are several possibilities:

- poor compensation of cable currents in the \(n,\beta\)-detectors and zero displacement on the experimental side

- neglect of grid-spacers, time-independent albedos and incorrect cross sections of control rods on the calculational side.

In Fig. 9 is presented the decrease of the coolant outlet temperature in the most affected fuel element B09. The comparison between measured and computed temperature is limited to 13 s, because the coolant recirculation takes about this time and this process is not modelled in IQSBOX. From about 12 s on the inlet temperature of the loop, supplying B10 and B09 begins to decrease. This is one of the reasons why the measured temperatures beyond this time drop below the calculated curve. In the beginning
SINGLE ROD DROP IN B 10

FIG. 7
of the transient the computed temperature decreases more rapidly than the measured values. One reason is certainly that the measured values are not corrected for a time lag of the measuring device. Its time constant is estimated to be about 1 s. This correction would reduce the discrepancy between measured and calculated values. The agreement between measurement and calculation is satisfactory and indicates that the use of a simple closed channel model is sufficient for the description of near-nominal conditions.

5 CONCLUSIONS

High computing costs and storage requirements were the main incentives for the development of several coarse mesh methods in the past. Yet even when using coarse mesh methods reduction of fast storage requirements by transfer of data in and out fast memory as it is needed in the calculation remains important in 3-D calculations. For this reason an advanced version of IGSBOX, consisting of NEMBOX and TORC/10/, which itself is an improved version of COBRA-IIIC, is being developed. The new code system uses an automated data management scheme which provides efficient transfer of data between central memory and mass storage devices.

The single rod drop presented here is the first measurement of a series, which are evaluated at present by means of IGSBOX. Further experiments of this kind are e.g.: reactor emergency shut down, load rejection to auxiliary load and switching off and on of a reactor coolant pump. The evaluation of some of these experiments will especially be useful for establishing the limits of the simple closed channel model.

The IGSBOX code accurately predicts the course of a transient caused by a single rod drop. All calculations were performed with a nominal set of neutronic and thermo-hydraulic data. The exponential transformation technique allowed the transient to be followed up to 15 s at reasonable costs in terms of computing time. In this way it could be shown that for near-nominal operating conditions, a closed channel model is quite adequate. We anticipate that for far off-nominal conditions where there are large gradients in power, mass flow, and inlet temperatures an open channel model permitting both energy and flow exchange between neighboring channels, is more appropriate.

ACKNOWLEDGMENTS

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SINGLE ROD DROP IN B 10
DETECTOR POSITION B 09

FIG. 8
Fig. 9 Decrease in Coolant Outlet Temperature of Fuel Element B 09
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Lathrop, K. D.: DTF-IV, a FORTRAN-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering, LA 3373
REVIEW OF SOME ACTIVITIES PERFORMED IN ITALY ON THE DEVELOPMENT
AND VERIFICATION OF CODES FOR THREE-DIMENSIONAL POWER DISTRIBUTION
CALCULATIONS IN LWRS

AMN    - A.G. Gandini, S. Grifoni, F. Labriola, V. Silvani
CISE   - G. Bottoni, M.M. Giorcelli, R. Guandalini, G. Vimercati
CNEN   - F. Pistella
ENEL   - G.M. Balestra, F. Di Pasquantonio

ABSTRACT

A review of some activities performed in Italy on 3D simulators is
given. Some of these activities contribute to the confirmation of methods
currently used in core design and operation, through operating and ex-
perimetal data at Garigliano and Caorsa power plants. On the other hand,
a few codes obtained from the MIT have been modified and applied both to
the usual benchmark problems and to critical situations. Besides, some
efforts have been devoted to the development of an essentially one-
group coarse mesh model (COMETA, now embodied into the three-dimensional
simulator CETRA); spectral effects arising from the presence of great
material heterogeneities are taken into account. Finally, the FEMSYN and
SYNTH-C codes based on the synthesis method have been developed.
1. INTRODUCTION

Three-dimensional calculations of power distribution are essential for the analysis of large LWR's.

This task is usually performed by computer codes called "simulators", designed to evaluate the core distribution of the quantities associated with power production (neutron flux, voids, temperatures, burnup etc.) and to specify their mutual influence in simulated reactor operations.

More specifically, the tasks of simulators are:

A evaluation of (one or few groups) neutron flux;
B computation of thermal and thermalhydraulic parameters associated with feedback effects;
C studies on fuel composition evolution over medium or long periods (Xe and burnup);
D simulation of control rods and (possibly) fuel assembly management;
E evaluation of detailed power distribution and main safety and operating margins.

In view of its wide range of applications from design and prediction calculations to "on-line" simulation, a simulator must meet at least the following requirements: (a) quantities of high economic importance must be evaluated with adequate accuracy; (b) the user may be not extremely experienced in the field; (c) the amount of input data evaluated by different programs or deriving from measurements on the power station under consideration, must be minimized; (d) owing to the frequent utilization of the program and the consequent practical and economic concerns, the software aspects (e.g. programming and result visualization) must be carefully considered.

Points C, D and E, though being an important part of the whole creative effort, are not troublesome from the physical and mathematical points of view. The impact of point B depends on whether a BWR or a PWR power plant is considered: nevertheless, in both cases, a correlative approach is used whose accuracy degree must not seriously affect the whole simulator efficiency and whose choice depends on the accuracy obtainable in point A.

From the physical and computational points of view the most serious problems are those concerning the neutron flux evaluation.

As it is well known, the starting point of all three-dimensional methods are the few group diffusion equations. The detailed description of a thermal reactor requires three or four energy groups and, if based on a finite difference approximation, can easily involve a million of mesh points. Consequently a number of alternative methods have been developed. These methods can be grouped in synthesis procedures, response matrix techniques, nodal schemes and finite element methods.

At present three-dimensional one-group coarse mesh diffusion models are currently used with confidence in the industry for BWR core analysis; the two-group model is more frequently used in PWR applications.
The frontier is nowadays the need of homogenization and collapsing methods producing few group homogenized constants suitable to adequately represent also highly heterogeneous structures by "coarse-mesh" methods, conceived for homogeneous elements.

The Italian activity in this field was carried out by different working groups, each emphasizing different aspects associated with simulator use, and organization. In order to logically frame the different activities, one can briefly list the steps to be accomplished in the major calculation programs:

a definition of the physical-mathematical model for each event to be simulated (events A, B, C and E);
b choice of numerical methods to solve problems defined at point A;
c specification of program structure and production of software;
d testing of the program performance on benchmark problems or, more generically, on reference code results;
e supply of suitable input data by allocating the program in a code chain (as shown in the following, particular care must be devoted to the assembly constants);
f adequacy evaluations of the whole code chain by comparison with experimental results.

Italian activities have covered all the above aspects, dealing with the development of codes (3-Dimensional neutronic Codes: COMETA /1/, /2/, 3DTD /3/, FEMSIN /4/; /3/ dimensional core simulators: BACONE /5/, /6/, CETHRA /7/, /8/, SYNTH-C /9/, and the confirmation of adequacy of simulators currently used in core design and operation (BWR simulator used at AMN /10/, BACONE) through operating and experimental test data from Italian power stations.

Results of COMETA and 3DTD codes have been compared with those of the open code QUANDRY /11/.

Nowadays particular care is devoted to improve the modelling aspects associated with task A and to confirm the adequacy of the program chains against experimental data: therefore a considerable part of this paper will be devoted to points a, d and f.

2. ITALIAN CONTRIBUTION TO DIFFERENT APPROACHES

The following description of the methods is only a summary outline since they have already been illustrated in detail elsewhere. Only a few particular aspects are touched upon here as they appear worthy of further investigation and interesting from the standpoint of a correct interpretation of the measurements.

2.1. Self-consistent approaches

2.1.a. 3D_Coarse mesh methods

The coarse mesh method used in COMETA has been developed to obtain, still retaining considerably simple formulation, a remarkable improvement as compared with the simple finite difference coarse mesh techniques. To be fruitful in physical problems the progress obtained in the solution of the one-group diffusion equation requires some analytical correlative adjustments extending the method applicability to both BWR and PWR core studies.
The method, whose original version is described in /1/, is derived from the Henry non-linear model of /12/.

The core is divided into homogeneous parallelepipeds (nodes).

The buckling of each node is assumed to be separable into three components
\[ B^2_x + B^2_y + B^2_z = B^2 \]  
which in turn are assumed to be constant nodewise.

The one-group flux is then a combination of either trigonometric (positive buckling) or hyperbolic (negative buckling) functions. In the \( x \) direction, for example, one has
\[ \phi(x) = A(y,z) \begin{cases} \sin (B \cdot x) + C(y,z) \\ \text{Sh} \\ \text{Ch} \end{cases} \begin{cases} \cos (B \cdot x) \\ \text{Sh} \\ \text{Ch} \end{cases} \]  

Interface averaged flux and current continuity is required. Adjacent nodes are coupled via the net interface current linearly depending on the average fluxes relevant to such nodes. In the \( x \) direction, for example, one has
\[ j^i_j = \frac{w^i_X - \bar{q}^i_X}{s^i_X/D^i_X + s^j_X/D^j_X} \]  
where \( s^i_d \) and \( W^i_d \) are functions only of buckling and width of the node \( n \) in the direction \( d \), \( D^n \) is the diffusion coefficient in node \( n \).

Therefore, to obtain the matrix needed to calculate the power distribution, it is necessary to know the bucklings which, however, are to be provided by the calculation itself, as they depend on interface current and node-averaged fluxes. Consequently, the coarse-mesh method, embodied into COMETA, must perform buckling iterations, until both power distribution and nodal buckling converge.

Conveniently chosen albedos simulate reflectors, not embodied into the core representation.

The method, giving satisfying results in one-group benchmark problems, becomes inadequate when, using conveniently energetically collapsed constants, it is applied to the IAEA two-group benchmark problem /13/. The greatest discrepancies occur in the nodes near the controlled assemblies or at the core-reflector boundary (the reflector in this case is embodied into coarse mesh discretization).

Then the need becomes apparent of a model extension that will somehow take into account the spectral effects at critical points though the one-group formulation is retained to minimize the computing time increment.

These effects may be partly considered by modifying the power obtained at the convergence of the one-group calculation; for this purpose the results of a conveniently simplified problem are used./14/
Spectral effects on the eigenvalue and the power shape even in uncritical nodes are taken into account by a source placed at the interfaces between adjacent nodes and proportional to the interface flux (blade model) /2/. This approach may be utilized in two completely different situations: inside the core to simulate thin, highly absorbing regions like a control rod (absorber blade) and both inside and at the core boundary to reproduce spectral effects due to adjacent material composition (spectral blade). It must be emphasized that, in the absence of localized absorption, the interface source is a mere expedient to reproduce two-group results by a one-group model.

Usually, at the core boundary, alternative expedients are applied like albedos or, when the reflector is explicitly taken into account, adjusted material constant. Both approaches introduce drawbacks.

The geometry and material distribution effects on the incoming/outgoing current ratio are not easily represented in the albedo approach. On the other hand, for an explicit reflector representation, one has to decide how many and which core and reflector nodes must be corrected, as well as the correction modalities. Beside in the latter case, if suitable measures are not applied, the gain obtained by accurately representing geometry and material distribution is nullified by the one-group model inadequacy.

The blade model allows the required modifications to be performed on the one-group model without using adjusted material constants.

The "absorber blade" is a device to save nodes in reactor simulation. Let the control rod be represented by a thin region \( k \) of convenient material composition and placed between two core regions \((i,j)\)

\[
\begin{array}{cccc}
\text{blade} & \hline
i & k & j \\
\hline
-h & 0 & +h \\
\end{array}
\]

In the blade model the \( i \) and \( j \) regions reach the middle of the \( k \) layer. At the interface between \( i \) and \( j \) regions, the following conditions hold

\[
\begin{align*}
\Phi^i_j &= \Phi^j_k = \Phi^k_j \\
J^i_j &= J^j_k; \quad J^j_i = J^j_k; \quad J^i_j + J^j_i = E \Phi^i_j
\end{align*}
\]

where \( E \) is the "blade factor" typical of the localized absorber.

One can easily verify that is a one-group scheme at \( k \) layer.
boundaries, the following relationships between flux and current are fulfilled.

\[ \dot{\varphi}^{ik} - \varphi^{kj} = \frac{Th}{D_B} \left( j^{jk} + j^{ik} \right) \quad (6) \]

\[ j^{ik} + j^{jk} = D_k^k Bh \left( \varphi^{ik} + \varphi^{kj} \right) \quad (7) \]

where \( B^2 = \sum_k^{D_k^k} \) is the non-multiplying \( k \) region buckling.

For \( h \to 0 \), equation (6) becomes the current definition as the flux difference and (7) becomes the balance equation on region \( k \), that is,

\[ \varphi^{ik} - \varphi^{kj} = \frac{h}{D_k^k} \left( j^{jk} + j^{ik} \right) \quad (6') \]

\[ j^{ik} + j^{jk} \approx D_k^k B h \left( \varphi^{ik} + \varphi^{kj} \right) = \sum_k^{D_k^k} h \left( \varphi^{ik} + \varphi^{ki} \right) \quad (7') \]

Equation (6') becomes equation (4) when symmetry conditions as to the blade middle plane hold and it is quite similar to condition (4) when \( h \) is small compared with \( D_k^k \). This condition is verified in a BWR when \( h \) may be identified as control rod semi-width.

When condition (4) holds, equation (7') becomes equation (5) and, if \( \sum h \) is not zero, it does not correspond to the usual current continuity condition. The term on the right hand of equation (7') represents the \( k \) region capture reaction rate; in a control rod this quantity, that cannot be neglected, represents a considerable part of the assembly capture rate.

COMETA equations, using continuity conditions (4) and (5), become

\[ \varphi^{ij} = \frac{\varphi^{i} \cdot \varphi^{j} + \varphi^{i} \cdot \varphi^{j}}{D_i^i D_j^j} \quad (8) \]

\[ j^{ij} = \frac{\varphi^{i} \cdot \varphi^{j} \left[ 1 + \frac{\varphi^{j}}{D_j^j} \right] - \varphi^{i} \cdot \varphi^{j}}{D_i^i D_j^j} \quad (9) \]

These equations obviously hold both for an "absorber blade" and a "spectral blade".
The "spectral blade" is quite similar to the "absorber blade" except that in this case the criterion adopted for selecting the extremely thin layer material characteristics is to get a "good" agreement between the real situation and a convenient sample problem. The procedure consists in deducing from the sample problem the values of \( \bar{q}^1_i, \bar{q}^j_i \) and \( J^i_{ij}/\bar{q}^i_{ij} \), and in evaluating \( \mathbf{E} \) using these values and equation (8) and (9).

The value of \( \mathbf{E} \) thus obtained is then considered typical at the interface considered in the problem under study.

The sample problem is described in /2/: maximum simplicity has been pursued in its formulation. Taking into account that the better the real situation is reproduced from the sample problem the better the results obtained, two different sample problems have been formulated: one applies when the spectral transient may be adequately represented with a one-dimensional model and the other is applied when reflector nodes share two interfaces with the core.

The original COMETA model, improved as previously described gives good results in IAEA benchmark type problems where the heterogeneous element structure in not considered or, anyway, is not determinant. Then the model, suitable for PWR node averaged power evaluation, needs some further corrections for BWR studies.

These further improvements /8/ required by the \( \text{H}_2\text{O} \) gap that weakens the connection between assemblies, consist in reducing both the blade coefficient \( \mathbf{E} \) and the "a posteriori" modification of the power obtained in the mere one-group scheme. In practice, inside the core, both "a posteriori" modification and "spectral blade" have been cancelled, and only a "absorber blade" is used for control rod simulation. Conveniently reduced "spectral blade" and "power modifications" are used on nodes at the core-reflector boundary: the reduction factors are deduced from a few problems previously solved taking into account that this "improvement in the improvement" depends more on geometry than on material composition.

2.1.b. Synthesis methods

For the last two decades the Single Channel Flux Synthesis (SCFS) method and its several variation have been in use for three-dimensional steady-state and time-dependent neutron flux solutions. The SCFS method takes advantage of the fact that the reactors are generally less heterogeneous in axial direction than in radial plane, thus allowing a 3D problem to be broken into a set of 2D trial function solutions followed by a one-dimensional calculation for the mixing functions.

In a multigroup SCFS method, the neutron flux of each group \( g \) is approximated by a linear combination of the form

\[
\phi^g(x,y,z) = \sum_{k=1}^{K} H^g_k(x,y) z^g_k(z) \quad g = 1,2,\ldots, G
\]

where \( G \) is the number of energy groups, \( H^g_k \) are precalculated two-dimensional trial functions and \( z^g_k(z) \) are mixing coefficients which become the actual unknowns of the problem.
The main factor blocking the widespread use of the synthesis method is the difficulty in choosing appropriate trial functions.

Most of the currently available synthesis codes use 2D trial functions generated by a FDM routine which is either built-in or coupled externally. These FDM calculations should use reasonably fine meshes in order to guarantee a good accuracy on the final 3D flux solution. Trial functions obtained by the finite element method (FEM) prove to give very accurate results using assembly sized meshes. Thus there is some good incentive in replacing FDM routine by a FEM routine for the generation of 2D trial functions in a SCFS code. Another advantage of using FEM is the possibility of concentrating meshes in regions of large flux gradients (e.g. control rod, reflector etc.).

Some applications of the last method could be made when large homogeneous/homogenized regions are not uncommon. In the explicit treatment of all the heterogeneties of fuel boxes however, the use of trial functions obtained via the finite difference method should be preferable since the advantage of employing coarse meshes in the case of the finite element method would be lost.

The SYNTH-C program /9/ solves both steady-state and time-dependent few-group diffusion problems by a space-time synthesis method with axially and time discontinuous trial functions \( H_k^G(x,y) \). The reactor height may be divided into several axial zones where different sets of trial functions can be defined, and the transient duration may be divided into several time segments for the same purpose.

The generation of trial and weight functions can be accomplished by an appropriate version of the finite difference program SQUID /15/.

The linear independence of trial and weight functions is of great importance in determining the convergence of the solution and the accuracy of the results. Actually a good indicator for linear dependence can be identified in the minimum eigenvalue of the CRAM matrix for each function (separately for trial and weight functions, group by group), which is exactly zero if and only if the functions are strictly linearly dependent. In SYNTH-C, possible sets of trial and weight functions are tested for linear independence using this methods.

The eigenvalue problem to obtain the mixing coefficients \( Z_k^G(z) \) is solved by the Wielandt method.

In SYNTH-C, three thermal-hydraulic models are available: adiabatic fuel heatup, WIGL /16/ and COBRA - IIIC/MIT /17/ models. At the development stage the SYNTH-C code was extensively tested /32/.

Program FEMSYN /4/ solves the multi-group diffusion equations in three dimension using a single channel continuous synthesis model.

The trial functions \( H_k^G(x,y) \) are obtained by a finite element routine treating any combination of rectangular and triangular elements. Linear, quadratic or cubic Langrange interpolation polynomial functions can be used. A locally variable bandwidth
storage scheme is used for the finite element matrices in order to facilitate solution by modified Choleski decomposition method.

Owing to the possibility of choosing rather large assemblies, the computation time for the trial function calculation is low, and the evaluation of the integrals needed for synthesis calculation may be performed analytically within each element.

The eigenvalue problem to obtain the mixing coefficients \( Z^g_k(z) \) is solved by the usual power method accelerated by an input over-relaxation parameter.

2.2. Calibrated methods

By "calibrated methods" one usually means approaches where some aspects of the theoretical method are improved using information previously obtained (experimentally or by calculations).

The "calibrated methods" more frequently used in BWR calculations are based on the finite difference coarse mesh 1.5 group diffusion theory. The mesh points are distributed approximately within one fast neutron mean free path.

Albedo type boundary conditions are applied at core reflector interface.

The one-group model in its simplest form

\[
- \nabla^2 \phi = B^2 \phi
\]  

(10)

is derived from three-group diffusion equations.

Adopting the following assumptions:

1. all neutrons are born in the fast group

2. spatial gradient of \( D_1 \) is neglected

3. most neutron leakage and diffusion over a mesh point takes place at fission energies (group 1). For slower energies (group 2 and 3), the leakage approaches the asymptotic expression

\[
- \nabla \cdot D g \nabla \phi_g = \sum_{g} \left( \frac{D g}{g} \right) \phi_g \quad g = 2, 3 \]  

(11)

4. the thermal and epithermal global flux shapes are similar to the fast distribution over a coarse mesh, that is

\[
\frac{\nabla \cdot D_3 \nabla \phi_3}{D_3 \phi_3} \sim \frac{\nabla \cdot D_2 \nabla \phi_2}{D_2 \phi_2} \sim \frac{\nabla \cdot D_1 \nabla \phi_1}{D_1 \phi_1}
\]  

(12)

or, assuming equality and using equations (11) and (12)

\[
B_3^2 = B_2^2 = B^2
\]  

(12')
$B^2$ is much less than 1 ($B^2 \ll 1$), the resulting material buckling takes the well known simple forms

$$B^2 = \frac{\frac{k_{\infty}}{k} - 1}{M^2 - \frac{A_{\infty}}{k}}$$  \hspace{1cm} (13)

where

$$k_{\infty} = \frac{\nu \sum f_1}{\sum R_1} + \frac{\nu \sum f_2}{\sum R_2} + \frac{\nu \sum f_3}{\sum R_3}$$

$$A_{\infty} = \frac{\nu \sum f_1}{\sum R_1} \left( M_2^2 + M_3^2 \right) + \frac{\nu \sum f_2}{\sum R_2} \frac{M_3^2}{M_3}$$

with

$$\sum R_j = \text{total removal cross section in the group } j$$

$$\sum f_j = \text{fission cross-section}$$

$$\sum_{SL} J = \text{slowing down cross section}$$

$$M_j = \text{migration area}$$

At the interface between reactor core and reflector fuel homogeneous boundary conditions are used:

$$D \nabla \phi + \Gamma \phi = 0$$ \hspace{1cm} (14)

where $\Gamma$ is a logarithmic derivative boundary-condition constant determined for top, bottom and radial calculations outside the three-dimensional simulator.

Equation (10) is solved by discretization using a first-order difference scheme.

It is possible improve the results in proximity of strong material heterogeneities (e.g. controlled assemblies) replacing $B^2$ in E q n. 11 by $B^2_g$, obtained by averaging the nuclear characteristics of the considered node with those of adjacent nodes. Instead of averaging the $B^2$ value obtained from equation 13 directly, is preferable to average the value of $M^2$ and $k_{\infty}$, ignoring the negligible contribution of $A_{\infty}$.
3. COMPARISON OF SELF-CONSISTENT APPROACHES

3.1 Coarse mesh methods

The COMETA /1/ /2/ 3DTD /3/ and QUANDRY /11/ codes have been considered.

The COMETA theory has been previously described in 2.1.a. section.

Both 3DTD and QUANDRY are three-dimensional programs developed mainly for dynamic analysis but can be successfully used for steady-state calculations. They are based on the MIT analytical nodal scheme /18/ but QUANDRY has the advantage of a quadratic approximation of the nodal transverse leakage (instead of the flat approximation used in 3DTD). The 3DTD program has been developed from ENEL-CRTN starting from the 2DTD program described in the Shoher thesis /19/; QUANDRY code on the contrary has been obtained from MIT with the kind permission of EPRI.

The comparison has been performed on the IAEA /13/ and LRA /20/ three-dimensional benchmark problems.

The IAEA problem represents on actant of a medium-sized PWR with two radial enrichment zones. The core is reflected by pure water. A number of fully and partially inserted rods, represented as smeared absorbers, cause a strongly varying non-separable 3D power distribution.

In addition the existence of a very sharp thermal flux peak in the radial reflector makes this a very difficult and challenging problem to be solved.

The LRA problem represents superprompt critical transient in a BWR reactors. The transient is induced by withdrawing the most reactive rod in cold situation. The results at initial steady state are frequently used to test results of static codes. At the initial time, the core is divided into two radial zones with different enrichments: both, internal and peripheral regions are nearly fully controlled.

Though the inserted rod situation is considered, axial and radial reflectors are represented by pure cold water regions. Considering that we are dealing with a BWR reactor, the more severe simplification adopted consists of the homogenization of the control rods and of any other element heterogeneity.

However the presence of a high radial power peaking factor (more than 2) with the peak power near the reflector makes the problem very hard to be solved.

The same programs have been also compared in the two-dimensional problem quoted in /8/. The more interesting characteristic of this benchmark is to emphasize in a not particularly critical situation, the importance of correctly taking into account the BWR assembly typical heterogeneities. Two versions of the problem are proposed: the same reactor situation is indeed considered with both heterogeneous and homogenized elements. Two types of element are involved, both in controlled and not-controlled situation. The homogeneous material constants have been obtained by boundary zero current element calculation in each situation. The flux weighting method has been used. Reference calculations have been made by
The results obtained in the two benchmark problems are quoted in table I.

<table>
<thead>
<tr>
<th>PROBLEM</th>
<th>REFERENCE SOLUTION</th>
<th>3DTD/45/(x)</th>
<th>QUANDRY/21</th>
<th>COMETA/31</th>
</tr>
</thead>
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<tr>
<td>IAEA 3D /38/</td>
<td>$k_{eff}$</td>
<td>1.02904</td>
<td>1.02963</td>
<td>1.02903</td>
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<tr>
<td>Ref Sol at (x, z) cm (o)</td>
<td>$P_{max} / P_{avg}$</td>
<td>2.301</td>
<td>2.265</td>
<td>2.294</td>
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<td>(+)QSBOX /10/</td>
<td>symmetry</td>
<td>170</td>
<td>170</td>
<td>170</td>
</tr>
<tr>
<td></td>
<td>computer</td>
<td>CDC 6600</td>
<td>IBM 370/158</td>
<td>IBM 370/158</td>
</tr>
<tr>
<td>CPU time</td>
<td>276 sec</td>
<td>5 min</td>
<td>159 sec</td>
<td>235 sec</td>
</tr>
<tr>
<td>symmetry</td>
<td>1/8</td>
<td>1/8</td>
<td>1/8</td>
<td>1/8</td>
</tr>
</tbody>
</table>

| LRA-3D /39/ | $k_{eff}$ | 15x15x30 | 15x15x30 | 15x15x30 |
| Ref Sol at (x, y) cm (o) | $P_{max} / P_{avg}$ | 99632 | 99644 | 99661 |
| QSBOX /10/ | symmetry | 3.195 | 3.2184 | |
| | computer | ---- | ---- | ---- | |
| CPU time | 160 sec | 360 sec | |
| symmetry | 1/8 | 1/8 | |

| LRA 2D /39/ | $k_{eff}$ | 15x15 | 15x15 | 15x15 |
| Ref Sol at (x, y) cm (o) | $P_{max} / P_{avg}$ | 2.161 | 2.222 | 2.164 | 2.1756 |
| QSBOX /10/ | symmetry | 97.5; 97.5 | 97.5; 97.5 | 97.5; 97.5 |
| CPU Time | CDC CYBER 175 | IBM 360/165 | IBM 360/165 | UNIVAC 1106 |
| symmetry | 255 sec | 15 sec | 7 sec | 53 sec |
| | 1/4 | 1/4 | 1/4 | 1/8 |

| Homogeneous Problem of /31/ | $k_{eff}$ | Variable <2.5 cm | 15 x 15 | 15 x 15 |
| Ref Sol at (x, y) cm (o) | $P_{max} / P_{avg}$ | 95017 | 95034 | 95223 |
| QS/ SQUID/34 | symmetry | 1.189 | 1.401 | 1.400 |
| CPU Time | UNIVAC 1105 | IBM 370/158 | IBM 370/158 | UNIVAC 1106 |
| symmetry | 2520 sec | 9 sec | 23 sec | 1/4 |
| | 1/4 | 1/4 | |

| Heterogeneous Problem of /31/ | $k_{eff}$ | Variable <2.5 cm | 15 x 15 | 15 x 15 |
| Ref Sol at (x, y) cm (o) | $P_{max} / P_{avg}$ | 82.5; 22.5 | 82.5; 22.5 | 82.5; 22.5 |
| QS/ SQUID/34 | symmetry | UNIVAC 1105 | UNIVAC 1106 | 1/4 |
| CPU Time | 2560 sec | 9 sec | 23 sec | | |
| symmetry | 1/4 | 1/4 | |

(o) Center node values: $x = y = 0$ at core center; $z = 0$ at core bottom
(x) The strong difference in computing times between QUANDRY and 3DTD is essentially due to a lack of optimization in the program organization and solution methods (e.g. 106 power iterations in 3DTD against 30 Wilkinson iterations in QUANDRY).
(+) $G_3 B^2$-approximation (quintic polynomial with quadratic transverse leakage).
As to the results of table I, one can observe that:

1) Assuming that the accuracy achieved in the problem considered is obtainable as a rule even in situations where a simulator is used (what is not absurd owing to the benchmark severe difficulties), one can deduce that the accuracy of the results of all the codes considered is quite sufficient. Obviously, the accuracy obtained with two-group models is higher than that of the one-group model, at least in situations where the comparison is possible.

2) The low computing time allows a not expensive use of the codes. In particular the high quality achieved in two-group code software implementation, is evident (even if the comparison of CPU time of different computers is always imprecise). For a correct evaluation of COMETA efficiency, one has to take into account that the version used is a "multipurpose" code, and not the BWR oriented one (embodied into CETHRA), where the neutron and thermalhydraulic models are coupled.

3) The 3DDT and QUANDRY theories are not comprehensive of devices to take into account assembly heterogeneities. The best efficiency of these codes (which are undoubtably powerful) is obtained when the core heterogeneities do not play too an important role. Another positive aspect of these two-group codes is their internal coherence that would guarantee performance reliability. This fact becomes particularly evident observing that a one-group approach requires a specific model for the power evaluation from the flux. On the other hand it is true that a one-group model such as COMETA seems not to suffer from this need for further theoretical considerations, but on the contrary it proves to be very efficient if applied to substantially heterogeneous situations for which it had been conceived, that is BWR core simulation.

3.2. Synthesis method

The 3-D IAEA benchmark problem /13/ was chosen in order to demonstrate the potentiality of the synthesis method.

The eigenvalue, the peak/average thermal flux value in core and its location, as computed by SINTH-C /9/ and FEMSYN /4/, are presented in table II. For the evaluation of trial functions in FEMSYN, triangular elements have been used mainly in controlled fuel bundles and in reflector region. Rectangular elements (20 x 20 cm) were used for most of the uncontrolled fuel bundles.

Results of a PDQ 7 /21/ fine mesh calculation and of IQSBOX /22/ were used as the reference value.

4. COMPARISON WITH EXPERIMENTAL DATA FOR CALIBRATED METHODS

4.1. Comparison between Garigliano data and BACONE results

The first seven cycles in the Garigliano nuclear power station (BWR, 150 MWe) were reproduced by BACONE code (BWR's Analysis with
<table>
<thead>
<tr>
<th>PROGRAM</th>
<th>PDQ 7</th>
<th>IQSBOX</th>
<th>SINTH C</th>
<th>FEMSYN</th>
</tr>
</thead>
<tbody>
<tr>
<td>METHOD</td>
<td>corner mesh 3D FDM</td>
<td>NEM</td>
<td>mesh centered FDM + synthesis</td>
<td>FEM + Synthesis</td>
</tr>
<tr>
<td>MESHES</td>
<td>68 x 68 x 76</td>
<td>17 x 17 x 17</td>
<td>137 x 137 x 305</td>
<td>183 x 90</td>
</tr>
<tr>
<td>POLYNOMINAL ORDER</td>
<td>——</td>
<td>4</td>
<td>——</td>
<td>2</td>
</tr>
<tr>
<td>NUMBER OF TRAIL FUNCT.</td>
<td>——</td>
<td>——</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>k&lt;sub&gt;effect&lt;/sub&gt;</td>
<td>1.02933</td>
<td>1.02910</td>
<td>1.02898</td>
<td>1.02922</td>
</tr>
<tr>
<td>CP time</td>
<td>67.8 min (CDC 6600)</td>
<td>4.8 min (CDC 6600)</td>
<td>(39.2) min (IBM 370/158)</td>
<td>(13 x 7) min (IBM 370/168)</td>
</tr>
<tr>
<td>$\theta_{th}$/ $\theta_{avg}$ in core</td>
<td>2.256</td>
<td>2.356</td>
<td>2.351</td>
<td>2.487</td>
</tr>
<tr>
<td>at (X,Y) cm</td>
<td>(32,32)</td>
<td>(30,30)</td>
<td>(32.5,32.5)</td>
<td>(30,30)</td>
</tr>
<tr>
<td>Z cm</td>
<td>175</td>
<td>170</td>
<td>172.5</td>
<td>175</td>
</tr>
</tbody>
</table>

(+) The members in brackets refer to trial function generation and synthesis calculation respectively.
Coupled NEutronics) /5/, which is a tridimensional simulator of a BWR core with a representation of the neutronic and thermohydraulic behaviour of the core versus irradiation.

As an input in the simulation, use was made of the nuclear constants of the fuel assemblies according to the procedure described in /23/. In BACONE, channel and bypass mass flow rates can be calculated directly with the code or determined by means of correlations whose coefficients are obtained from off-line calculations. In this comparison the second option has been used, and the correlation coefficients were obtained by suitable thermalhydraulic codes described in /24/.

Fig. 1-4 compare the radial power distributions with γ-scannings performed for BOC 1A, EOC 1A, EOC 2 and EOC 5.

The comparisons indicate that in the presence of control rods (BOC 1A) (fig. 1), the power of the adjacent assemblies is underrated. This underrating is corrected with the "MEDIE" version of the code which averages the buckling values (cfr. para 2.2. Eqn. 13).

Another observation is that in any cycle studied, the effect of the reflector on the peripheral assemblies was not adequately represented (the power of the assemblies near the reflector was generally underrated). Anyway these assemblies generate much less power than the central ones, on which thermal limits are checked for proper plant operation. A study is under way to take the reflector effect on the peripheral assemblies more accurately into account.

Another fact that was revealed by the radial comparison (EOC5) is that the calculation of the power of adjacent assemblies having very different characteristics (uranium, plutonium-island, all-plutonium assemblies) gives much larger deviations even though the calculated values are conservative.

The axial curves, related to the various operating cycles, representative of the experimental data obtained from γ-activation of the assemblies and of the in-core TIP readings during plant operation /25/ are given in figs. 5-6 and 7-8, respectively. The results of BACONE calculations, also obtained with the "MEDIE" version, are represented in the same figures. The map of TIP position is given in fig. 9.

The comparison indicate that the calculated values are fairly consistent with the operating data.

Finally one can say that these experimental comparisons demonstrated that on the whole the results obtained with the BACONE code are satisfactory for the user's requirements even though in quite particular situations the results are less accurate. (but can be improved with better calculation models).

4.2 Comparison between Caorso experimental data and AMN simulator results /26/.

In support of the adequacy and accuracy of core design methods, Ansaldo Meccanico Nucleare (AMN) carried out several experimental tests during Caorso NPS start-up period. Control rod calibration (cold condition) and in particular axial flux measurements in localized cold criticals are severe tests of the three-dimensional model.

- 297 -
The three-dimensional BWR Core Simulator /10/ currently used at ANL is a coupled nuclear thermal-hydraulic program; the nuclear model consists of a finite-difference, coarse mesh, 1.5 group fast flux static diffusion theory.

The program is used for detailed three-dimensional design and operational calculations of BWR neutron flux and power distributions and thermal performances and for target exposure distribution and cycle length predictions.

The results presented herein contribute to confirm the accuracy in shut-down margin evaluation and to support the adequacy of the diffusion coarse mesh flux and power solution, which in turn affect safety, fuel cycle economics and plant performances.

Cold critical measurements /27/ /28/ /29/ /30/

A localized cold critical measurement provides spatial thermal epithermal and fast flux distributions for a critical configuration closely representing the cold one-stuck rod configuration, an important constraint, in term of shut-down margin, in BWR design and operation.

The very steep radial and axial flux gradient and the axially varying burn-up and hystorical void make this a severe test of the three-dimensional model and of the ability of the coarse mesh diffusion theory to accurately predict nuclear characteristics.

Two localized cold critical measurements were performed at ~ 1200 MWD/T, one in a central region of the core and the other in a peripheral one, by the withdrawal of two adjacent control rods in each zone.

In both critical configurations two full-length axial wire assemblies, each of these containing a copper a gold and a nickel wire, were irradiated to obtain a measurement of the thermal epithermal and fast axial flux distributions at two different radial positions. In each zone, the flux wire assemblies were inserted into two TIP guide tubes, one diagonally adjacent to the two withdrawn rods, and the other several bundles away from withdrawn rods (see fig. 10).

Criticality was achieved in both cases with the two adjacent rods about 50% withdrawn.

The prediction of the core eigenvalue and fast flux distribution was performed using the three-dimensional BWR simulator program, considering in detail the actual operating history.

The normalized fast flux distribution is compared directly to the normalized nickel activation distribution.

The axial distribution in each flux wire location was calculated by averaging the nodal fast flux of the four bundles surrounding the flux wire location.

For each localized critical the flux distributions in both wire localisations are normalized to enable a comparison of the magnitude of the flux distribution in the two radial positions.
The experimental copper, gold and nickel activation distributions are shown in fig. 11 and 12 (central and peripheral localized cold criticals) (ref. 29).

The similar shape of the thermal, epithermal and fast spatial activation distributions justifies approximations in the coarse mesh fast flux solution.

The comparison of the measured nickel wire activation and the calculated fast flux distributions for both flux wire locations is shown in fig. 13 and 14 (central and peripheral criticals). The predicted fast flux distributions agree well at both flux wire locations at the peak agreement is within 4% in the central zone and within 3% in the peripheral zone. The experimental uncertainty is about ± 1%.

In addition to the axial shape the BWR core simulator program demonstrates good accuracy in predicting the radial flux distribution for the local criticals.

The predicted critical eigenvalues for the experiments after period and temperature correction agree closely with the expected eigenvalue in cold conditions at the corresponding core average exposure.

In addition to the two localized criticals, a cold dispersed critical has been performed at the same exposure. The calculated critical eigenvalues for localized and dispersed cold criticals are within a narrow range of 0.001ΔK.

**Control rod calibration /31/**

The control rod calibration test was performed during the first phase of the heat-up.

Initial conditions were: recirculations pumps at minimum speed, temperature of the moderator at 40°C, all the control rods inserted.

Rods were withdrawn until criticality was reached; then the rod following in the sequence, was calibrated (see fig. 10).

By this experience three different comparisons with calculated results were performed:

a) Control rod worth

The calibration was performed at 40°C until the 32nd notch was withdrawn, from there on the temperature was allowed to raise at 45.7°C. This was necessary to avoid a short period with the complete withdrawal of the rod being calibrated.

The measured values at 36, 40 and 48 notches have been corrected to 40°C. The experimental and calculated results are compared in fig. 15.

b) Moderator temperature coefficient

During the control rod calibration the reactor period was taken with the same rod pattern at 40°C and 45.7°C; this resulted in a measure of the temperature coefficient of 11.3 \( \times 10^{-5} \pm 0.4 \times 10^{-5} \) ΔK/K°C in agreement with the calculated value /31/ within a few percents.
c) Critical eigenvalues

The approach to criticality was made at two different temperatures, 27°C and 40°C. The values of the bias at 20°C and 40°C were very close each other and lower than 0.3%ΔK.

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**GARIGLIANO NUCLEAR POWER STATION**

\[ \Delta = \frac{T - E}{E} \]

<table>
<thead>
<tr>
<th>Exp. data</th>
<th>( \Delta % ) Bacone &quot;medie&quot;</th>
<th>( \Delta % ) Bacone &quot;no medie&quot;</th>
</tr>
</thead>
</table>

- Notches out

**FIG. 1 - BOC 1 A - POWER DISTRIBUTION AND PERCENT DIFFERENCE BETWEEN BACONE RESULTS AND EXPERIMENTAL DATA**

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**GARIGLIANO NUCLEAR POWER STATION**

<table>
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\[ \Delta = \frac{T - E}{E} \]

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**FIG. 2 - EOC 1A - POWER DISTRIBUTION AND PERCENT DIFFERENCE BETWEEN BACONE RESULTS AND EXPERIMENTAL DATA**
GARIGLIANO NUCLEAR POWER STATION

FIG. 3 - EOC 2

POWER DISTRIBUTION AND PERCENT DIFFERENCE BETWEEN BACONE RESULTS AND EXPERIMENTAL DATA
### FIG. 4 - EOC 5

POWER DISTRIBUTION AND PERCENT DIFFERENCE BETWEEN BACONE RESULTS AND EXPERIMENTAL DATA

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**Exp. data**

**Bacone "no medie"**

**Δ%**

**σ**

Bacone "no medie" **6.8%**

**Δ·T·E**

**E**
FIG. 5 -- Comparison of γ scanning data with data calculated with BACONE code
FIG. 6 -- Comparison of γ scanning data with data calculated with BACONE code
FIG. 7 -- Comparison of TIP readings with data calculated with BACONE code
FIG. 8 -- Comparison of TIP readings with data calculated with BACONE code
Fig. 10 - Core Map
Fig. 1.1 - Experimental activity distributions
CAORSO COLD CONDITION

PERIPHERAL ZONE

○ AU
△ CU
+ NI

TIP POSITION (12, 05)

TIP POSITION (12, 37)

DISTANCE (CM)

Fig. 12 - Experimental activity distributions
Figure 13 Comparison of Measured to Predicted Fast Flux Distribution - Central Zone
Figure 14  Comparison of Measured to Predicted Fast Flux Distribution - Peripheral Zone
Fig. 15: Comparison Between the Calculated and Experimental Control Rod Worth
POLESTAR-2F/3F CODE FOR
POWER MAPPING AND REFUELING ANALYSES
OF HWR-FUGEN

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A computer program POLESTAR-2F/3F has been developed to carry out power mapping and refuelling analyses of the 165 MWe HWR-Fugen; a pressure tube type, heavy water moderated, boiling light water cooled, and Pu + MOX fuelled reactor. The program has both 2 and 3 dimensional versions, with their unique characters in effective use of data library system, short computation time, and also in easy I/O controls to specify the complication of core layout loaded with various fuels in free loading patterns. The numerical experiments have shown a satisfactory result compared with the operating data of the HWR-Fugen, and also with the other computer code simulations.

I. Introduction

A computer program POLESTAR-2F/3F is a 2 and 3-dimensional power mapping and refuelling analysis code for pressure tube type heavy water reactors, and is specially developed for the HWR-Fugen/1/ which uses plutonium MOX fuel as well as enriched UO₂ fuel. From the fuel cycle strategy of the HWR-Fugen, it is expected to use various fuels in mixed bed loading and also with free loading patterns. The POLESTAR code therefore puts an emphasis on easy I/O controls to specify such reactor conditions. Although the program is developed primarily for the HWR-Fugen, it would commonly be used for any pressure tube type reactors.

The main part of the POLESTAR code calculates a gross power distribution by a coarse mesh one-group diffusion approximation, and proceeds to the core burnup calculation based on this spatial distribution. For each burnup, refuelling, and other control step, the program automatically refreshes the core cross section sets by transferring the library data as to match with the changing reactor conditions.

Detailed burnup data of fuel bundles are separately calculated by any of the established multigroup cell burnup codes, and compiled as two group constants. These data are stored in the data library of the POLESTAR code, by putting ID No. to each fuel type, and are converted to one group constants when used in the main program of the POLESTAR.

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Fuel design of prototype Fugen-HWR

Fuel
Fuel materials: Pu-NU, MOX, Enriched UO₂
Enrichment, MOX(%) PUF: 0.55/0.55/0.8
UO₂(%) U-235: 1.5/1.5/1.5
Pellet diameter(mm): 14.4
Density(g/cm³): 10.4

Bundles:
Fuel pins: material: Zircaloy-2
od(mm): 16.42
thickness(mm): 0.86
Number of pins per bundle: 28
Effective length of bundle (mm): 3,700
Min. spacing between pins (mm): 2.1

Pressure tube:
material: HT Zr-2.5% Nb
i.d.(mm): 117.8
thickness(mm): 4.3

Calandria tube:
material: Zircaloy-2
i.d.(mm): 156.4
thickness(mm): 1.9

Fig. 1 Cross Sectional View of the Prototype Fugen Fuel Assembly
Any fuels, if once stored in this library system, can be considered for loading to the reactor and analysed by the POLESTAR code. Some of the fuels already stored in this library system are: E, UO₂, Pu-NU MOX, Pu-DU MOX, LWR-HWR tandem MOX, Th₀₂, Pu-Th MOX, Pu-NU-Th MOX, etc., each having ring array bundle structures.

The core layout in the POLESTAR code is described by a free format method, i.e., all fuel locations and fuel types loaded therein are specified by individual ID numbers. Hence, the input control of refuelling, for example, can be simply specified by indicating ID Nos. of refuelling channels and reload fuels.

The POLESTAR-2F/3F code edits fuel burnup, Kₘ, neutron flux, channel power, radial power peaking, MLHR, LPF., etc., for each individual channel in the reactor, and at each burnup or control step. The 3-dimensional version also edits axial informations, concerning to those items.

The program also edits the average values of these informations for any arbitrary spatial regions, including such cases which consist of the scattered fuel channels. This is a unique aspect of the program, and is quite effective in carrying out core management of the reactor which is loaded with varieties of fuels in scattered distributions.

The intention of this paper is to describe a general outline of the POLESTAR code, together with some example calculations using UO₂ and MOX fuels. The start-up physics measurements of the 165 MWe Fugen reactor have also been studied in those calculations.

II. Data Library System

In the POLESTAR-2F/3F program, the detailed burnup data of fuel bundle cell shall be stored in the data library. These data are separately prepared by using any of the detailed multigroup cell burnup codes such as METHUSELAH-II/2/, WIMS-D/3/, CLUSTER/4/, etc. Presently, METHUSELAH-II code is joint to this POLESTAR library system, i.e., a supplementary program automatically produces the POLESTAR library data using an output tape of the METHUSELAH-II.

Those library data are prepared for each fuel type, and called to the POLESTAR program to carry out core burnup and refuelling calculations. The data compiled in this library system are:

(1) Name of fuel type and its ID No.

(2) Informations of the fuel bundle structure. (See Fig. 1.)

(3) Fuel weight in the bundle.

(4) Fuel cell nuclear data given for each successive burnup step (bundle average burnup, cell Kₘ, fast and thermal neutron fluxes, Fermi age and diffusion area, 2 group nuclear constants, local peaking factor, etc.)

(5) Fuel contents of the bundle at each burnup step (Pu and U contents with their isotopic classification, conversion ratio, etc.).

(6) Reactivity coefficients of the unit fuel cell for each burnup step (void coefficient, fuel temperature coefficient, moderator temperature coefficient, and power coefficient.).
Fig. 2 Flow Chart of POLESTAR-2F/3F Program
Those library data are prepared for arbitrary steps of burnup, at every 1,000 MWD/TF for example, and any intermediate burnup data between these steps are generated by linear interpolations. The two group nuclear constants compiled in this data library are converted to the one group when used in the POLESTAR calculations.

The reactivity coefficients are generally evaluated by off-line calculations using any of the detailed cell burnup codes, and shall be stored in the library. Sometimes, the calculated results of reactivity coefficients, especially the void coefficient, are not accurate enough to describe a real reactor performance. When those reactivity coefficients are already known, or at least partially known from the operational experiences, the experimentally corrected values of those coefficients shall be stored in the data library instead of the pure calculations.

These library data are closely linked to the main part of the POLESTAR program, and any changes of reactor conditions due to burnup, control, refuelling, etc., are described by transferring the necessary data from the library. The calculational flow chart of the POLESTAR program is first shown in Fig. 2, and the analytical model of the program will be explained in the following section.

III. Analytical Models

1. Diffusion Equations for Neutron Flux

The POLESTAR program employs a coarse mesh one group diffusion approximation to describe a global core flux distribution, but with some flux shape corrections against reflector and distributed void effects. Its basic machinery is expressed in difference equations in which each fuel location is represented by a single spatial mesh point of X-Y plane. Those difference equations are:

\[
\begin{align*}
2-\text{Dim}: \quad & \frac{1}{h^2_T} \left[ \phi_{i-1,j} + \phi_{i+1,j} + \phi_{i,j-1} + \phi_{i,j+1} - 4\phi_{i,j} \right] \\
& + \left\{ \frac{1}{M^2_{i,j}} \left( K_{i,j} - 1 \right) + \mu^2_T \right\} \phi_{i,j} = 0, \\
\end{align*}
\]

\[
\begin{align*}
3-\text{Dim}: \quad & \frac{1}{h^2_T} \left[ \phi_{i-1,j,k} + \phi_{i+1,j,k} + \phi_{i,j-1,k} + \phi_{i,j+1,k} - 4\phi_{i,j,k} \right] \\
& + \frac{1}{h^2_x} \left[ \phi_{i,j,k-1} + \phi_{i,j,k+1} - 2\phi_{i,j,k} \right] + \left\{ \frac{1}{M^2_{i,j,k}} \left( K_{i,j,k} - 1 \right) \right\} \phi_{i,j,k} = 0, \\
\end{align*}
\]

where \( \phi_{i,j} / \phi_{i,j,k} = 2/3 \) dimensional neutron fluxes in the spatial segments \((i,j)/(i,j,k)\),

\( h_T \) = calculational mesh spacing in X-Y plane,

\( h_x \) = calculational mesh spacing in Z-direction,

\( M^2_{i,j}/M^2_{i,j,k} = \) neutron migration areas in spatial segments \((i,j)/(i,j,k)\),

\( K_{i,j}/K_{i,j,k} = K_w \) value of fuel segment cells \((i,j)/(i,j,k)\),

\( K_{eff} \) = effective multiplication factor of the reactor (= eigenvalue of the original diffusion equation),

\( \mu^2_T \) = axial buckling (needed in the 2-dimensional case only).
It is noted that the difference equation in the X-Y plane is expressed by taking only 4 spatial points \((i-1,j),(i+1,j),(i,j-1),(i,j+1)\) immediately surrounding the segment \((i,j)\), and this character is fully utilized to specify the core layout and arbitrary refuelling patterns. To express the core layout, the ID No. of each individual fuel channel shall be listed together with those of and 4 spatial points in the following form, i.e.,

\[
\text{SEGMENT } I, K, I_1, I_2, I_3, I_4
\]

where
\[
I = \text{ID No. of the } i\text{-th fuel channel},
\]
\[
K = \text{ID No. of the fuel loaded in the } i\text{-th channel},
\]
\[
I_1 - I_4 = \text{ID Nos. of the surrounding fuel channels}
\]

This method greatly simplifies many complicated I/O controls of the core management, i.e., in refuelling, fuel shuffling, CR pattern alteration, and in other reactor control actions. The method herewith is called a free format system, and the ID No. assignment for the 165 MWe Fugen reactor is shown in Fig. 3 as an example.

To solve the original difference equations, the 3-dimensional Eq. (2) is taken up and explained. Rearranging Eq. (2) with respect to \(\phi_{i,j,k}\), one has,

\[
\phi_{i,j,k} = \frac{(\phi_{i-1,j,k} + \phi_{i+1,j,k} + \phi_{i,j-1,k} + \phi_{i,j+1,k}) h_t^2 + (\phi_{i,j,k-1} + \phi_{i,j,k+1}) h_t^2}{4 h_t^2 + 2 h_t^2 \left( \frac{K_{i,j,k}}{M_{i,j,k}} - 1 \right)}
\]

(3)

The initial values are first given to \(\phi\)'s and \(K_{\text{eff}}\) on the RHS of this equation, and the calculated \(\phi_{i,j,k}\) on the LHS replaces \(\phi\)'s on the RHS by an iterative method. At each iterative step, \(K_{\text{eff}}\) value is renewed by the following method.

Integration of Eq. (2) gives,

\[
\sum_{i,j,k} (\phi_{i-1,j,k} + \phi_{i+1,j,k} + \phi_{i,j-1,k} + \phi_{i,j+1,k} - 4 \phi_{i,j,k}) h_t^2
\]

\[
+ \sum_{i,j,k} (\phi_{i,j,k-1} + \phi_{i,j,k+1} - 2 \phi_{i,j,k}) h_t^2
\]

\[
= - \sum_{i,j,k} \frac{h_t^2}{M_{i,j,k}} \left( \frac{K_{i,j,k}}{K_{\text{eff}}} - 1 \right) \phi_{i,j,k}
\]

(4)

The 1st term of the LHS of Eq. (4) becomes

\[
\sum_{i,j,k} (\phi_{i-1,j,k} + \phi_{i+1,j,k} + \phi_{i,j-1,k} + \phi_{i,j+1,k} - 4 \phi_{i,j,k}) h_t^2
\]

\[
= - \sum_{i,j,k} n_{i,j,k} \left\{ \phi_{i,j,k} \in \text{Zero}(X,Y) \right\} h_t^2
\]

(5)

where \(\phi_{i,j,k} \in \text{Zero}(X,Y)\) = neutron flux \(\phi_{i,j,k}\) in the segment having zero flux boundaries on adjacent XY faces,

\[n_{i,j,k} = \text{number (either 1, 2, or 3) of zero flux boundary faces of the segment having flux } \phi_{i,j,k} \in \text{Zero}(X,Y)\].

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Similarly, the 2nd term of the LHS of Eq. (4) becomes

\[
\sum_{i,j,k} \left( \phi_{i,j,k-1} + \phi_{i,j,k+1} - 2\phi_{i,j,k} \right) h_{i,j}^2 = - \sum_{i,j,k} \left\{ \phi_{i,j,k} \in \text{Zero}(Z) \right\} h_{i,j}^2
\]  

(6)

where \( \phi_{i,j,k} \in \text{Zero}(Z) \) = neutron flux \( \phi_{i,j,k} \) in the segment having a zero flux boundary on an adjacent Z face.

The relations given by Eq. (5) and (6) are resulted from the cancellation of internal spatial fluxes in integrating process, and only expressed by the zero flux boundary conditions. Hence, Eq. (4) now takes the following form.

\[
h_{i,j}^2 \sum_{i,j,k} n_{i,j,k} \left\{ \phi_{i,j,k} \in \text{Zero}(X,Y) \right\} + h_{i,j}^2 \sum_{i,j,k} \left\{ \phi_{i,j,k} \in \text{Zero}(Z) \right\} \\
= h_{i,j}^2 h_{i,j}^2 \sum_{i,j,k} \frac{1}{M_{i,j,k}^2} \left( \frac{K_{i,j,k}}{K_{\text{eff}}} - 1 \right) \phi_{i,j,k} 
\]

(7)

Rearranging the above equation with respect to \( K_{\text{eff}} \), one has,

\[
K_{\text{eff}} = \frac{\sum_{i,j,k} \frac{K_{i,j,k}}{M_{i,j,k}^2} \phi_{i,j,k}}{\sum_{i,j,k} \frac{1}{h_{i,j}^2} n_{i,j,k} \left\{ \phi_{i,j,k} \in \text{Zero}(X,Y) \right\} + \sum_{i,j,k} \frac{1}{h_{i,j}^2} M_{i,j,k}^2 \phi_{i,j,k}} 
\]

(8)

The value of \( K_{\text{eff}} \) is calculated by this equation, and recycled to Eq. (3) together with \( \phi_{i,j,k} \) obtained from each iterative step.

To accelerate convergence in these iterative calculations, the following method is applied to \( \phi_{i,j,k} \) and \( K_{\text{eff}} \), i.e.,

\[
\phi_{i,j,k}^{(n)} = \alpha_{i,j,k}^{(n)} + \Gamma(\alpha_{i,j,k}^{(n)} - \phi_{i,j,k}^{(n-1)}) 
\]

(9)

\[
K_{\text{eff}}^{(n)} = \beta^{(n)} + \Gamma(\beta^{(n)} - K_{\text{eff}}^{(n-1)}) 
\]

(10)

where \( \phi_{i,j,k}^{(n)} \), \( \phi_{i,j,k}^{(n-1)} \) = evaluated values of \( \phi_{i,j,k} \) at \( n \)-th and \( (n-1) \)-th iterative steps,

\( K_{\text{eff}}^{(n)} \), \( K_{\text{eff}}^{(n-1)} \) = evaluated values of \( K_{\text{eff}} \) at \( n \)-th and \( (n-1) \)-th iterative steps,

\( \alpha_{i,j,k}^{(n)} \) = calculated values of \( \phi_{i,j,k}^{(n)} \) from Eq. (3), but prior to applying the present acceleration method,

\( \beta^{(n)} \) = calculated value of \( K_{\text{eff}}^{(n)} \) from Eq. (8), but prior to applying the present acceleration method,

\( \Gamma \) = acceleration constant ( = 0.6 ).

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Fig. 3 Spatial Node ID No. of POLESTAR - 2F/3F

Fig. 4 Convergence Profile of Iterative Calculations
An acceleration constant, $\Gamma = 0.6$, is employed as a most appropriate value in the present program. This was examined by numerical experiments for the HWR-Fugen core, and the convergence profile obtained therewith is shown in Fig. 4.

As for the convergence criteria, the following restrictions are given, i.e.,

$$\left| \frac{K^n_{\text{eff}} - K^{(n-1)}_{\text{eff}}}{K^n_{\text{eff}}} \right| \leq \varepsilon_1, \quad \varepsilon_1 = 0.00001, \tag{11}$$

$$\left| \frac{\phi_{i,j,k}^{(n)} - \phi_{i,j,k}^{(n-1)}}{\phi_{i,j,k}^{(n)}} \right| \leq \varepsilon_2, \quad \varepsilon_2 = 0.001, \tag{12}$$

where the spatial nodes $(i, j, k)$ of fuelled region are only considered. The iterations come to the end when these criteria are both satisfied.

2. Flux Shape Corrections

(1) Reflector Effect to Flux Shape

Since the original diffusion equations of the POLESTAR-2P/3F are given in a coarse mesh one-group model, they do not describe the precise shape of thermal neutron flux close to the reflector boundaries. To avoid such problems, various authors used the fitting of albedos at the core boundary by using an iterative method. The typical examples are found in FLARE/5/ and LAYMON/6/ codes, but its fitting process is thought to be tedious although the method works well. The 2 group model can avoid this difficulty as in the case of the ZADOC code/7/, but it is practically limited to the 2-dimensional analysis to save computer time. Recently, B. Lin, et al/8/ proposed the 1 1/2 group model which simulates 2-group diffusion theory but neglecting the leakage term in the thermal group equation.

In the present case dealing with HWR, it is pointed out that the reflector effect is not so strong as that of LWR, and therefore the authors proposed to correct the peripheral flux shape by simply multiplying edge factors to the flux $\phi_{i,j,k}$ given by the one group diffusion equation. The authors studied the reflector effects by the 2-group diffusion simulations using the CITATION code/9/, and the edge factors were evaluated for various core conditions. These edge factors are them stored in the data library, and the corrected flux is given by

$$\phi_{i,j,k} = (1 + C_{i,j,k}) \phi_{i,j,k} \tag{13}$$

where the equality sign is for the FORTRAN statement, and the edge factor $C_{i,j,k}$ takes the non-zero values only in the peripheral region of the 2-lattice spacing from the reflector boundary. It is noted that no correction is made to the $K_{\text{eff}}$ value (eigenvalue) after this flux shape correction, because the $K_{\text{eff}}$ is determined by the total flux including fast and thermal groups. With the employment of this edge factor method, the POLESTAR program virtually works the same way as a program using the 2-group model, and saves a big amount of computer time.

(2) Void Effect to Flux Shape

In the previous codes such as FLARE/5/ and LAYMON/6/, the void distributions are first generated from the calculated power distributions, where the obtained void distributions are then used to re-calculate the flux and power distributions. This requires an iterative process until the flux calculation converges, and also requires some more computer time.
The original 3-dimensional diffusion equation, Eq. (2), uses the nuclear constants based on the average void condition of the reactor, and this is quite effective to save computer time. However, the vertical flux shape is somewhat influenced by the void distributions. It is noted that the HWR-Fugen's void reactivity coefficient is much smaller than BWR's; and in fact, the zero void coefficient is the design target set for this reactor. Thus, the distributed void effect to the axial flux of the HWR-Fugen would not be very strong as the BWR case. This comes from the fact that the void is generated only in the H2O coolant space in the fuel bundles, while the big D2O moderator space stays unchanged where neutrons are mostly thermalized.

With this background, the distributed void effect on the axial flux has been studied by numerical experiments. It is now understood that the distributed void has a small effect of spatial flux shift over the axial direction, but it can best be corrected by a simple linear function as shown below.

\[
\phi_{i,j,k} = 1 + \alpha_v (8.5 - Z_k) \phi_{i,j,k},
\]

where the equality sign is again for the FORTRAN statement, and

\[\phi_{i,j,k} = \text{neutron flux calculated in average void condition},\]

\[\alpha_v = \text{constant of axial flux shape correction},\]

\[Z_k = \text{axial space node (center = 8.5)}.\]

The constant \(\alpha_v\) depends on the void reactivity coefficient, and it takes positive, zero, or negative value corresponding to the value of void reactivity coefficient. For the Fugen initial core, \(\alpha_v = 0.03\), for example.

3. Control Rod Calculations

The annular control rods employed in the HWR-Fugen can be most effectively calculated by the absorption area method\(^{10}\), and this analytical technique was fully utilized in the control rod design calculations of the 165 MWe prototype reactor. The method was originally described by a 3-group diffusion model, but the result is applied to the POLESTAR's one group calculations with some adjustments.

To evaluate the CR effect, the "controlled super-cell" is first considered, which consists of 4 fuel channels in 2 x 2 matrix with an annular CR at its center. The absorption area is related to the total number of neutrons lost to the CR, and it is expressed in terms of the equivalent area of slowing down source neutrons. For the 1\textsuperscript{st}-group neutrons, it is given by

\[
A_i = \frac{4\text{th-group neutron absorption in the CR}}{\text{slowing down density into the 1\textsuperscript{st} group}} = -2\pi r_s J_1(r_o) \sum_{s=1}^{5} \phi_{s-1},
\]

where \(r_o\) is the radius of the CR and \(-J_1(r_o)\) is the neutron current into the CR surface. To evaluate the \(A_i\)'s, it is assumed that

1) The fast neutrons are not absorbed by the CR and the slowing down source distribution to the epithermal group is flat.

2) The flux in the super-cell calculation is a function of the radial distance \((r)\) only.

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Then, epithermal and thermal fluxes in the controlled super-cell obey

\[ \nabla^2 \phi_2 - \left( \frac{1}{L_1} \right) \phi_2 + \frac{Q}{D_2} = 0 \]  
\[ \nabla^2 \phi_3 - \left( \frac{1}{L_1} \right) \phi_3 + \left( \Sigma_{sd_1}/D_3 \right) \phi_3 = 0 \]  
\[ (16) \]  
\[ (17) \]

where \( L_2 \) and \( L_3 \) are the diffusion lengths for epithermal and thermal neutrons, \( D_2 \) and \( D_3 \) are the diffusion constants, \( \Sigma_{sd_1} \) is the slowing down cross section from epithermal group, and \( Q \) is the fast-neutron slowing down source. The boundary conditions applied for these equations are

1) the logarithmic-derivative boundary condition at the CR surface

2) the flat boundary condition at the outer boundary of the super cell.

The second condition expresses the shadowing effect of the adjacent CRS spaced uniformly.

The epithermal and thermal flux distributions obtained as solutions of Eqs. (16) and (17) yield the absorption areas for each group of neutrons by using the definition, i.e., Eq. (15):

\[ A_1 = 2 \pi r_o L_1 \left[ \alpha(2) + d_1/L_2 \right]^{-1} \]  
\[ A_2 = \frac{2 \pi r_o L_2}{\epsilon} \left\{ \frac{L_2}{L_3} \left( 1 - \frac{L_1}{L_2} \right) \right\}^{-1} \left[ \alpha(2) + d_1/L_2 \right]^{-1} + \zeta \left[ \alpha(3) + d_3/L_3 \right]^{-1} \]  
\[ (18) \]  
\[ (19) \]

where \( \epsilon = 1 - \alpha(2) \left[ \alpha(2) + d_1/L_2 \right]^{-1} \)

\[ \zeta = 1 - \left( 1 - \frac{L_1}{L_2} \right) \left[ \alpha(2) + d_3/L_3 \right] \left( \alpha(2) + d_1/L_2 \right)^{-1} \]  
\[ (20) \]  
\[ (21) \]

\[ \alpha(i) = \frac{I_i \left( R_o/L_1 \right) K_i \left( r_o/L_i \right) + K_i \left( R_o/L_i \right) I_i \left( r_o/L_i \right)}{I_i \left( R_o/L_1 \right) K_i \left( r_o/L_i \right) - K_i \left( R_o/L_i \right) I_i \left( r_o/L_i \right)} \]  
\[ (22) \]

\[ \alpha(2) = \frac{I_1 \left( R_o/L_2 \right) K_1 \left( r_o/L_2 \right) + K_1 \left( R_o/L_2 \right) I_1 \left( r_o/L_2 \right)}{I_1 \left( R_o/L_2 \right) K_1 \left( r_o/L_2 \right) - K_1 \left( R_o/L_2 \right) I_1 \left( r_o/L_2 \right)} \]  
\[ (23) \]

where \( I_0 \), \( I_1 \), \( K_0 \), and \( K_1 \) are the Bessel functions, \( R_o \) is the effective radius of the super cell, \( d_1 \) and \( d_3 \) are the linear extrapolation distances for the epithermal and thermal neutron fluxes on the CR absorber surface.

The three-group diffusion equations in the reactor can be described in the forms

\[ -D_1 \nabla^2 \phi_1 + \Sigma_{d_1} \phi_1 + \Sigma_{s_1} \phi_1 = \nu \Sigma_{f_1} \phi_1 + \nu \Sigma_{f_2} \phi_2 + \nu \Sigma_{f_3} \phi_3 \]  
\[ -D_2 \nabla^2 \phi_2 + \Sigma_{s_2} \phi_2 + \Sigma_{d_2} \phi_2 = F_1 \Sigma_{sd_1} \phi_1 \]  
\[ -D_3 \nabla^2 \phi_3 + \Sigma_{s_3} \phi_3 = F_2 \Sigma_{sd_2} \phi_2 \]  
\[ (24) \]  
\[ (25) \]  
\[ (26) \]

where \( F_1 = (A_c - A_1)/A_c \)

\[ A_c = \text{area of the controlled super cell.} \]  
\[ (27) \]

- 329 -
The last equation expresses the reduction rate of the slowing down source neutron to the i'th energy group due to the CR in the controlled super cell. If the flux distribution is represented using the super-cell buckling, i.e., \( \gamma^2 \Phi_i = B_i^2 \Phi_i \), the reduced fission source in the following form also gives the correct multiplication factor, instead of adjusting slowing down source neutrons, i.e.,

\[
\nu \Sigma f_z \rightarrow F_2 \nu \Sigma f_z, \quad \nu \Sigma f_z \rightarrow F_3 \nu \Sigma f_z
\]

(28)

In short, the reduced fission source, defined in the above relation (28), is applied to the controlled super-cell region when carrying out the whole core diffusion calculations. The calculational accuracy of this technique has been already studied by the DCA critical experiments/10/ and also by the operational experience of the Fugen reactor itself, where the results were judged quite satisfactory.

As mentioned previously, the POLESTAR data library stores the 2 group nuclear constants, and the reduced fission source is applied only to the thermal constant of the controlled super-cell region, i.e.,

\[
\nu \Sigma f^{\text{thermal}} \rightarrow F_2 F_3 \nu \Sigma f^{\text{thermal}}
\]

(29)

The values of \( F_2 \) and \( F_3 \) are taken from the Fugen CR design calculations, and they are in the range; \( F_2 = 0.95 \pm 0.06 \), and \( F_3 = 0.85 \pm 0.08 \).

In the POLESTAR-2P calculations, an additional factor \( S(Z_k) \) is multiplied to the reduced fission source, i.e.,

\[
\nu \Sigma f^{\text{thermal}} \rightarrow \left(1 - (1 - F_2 F_3) S(Z_k)\right) \nu \Sigma f^{\text{thermal}}
\]

(30)

where \( S(Z_k) \) is a constant and varies in the range \( 0 \leq 1.0 \) following \( S \)-curve of the CR insertion.

4. Burnup and Refuelling

1. Burnup calculation

Once the neutron flux is evaluated with some necessary shape corrections as mentioned, the POLESTAR program then proceeds to the calculation of power and burnup distributions. The power distribution \( P_{i,j,k} \) (or \( P_{i,j} \) in the POLESTAR-2P) is directly obtained from the flux \( \Phi_{i,j,k} \) (or \( \Phi_{i,j} \)), by multiplying with the fission cross section \( \Sigma_f(B_{i,j,k}) \) given at each burnup condition. The \( \Sigma_f(E)_s \) are all stored in the data library for each fuel type and taken into this calculation by data transfer.

By using the \( P_{i,j,k} \) obtained in the previous step, the fuel burnup calculation then follows for any period of time specified by the input control. Generally, the burnup time step of 5 \( \leq \) 30 days is chosen depending on the purpose of calculations. At the end of each burnup step, the nuclear constants are all replaced to match with the new burnup conditions, and the \( K_{\text{eff}}, \Phi_{i,j,k} \) and \( P_{i,j,k} \) are recalculated. If the \( K_{\text{eff}} \) becomes smaller than some specified value (e.g. \( K_{\text{eff}} \leq 1.005 \)), the reactivity control takes place by replacing the necessary nuclear constants (withdrawal of CRs, or withdrawal of liquid poison from D0 moderator), and all the calculations are repeated from the beginning. The burnup calculations come to the end when no more control reactivity is available for further burnup, otherwise the reactor is to be refuelled.

- 330 -
(2) Refuelling calculation

The refuelling sequence and its pattern are specified by the input control, and any fuels in the POLESTAR data library can be loaded at any desired locations of the reactor. Shuffling calculation of incore fuels is also possible, and it is very easily done.

Generally, the basic principle for selecting the refuelling or shuffling pattern is that the power peaking must become smaller than some specified limit, wherein the larger discharge burnup is sought for. The data of the discharged fuels such as burnups, Pu contents, U contents, etc., are all recorded for each individual bundle.

5. Output Edit

An example of the POLESTAR-3F output edits is partly shown in Table I, which has been calculated for the 165 MWe prototype HWR-Fugen reactor. This shows one aspect of the burnup step, and the unique feature of this output format is that it lists the important parameters of the every incore fuel, compacted in a single page. The output edits on some of the important parameters are briefly summarized in the following.

(1) Neutron Multiplication Factor

1) Core $K$-effective

\[ K_{eff} = \text{obtained by Eq. (8).} \]

2) Fuel channel $K$-infinity, $K_{\infty} (i,j)$.

\[ K_{\infty}(i,j) = \sum_{k \in F} \phi_{i,j,k} \cdot K_{\infty}(i,j,k) / \sum_{k \in F} \phi_{i,j,k} \]  \hspace{1cm} (31)

where \( K_{\infty}(i,j,k) \) = $K$-infinity at each spatial node \((i,j,k)\), \( \phi_{i,j,k} \) = normalized flux at each spatial node \((i,j,k)\), \( \sum_{k \in F} \) = axial integral in the fuelled region.

(2) Neutron Flux

1) Normalized flux distribution, \( \phi_{i,j,k} \cdot \)

\[ \phi_{i,j,k} = N_{i,j,k} \cdot \phi_{i,j,k} / \sum_{i,j,k \in F} \phi_{i,j,k} \]  \hspace{1cm} (32)

where \( N_{i,j,k} \) = total number of spatial nodes in the fuelled region, \( \phi_{i,j,k} \) = neutron flux after flux shape correction, \( \sum_{i,j,k \in F} \) = 3-dim. integral in the fuelled region.

ii) Normalized channel flux, \( \phi_{i,j} \cdot \)

\[ \phi_{i,j} = \sum_{k \in F} \phi_{i,j,k} / N_k \]  \hspace{1cm} (33)

where \( N_k \) = number of axial nodes in the fuelled region.
(3) Thermal Power

1) Normalized power distribution, $P_{i,j,k}$

$$P_{i,j,k} = N_{ijk} \cdot \frac{\sum_{i,j,k} \phi_{i,j,k}}{\sum_{i,j,k \in F} \phi_{i,j,k}}$$

(34)

where $\sum_{i,j,k} \phi_{i,j,k}$ = fission cross section at each spatial node $(i,j,k)$.

ii) Channel power peaking, $P_{i,j}$

$$P_{i,j} = \sum_{k \in F} P_{i,j,k} / N_k$$

(35)

iii) Channel power (MW), $CHP(i,j)$.

$$CHP(i,j) = P_e \cdot P_{e,j} / N_{ij}$$

(36)

where $N_{ij}$ = number of fuel channels,

$P_e$ = core thermal power (MW).

iv) Channel power to coolant (MW), $CHP^*(i,j)$.

$$CHP^*(i,j) = f_{eff} \cdot CHP(i,j)$$

(37)

where $f_{eff}$ = fraction of channel power to coolant, and it is specified by the input.

v) Axial power peaking, $P_x(i,j)$.

$$P_x(i,j) = \text{MAX}_k \{P_{i,j,k}\} / P_{i,j}$$

(38)

(4) Linear Heat Rate

1) Maximum linear heat rate in bundle (KW/cm), $MLHR(i,j)$.

$$MLHR(i,j) = \frac{1000}{h_s} \cdot f_{eff} \cdot P_e \cdot \text{MAX}_k \left\{ \frac{P_{i,j,k}}{N_{ijk}} \cdot \frac{L_p(i,j,k;E)}{N_{rod}(i,j)} \right\}$$

(39)

where $L_p(i,j,k;E)$ = local power peaking at each spatial node $(i,j,k)$ and exposure $E$, and taken from the POLESTAR data library,

$N_{rod}(i,j)$ = number of fuel pins of the bundle $(i,j)$.

ii) Maximum linear heat rate in core (KW/cm), $MLHR$.

$$MLHR = \text{MAX}_{i,j} \{ MLHR(i,j) \}$$

(40)

(5) Fuel Burnup

1) 3-dim. burnup distribution (MWD/TF), $E(i,j,k;t)$.

$$E(i,j,k;t) = E(i,j,k;\Delta t) + \Delta t \cdot \frac{P_e \cdot P_{i,j,k}}{N_{ijk}} / W(i,j)$$

(41)

where $\Delta t$ = burnup step time span (days),

$W(i,j)$ = weight of oxide fuel in channel (tons).
### Table II  Benchmark Problems on Fugen Start-up Tests

<table>
<thead>
<tr>
<th>Code</th>
<th>25%</th>
<th>50%</th>
<th>75%</th>
<th>100%</th>
<th>CPU Time (sec.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>POLESTAR-2F</td>
<td>1.00477</td>
<td>1.01008</td>
<td>1.00867</td>
<td>1.00847</td>
<td>3.7</td>
</tr>
<tr>
<td>POLESTAR-3F</td>
<td>1.00098</td>
<td>1.00450</td>
<td>1.00271</td>
<td>1.00209</td>
<td>45.9</td>
</tr>
<tr>
<td>LATMON</td>
<td>1.00644</td>
<td>1.00640</td>
<td>1.00343</td>
<td>1.00288</td>
<td>54.0</td>
</tr>
<tr>
<td>ZADOC</td>
<td>1.01214</td>
<td>1.01595</td>
<td>1.01489</td>
<td>1.01531</td>
<td>33.8</td>
</tr>
</tbody>
</table>

Core condition (Experiment, $K_{eff} = 1$)

<table>
<thead>
<tr>
<th>Core BU (GW/TH)</th>
<th>$1^8B$(ppm)</th>
<th>CR (Full in: 16.0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25%</td>
<td>97.4</td>
<td>6.43</td>
</tr>
<tr>
<td>50%</td>
<td>258.3</td>
<td>6.42</td>
</tr>
<tr>
<td>75%</td>
<td>445.0</td>
<td>5.92</td>
</tr>
<tr>
<td>100%</td>
<td>703.0</td>
<td>5.24</td>
</tr>
</tbody>
</table>

### Table III  Core Informations of Initial Cycle (Cycle No.0, POLESTAR-2F)

<table>
<thead>
<tr>
<th>Cycle No.</th>
<th>Days at EOC</th>
<th>Average core burnup (GW/TH)</th>
<th>Ch. power peaking Value</th>
<th>Max. L.H.R (Kw/cm)</th>
<th>Keff</th>
<th>$1^8B$ (ppm)</th>
<th>Axial peaking factor</th>
<th>Control rod pattern (Full in: 16.0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-1</td>
<td>BOC EOC 40</td>
<td>0.0 6.52</td>
<td>1.353 1.308 13</td>
<td>0.466 0.450</td>
<td>1.0148 1.0029</td>
<td>6 1.306</td>
<td>L:11.0, K:12.0</td>
<td></td>
</tr>
<tr>
<td>0-2</td>
<td>BOC EOC 80</td>
<td>0.652 1.304</td>
<td>1.293 1.253 13</td>
<td>0.445 0.430</td>
<td>1.0143 1.0026</td>
<td>5 1.306</td>
<td>L:11.0, K:12.0</td>
<td></td>
</tr>
<tr>
<td>0-3</td>
<td>BOC EOC 120</td>
<td>1.306 1.956</td>
<td>1.235 1.210 15</td>
<td>0.428 0.427</td>
<td>1.0145 1.0030</td>
<td>4 1.306</td>
<td>L:11.0, K:12.0</td>
<td></td>
</tr>
<tr>
<td>0-4</td>
<td>BOC EOC 160</td>
<td>1.956 2.608</td>
<td>1.164 1.154 27</td>
<td>0.458 0.452</td>
<td>1.0166 1.0042</td>
<td>3 1.427</td>
<td>M:2.0, E:4.5, K:13.0, J:6.0</td>
<td></td>
</tr>
<tr>
<td>0-5</td>
<td>BOC EOC 210</td>
<td>2.608 3.423</td>
<td>1.153 1.151 34</td>
<td>0.452 0.449</td>
<td>1.0174 1.0038</td>
<td>2 1.427</td>
<td>M:2.0, E:4.5, K:13.0, J:6.0</td>
<td></td>
</tr>
<tr>
<td>0-6</td>
<td>BOC EOC 250</td>
<td>3.423 4.076</td>
<td>1.159 1.131 9</td>
<td>0.401 0.399</td>
<td>1.0147 1.0033</td>
<td>2 1.319</td>
<td>L:6.0, E:4.5</td>
<td></td>
</tr>
<tr>
<td>0-7</td>
<td>BOC EOC 290</td>
<td>4.076 4.728</td>
<td>1.109 1.118 27</td>
<td>0.398 0.399</td>
<td>1.0172 1.0042</td>
<td>1 1.319</td>
<td>L:6.0, E:4.5</td>
<td></td>
</tr>
<tr>
<td>0-8</td>
<td>BOC EOC 340</td>
<td>4.728 5.543</td>
<td>1.115 1.110 27</td>
<td>0.394 0.394</td>
<td>1.0184 1.0046</td>
<td>0 1.319</td>
<td>L:6.0, E:4.5</td>
<td></td>
</tr>
<tr>
<td>0-9</td>
<td>BOC EOC 350</td>
<td>5.543 5.706</td>
<td>1.165 1.159 3</td>
<td>0.418 0.416</td>
<td>1.0075 1.0047</td>
<td>0 1.392</td>
<td>M:2.0, E:4.5, K:13.0</td>
<td></td>
</tr>
<tr>
<td>0-10</td>
<td>BOC EOC 360</td>
<td>5.706 5.869</td>
<td>1.133 1.148 3</td>
<td>0.389 0.425</td>
<td>1.0036 1.0037</td>
<td>0 1.436</td>
<td>M:2.0, E:3.0</td>
<td></td>
</tr>
</tbody>
</table>

Initial core: 0.66% Pu NOX(96) + 1.5% UO2(124) + Sp.Fuel(4)
ii) Channel burnup, \( E(i,j,t) \), \( E^*(i,j,t) \)

\[
E(i,j,t) = \sum_{k \neq F} E(i,j,k;t) / N_k \quad \text{(MWD/TF)}
\]

\[
E^*(i,j,t) = C_f E(i,j,t) \quad \text{(MWD/TM)}
\]

where \( C_f = W_{\text{fuel}} / W_{\text{metal}} = 1.134 \) \hspace{1cm} (44)

iii) Average burnup of in-core fuels, \( E_c(t) \), \( E_c^*(t) \).

\[
E_c(t) = \sum_{i,j} E(i,j,t) \cdot w(i,j) / \sum_{i,j} w(i,j) \quad \text{(MWD/TF)}
\]

\[
E_c^*(t) = C_f E_c(t) \quad \text{(MWD/TM)}
\]

IV. Numerical Experiments

To study the reliability and validity of the POLESTAR calculations, several numerical experiments have been carried out and compared either with the Fugen operating data or with the other simulator calculations. Some representing results are shown in this section.

1. Benchmark Problem on Fugen Start-up Test

(1) \( K_{eff} \) and CPU time

The start-up test of the 165 MW\(e \) Fugen reactor were taken up as a benchmark problem; and the POLESTAR calculations, together with the other simulations (by ZADOC and LAYMON), have been compared with the Fugen operating data at 25, 50, 75 and 100% of its rated power. Shown in Table II are the benchmark tests on \( K_{eff} \) and CPU time requirements, where \( K_{eff} = 1 \) is considered to be the experimental value. All results seem satisfactory within the limit of calculational error, but the POLESTAR has the advantage in CPU time resulted from the simplified method presented in this work.

(2) Channel power distributions

The benchmark test on power distributions is next shown in Figs. 5 ~ 6 for the case when the Fugen first achieved 100% of its rated power, and again, the result seems reasonable for all simulations. In this benchmark test, the POLESTAR gave a little smaller peaking compared with the other simulations, but it will be improved very easily by adjusting the control rod constants. The distributions given from the on-line process computer are here considered as the experiments, but they are actually the results of power mapping by the LAYMON code with some fitting adjustments to the in-core monitor readings at distributed space points.

2. Burnup Profile of Initial Core

(1) Core burnup

Numerical examination of the initial core burnup is of special interest because its calculational accuracy determines the reliability of the POLESTAR code for the long range burnup and refuelling program. In this respect, the initial core burnup have been numerically studied by the 2D and 3D versions of the POLESTAR, and they both gave approximately the same core burnup. The results are summarized in Table III, wherein the 2-D calculations are only listed because
Fig. 5 Radial Power Distribution in HWR-Fugen (at 100% Power level)

Fig. 6 Radial Power Distribution in HWR-Fugen (at 100% Power level)
they are continued to the forthcoming refuelling analyses in the present example. However, the axial peaking factors given herewith are taken from the 3-D calculation.

The core average burnup expected at the end of this initial load cycle will be 5,870 MWD/THM by the POLESTAR code prediction. On the other hand, the 165 MWe Fugen reactor has achieved the core average BU of about 4,000 MWD/THM by the end of Sept. 1979; and by extrapolating this result to the zero control reactivity, the POLESTAR prediction (5,870 MWD/THM) is now certified with an accuracy of ±100 MWD/THM.

(2) Profile of 3-D power distributions

The transition of 3-dimensional power distributions with core burnup is here illustrated by quoting the POLESTAR calculations for the initial burnup cycle. The radial (channel) power distributions are shown in Figs. 7~8, where it is shown that power flattening is pretty well achieved by selecting an appropriate CR pattern for each step. The CRs are almost withdrawn at the end of the cycle (step 4 ~ 5), but the flattening is still held due to the core burnup. The behavior of axial power distributions are then shown in Fig. 9 taking a fuel No. 23 as an example, where the dotted line indicates the distribution immediately after the channel being refuelled. The power peaking first appears in the lower half of the core due to the CR insertion, and it gradually moves to the upper half as the CRs are withdrawn with burnup.

3. Example of Refuelling Calculations

(1) Refuelling pattern and its sequence

Any refuelling patterns can be selected for the POLESTAR calculations. Here, the so-called 6 ↔ 9 batch transition refuelling sequence shown in Figs. 10 ~ 11 is taken up, and refuelling calculations have been made as shown below.

Initial core:

<table>
<thead>
<tr>
<th>Fuel Type</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>NU + 0.66% PuF MOX</td>
<td>(96 Ass.)</td>
</tr>
<tr>
<td>1.5% E.UO₂</td>
<td>(124 Ass.)</td>
</tr>
<tr>
<td>2.5/1.5% E.UO₂</td>
<td>(4 Ass.)</td>
</tr>
</tbody>
</table>

1 ↔ 6 cycle reload: NU + 0.66% PuF MOX (6 batch refuelling)

7 ↔ 15 cycle reload: NU + 1.1% PuF MOX (9 batch refuelling)

The POLESTAR-2F code was used in this trial calculation just for saving the CPU time, but the case can also be treated very easily by the 3F code if desired. The results are summarized in Tables IV ~ V, and transition of discharge fuel exposure is graphically shown in Fig. 12.

The dotted line in Fig. 12 shows the case when the LWR-HWR tandem MOX is chosen as reload fuel instead of the regular NU + 0.66% PuF MOX. The information for such a refuelling case are shown in Table VI. The used LWR fuels generally contain about half as much fissile part as the fresh ones, including plutonium and 235U tail. This fissile content is quite close to the initial fuel of the prototype Fugen reactor, and the studies showed that use of such tandem MOX fuels (reprocessed and fabricated without separating Pu) is quite feasible on the basis that their fissile contents are known prior to loading to the reactor. The behavior of radial channel power peaking through these refuelling cycles is also shown in Fig. 13, where its maximum can be sustained below 1.5 which is a value to keep ML/NR well below the operational limit of 17.5 KW/ft.
Fig. 7 Transition of Channel Power Distribution (initial cycle)

Fig. 8 Transition of Channel Power Distribution (initial cycle)
V. Discussions and Conclusions

The outline of the power mapping and refuelling program POLESTAR-2F/3F has been described. Some numerical experiments have also been made and compared with the Fugen operating data or with the other computer simulations. The results are judged to be reasonable, and in fact, the POLESTAR-2F/3F code is now fully utilized to plan the future refuelling program of the 165 MWe HWR-Fugen. The developed computer program is considered to have advantages in the following aspects.

Effective data library system: The detailed burnup data of fuel bundles, calculated by any of the established multigroup cell burnup codes, are stored in the library, and taken into the main part of POLESTAR calculations when in necessity. By this method, the fuel bundle informations are always given in detail although the gross core calculation uses a coarse mesh one group model.

Short computation time and flux shape corrections: By eliminating the process of albedo fittings and void iterations, the computation time is shortened compared with the other computer codes used for the same purpose. Instead, the flux shape corrections are made against reflector and distributed void effects. The coolant void reactivity is generally very small in the HWR-Fugen, and its influence on the axial power distribution is a small and smoothing effect. Hence, the simple flux shape correction method works very well.

Easy I/O control: The input and output specifications are very much simplified by using a free format method, i.e., each fuel channel is given with its own ID number and any layouts of the core are expressed by listing these ID numbers. Thus, alterations of the CR pattern, refuelling, shuffling, and other spatial control actions are very easily specified. In addition, zone grouping of the core informations becomes a very easy process.
### Table IV Informations of 6→9 Batch Transition Refuelling (POLESTAR-2F) (during 6 batch refuelling)

<table>
<thead>
<tr>
<th>Cycle No.</th>
<th>Days at EOC</th>
<th>No. of loaded fuels</th>
<th>Discharge fuel exposure (GWD/TH)</th>
<th>Discharge core burnup (GWd/TH)</th>
<th>Average core burnup (GWd/TH)</th>
<th>Ch. power peaking</th>
<th>Control rod pattern (Full in : 16.0)</th>
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Initial core: 0.662% Pu MOX, and 1.5% enriched UO;
Reload fuels: 0.662% Pu MOX.

### Table V Informations of 6→9 Batch Transition Refuelling (POLESTAR-2F) (after entering to 9 batch refuelling)

<table>
<thead>
<tr>
<th>Cycle No.</th>
<th>Days at EOC</th>
<th>No. of loaded fuels</th>
<th>Discharge core burnup (GWd/TH)</th>
<th>Average core burnup (GWd/TH)</th>
<th>Ch. power peaking</th>
<th>Control rod pattern (Full in : 16.0)</th>
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<td></td>
<td>14.07</td>
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</table>

Discharged fuels: 0.662% Pu MOX (7 1/4 cycles), 1.12% Pu MOX (15 cycle)
Reload fuels: 1.12% Pu MOX.
Fig. 12 Transition of Discharge Exposure in 6→9 Batch Refuelling

Fig. 13 Transition of Channel Power Peaking in 6→9 Batch Refuelling
Table VI  Informations of Refuelling with LWR-HWR Tandem Fuels (POLESTAR-2F)

<table>
<thead>
<tr>
<th>Cycle No.</th>
<th>Days at BOC</th>
<th>No. of reload fuels</th>
<th>Discharge fuel burnup (GWd/THM)</th>
<th>Average core burnup (GWd/THM)</th>
<th>Ch. power peaking</th>
<th>Max. L.U.R. (kW/cm)</th>
<th>Keff</th>
<th>(^{137})Ig (ppm)</th>
<th>Control rod pattern (Full in: 16.0)</th>
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<td>1</td>
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<td>0.445</td>
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Initial core: 0.66% Pu MOX, and 1.2% enriched UO₂
Reloaded fuels: L-H tandem MOX

Bibliography


Summary of the Session 4

Résumé de la Séance 4

M. Melice

1. Zolotar's 3-level classification of core simulators is very appropriate. The amount of adjustment should diminish as the level increases; however, he is quite right in stating that, solving correctly the diffusion problem by means of a good coarse mesh simulator is only part of the solution because the value of the results depends on the quality of node homogenization, and its usefulness depends on the possibility to recover the fine structure of the flux by proper factorization or imbedded calculation techniques. This de-homogenization phase should also allow to account for the non-uniformity of fuel exposure within the node.

2. Several coarse mesh methods of level 3 which have been presented at the meeting are based on the same separation principle: the detailed flux distribution within the node is handled by means of neutron balances performed in each direction successively and operating on transversally averaged macroscopic cross-sections.

This local analysis provides coarse mesh inter-nodal coupling relations which are solved on the multi-dimensional representation of the core.

It may be of interest to compare how the separation principle works in the various methods.

2.1. In the analytical method (COMETA, MUSIC, BIDNOD, QUARRY, MERCATOR-XY, CETHRA, ...) the node must be strictly homogeneous (node-wise constant diffusion macroscopic cross-sections).

Then, the flux in each direction can be represented in terms of single buckling analytical natural modes whenever the transverse leakage of these modes may be approximated by a node-wise constant transverse buckling or leakage source.

The method produces nodal diffusion equations directly in terms of average nodal fluxes but, as the node bucklings depend on the eigen value and fluxes of the core problem, the method is non-linear, and the coupling coefficients must be improved iteratively in an additional outer loop.

Since the node bucklings are derived from the material bucklings, the analytical fluxes satisfy exactly the diffusion equation within each node, and the accuracy of the method is only limited by the approximations regarding the transverse leakage.

2.2. In the Nodal Expansion Method (MEDIUM, ...) the node does not need to be strictly homogeneous but the variation of cross-sections must be smooth enough that the flux may be approximated by polynomials. The latter have just the order (4th order splines) consistent with inter-nodal continuity relations. The method can accept transverse leakage if arbitrary shape, which is approximated by a quadratic smoothing of the average values provided by the core diffusion problem.

Because of its polynomial representation, the flux satisfies the node diffusion equation in an average manner only (in weighted residuals sense).
2.3. The Green Functions Method (NGFM) requires homogeneous nodes in order to use analytical Green functions of 1-D diffusion operator with constant diffusion and group removal coefficients. Like in the polynomial method, the transverse leakage may be of arbitrary shape and is handled explicitly. It is represented, like the volumic source by a quadratic modulation of average values. This lower order approximation is acceptable because it affects the source rather than the flux itself and that the internodal continuity conditions are satisfied "by construction".

Last two methods are linear but produce coupling relations in terms of partial currents.

It appears that the accuracy of the above methods is mostly limited by the way the transverse leakage is approximated.

2.4. HEXBU method is another interesting example of how the separation principle can be used in an analytical method. Uniformity of node is assumed to calculate the material bucklings of the analytical modes.

Separation of fundamental buckling in the Z direction is assumed, which is a fair approximation, but, contrarily to the other analytical methods, no separation in the XY plane is assumed. The XY component of the fundamental mode is rather approximated by a polynomial finite element covering the hexagonal node and fitted, on an average, to the XY component of the fundamental buckling. The transient mode is approximated by plane exponential waves. The free parameters of this flux representation are improved iteratively in a buckling iteration step.

This hybrid approach combines the advantages and avoids some disadvantages of the analytical and finite elements methods.

Profit is taken from the material bucklings but the questionable (especially in hexagonal geometry) separation of analytical modes in the XY plane is avoided. Finite elements representation is used without having to handle the large band matrix problem of pure finite elements solution.

3. Another point of interest which would deserve further discussion is the use of the separation principle extended to the energy variables in order to reduce formally a multi-group to an 1-group-problem.

This can be achieved (MERCATOR, MUSIC) by handling implicitly the leakage of the driving fundamental mode or flux, and explicitly the leakage of the driven mode.

The main interest of the formal 1-group reduction is that the dimension of the core problem is reduced to such a low level that the flux problem can be solved directly rather than interatively, and lends itself to using powerful WIELANDT-type acceleration methods to obtain not only fundamental mode but also, at marginal time, the source importance functions related to useful flux functionals (MERCATOR-Z).
Session 5

Chairman - Président
Dr. A. KAVENOKY
(France)

Séance 5
CALCULS DE SUIVI A TROIS DIMENSIONS D'UN REACTEUR PWR EXPERIMENTAL EN EXPLOITATION : CAP 1800

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Service d'Etudes des Réacteurs et de Mathématiques Appliquées
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Le système de codes de calcul NEPTUNE présenté à la conférence de
HAMBourg /1/ est appliqué au calcul du suivi de l'évolution d'un réacteur PWR
expérimental d'une puissance de 100 MWth situé à CADARACHE.

Les éléments combustibles de ce réacteur, la Chaufferie Avancée Prototype,
sont identiques à ceux des PWR 900 MWe à la hauteur près. Les caractéristiques
thermohydrauliques sont aussi comparables à celles d'un réacteur PWR de 900 MWe.

L'évolution du coeur à trois dimensions est calculée par deux méthodes.
La première est un calcul fin utilisant une méthode de synthèse, la seconde est
une méthode aux éléments finis portant sur des mailles larges. Ces deux calculs
font appel aux modules ICARE et TRIDENT du système NEPTUNE.

Les résultats des deux méthodes sont comparés : réactivité, distributions
de puissance ... On compare également les résultats de calcul aux mesures de flux
réalisées périodiquement à l'aide de l'instrumentation interne.

INTRODUCTION

La part croissante de l'électricité d'origine nucléaire en France
nécessite une qualification des combustibles aux sollicitations induites par le
suivi de charge (programme prévisionnel de production adapté à la consommation)
et le téléégargage (réglage autour d'une valeur de consigne de la puissance
fournie en fonction de la demande). Une expérience contribuant à cette qualification
pour les combustibles de type 17 x 17 des réacteurs PWR de 900 MWe, est effectuée
dans un réacteur expérimental du CEA situé à CADARACHE : la Chaufferie Avancée
Prototype (CAP).

La représentativité de l'essai repose, en grande partie, sur les calculs
de coeur, puisque les conditions de fonctionnement du réacteur expérimental sont
déterminées de façon à reproduire les variations locales de densité de puissance
calculées pour un réacteur PWR de 900 MWe en exploitation.

Nous présentons ici la comparaison de quelques paramètres de l'exploita-
tion du réacteur expérimental au cours du cycle 1, calculés par deux modules à trois
dimensions du système de codes NEPTUNE présenté à la conférence de HAMBourg /1/.
L'un de ces modules permet un calcul fin, crayon par crayon par une méthode de
synthèse, l'autre, un calcul à mailles larges par la méthode des éléments finis.

\* Agent COGEMA, détachée au SERMA
A - B - C - D

GROUPES DE BARRES DE CONTRÔLE

Figure 1
I/ PRESENTATION DU REACTEUR

Le réacteur CAP est un réacteur à eau légère pressurisé d'une puissance de l'ordre de 100 Mth, de type intégré : le générateur de vapeur est situé immédiatement au-dessus de la cuve contenant le cœur.

Ce réacteur permet d'irradier simultanément 12 assemblages identiques à la longueur près aux assemblages équipant les réacteurs de puissance.

Les grappes de contrôle constituées de crayons de Hafnium agissent deux par deux (un seul mécanisme pour deux grappes) sur quatre assemblages en périphérie du cœur. Quatre autres grappes destinées à la sécurité sont en position haute (figure 1).

Les variations lentes de réactivité sont contrôlées par du bore soluble dissous dans l'eau du modérateur. L'excès de réactivité en début de vie est compensé par des poisons consommables : au cycle I du réacteur, les 12 assemblages comportent chacun 12 crayons contenant un mélange d'oxyde d'uranium et d'oxyde de gadolinite (3 % en masse de Gd₂O₃). Les quatre assemblages centraux comportent en plus 12 crayons de pyrex (verre boraté à 12,5 % en masse de B₂O₃) et 12 crayons de hafnium placés dans les trous d'eau ; ces crayons sont tronqués axialement de 12 cm.

Les conditions thermohydrauliques sont comparables à celles d'un réacteur PWR 900 MWe du programme français actuel :

- pression de fonctionnement : 15 M Pa
- vitesse moyenne du réfrigérant : 2600 Kg/m²/s
- température moyenne du modérateur : 285 °C

Les dimensions et les caractéristiques principales des crayons standards, hormis la longueur, sont exactement les mêmes que celles des crayons qui équipent les centrales de puissance (tableau I). L'enrichissement de l'uranium est toutefois de 6,2 % (sauf dans les crayons gadolinités où il est de 5,1 %), le cœur étant conçu pour atteindre sans rechargement un épuisement moyen de 30 000 MWh/t sur les quatre assemblages centraux.

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Tableau I
Caractéristiques des assemblages combustibles
2/ CALCULS DE SUIVI DU COEUR À TROIS DIMENSIONS

2.1. Bibliothèques de sections efficaces

Les bibliothèques de sections efficaces sont établies à partir du code de transport multigroupe APOLLO /2/ qui fait également partie du système NEPTUNE. Les calculs sont faits en option multiculture et utilisent le formalisme de Roth. La concentration en bore soluble est maintenue constante et le calcul est fait à Laplacien critique.

Les sections efficaces par cellule, à quatre macrogroupes d'énergie, pour les calculs fins, sont corrigées de l'effet transport-diffusion, puis paramétrées en fonction de la concentration d'un corps évoluant. Les sections efficaces moyennes à deux macrogroupes sur l'ensemble des cellules constituant un assemblage, sont essentiellement des sections macroscopiques et sont tabulées en fonction de l'épuisement en MWj/t. Ces sections sont directement utilisées par le code de calcul à mailles larges.

2.2. Calculs fins par une méthode de synthèse variationnelle

Ce calcul utilise le module ICARE du système NEPTUNE. Le code ICARE utilise une méthode de synthèse monocanale continue /3/: le flux à trois dimensions est obtenu par le mélange de fonctions d'essais qui sont elles-mêmes solutions de l'équation de la diffusion à deux dimensions dans des tranches radiales choisies du réacteur. On a utilisé en général 6 fonctions d'essai qui ne sont pas nécessairement recalculées à chaque pas d'évolution.

Le cœur est décrit explicitement crayon par crayon, le maillage de calcul comporte 115 x 99 x 19 points en x, y, z, soit 216 315 points. Le nombre decellules d'évolution est de 55 488, on a, en effet, pris radialement, une cellule par crayon, et 12 cellules en axial.

Le réflecteur radial (baffle acier de 2 cm d'épaisseur) est représenté explicitement, les réflecteurs axiaux sont homogénéisés.

2.3. Calcul à mailles larges par la méthode des éléments finis

Ce calcul utilise le module TRIDENT de NEPTUNE. Le flux est approché dans les pavés par des polynômes que nous avons choisis du second degré en xy (interpolation parabolique) et du premier degré en z (interpolation linéaire). Chaque assemblage est divisé radialement en 4 mailles égales et axialement en 18 mailles : on a au total 2 592 pavés homogènes pour décriter le cœur. Le réflecteur radial est homogénéisé /4/, de même que les réflecteurs axiaux. Pour le réflecteur radial, les sections efficaces macroscopiques équivalentes sont calculées en fonction de la concentration en bore soluble. Le calcul de cœur est en effet très sensible à ces sections efficaces étant donnée l'importance des fuites radiales (6 12 000 pcm). La précision demandée est de 1 pcm sur la valeur propre et de 10^-3 sur le flux.

Ce calcul par la méthode des éléments finis est évidemment moins coûteux que le calcul fin par la méthode de synthèse (facteur 6 environ).

2.4. Comparaison des résultats de calcul

2.4.1. Réactivité

L'efficacité du bore soluble calculée en début de vie, sans xénon autour de 750 ppm est de :

<table>
<thead>
<tr>
<th>Code</th>
<th>1e3 EDP-pcm/ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICARE</td>
<td>5,94</td>
</tr>
<tr>
<td>TRIDENT</td>
<td>5,86</td>
</tr>
<tr>
<td>MESURE</td>
<td>5,9</td>
</tr>
</tbody>
</table>
Les courbes de concentration en bore critique obtenues par les deux calculs sont représentées sur la figure 2. Ces courbes sont faites dans les conditions moyennes de l'irradiation : barres A et B à 1 200 mm au-dessus du bas combustible, température moyenne du modérateur de 285 °C, équilibre xénon, les niveaux de puissance du réacteur étant de 104 MW de 0 à 2 500 MWj/t, 95 MW de 2 500 à 8 000 MWj/t, 93 MW de 8 000 à 10 000 MWj/t et 97 MW de 10 000 MWj/t à la fin du cycle. On a également représenté sur cette figure les résultats des prélèvements effectués par l'exploitant ramenés aux mêmes conditions.

Pour chaque calcul, une valeur propre moyenne de recalage a été déterminée sur la durée du cycle. La courbe expérimentale se situe entre les deux calculs et montre une légère remontée de réactivité vers la mi-cycle, qui n'apparaît pas dans le calcul TRIDENT, mais est amplifiée dans le calcul ICARE. Ce phénomène lié à la disparition du gadolinium se traduit par une différence au niveau des deux calculs, liée vraisemblablement à un effet de structure fine. L'écart brut entre les réactivités calculées est de l'ordre de 500 pcm, chaque calcul ne s'écarte pas de la courbe expérimentale de plus de 300 pcm.

2.4.2. Densités de puissance

Sur la figure 3, on a représenté la densité de puissance par assemblage en début de vie, à mi-cycle et en fin de cycle. L'écart ne dépasse pas 3 % à la périphérie et 2 % dans les assemblages centraux. Nous n'avons pas représenté sur ces figures les assemblages expérimentaux situés aux angles et qui dégagent environ 5 % de la puissance du cœur, le calcul de la puissance dans ces assemblages nécessite, en effet, un traitement spécifique notamment pour les sections efficaces des structures radiales à deux dimensions.

2.5. Mesures internes d'activités

Le cœur comporte six conduits d'instrumentation interne situés dans les assemblages positionnés en A3, B4, B2, B3, C2, C3 (figure 1). Dans les assemblages centraux, ces conduits sont au centre de l'assemblage, mais pour les deux assemblages périphériques, ils sont situés en bordure. Ces conduits peuvent être équipés de fils de Ti-Cu, qui s'activent sous flux dans le cœur et sont ensuite comptés sur un banc automatique. Ces mesures périodiques sont dépouillées par les deux méthodes de calcul et les écarts entre les deux dépouillements sont reportés dans le tableau II. Les sections efficaces du cuivre sont issues du calcul de transport initial, pour le calcul fin, elles sont ajustées de l'écart transport-diffusion.

<table>
<thead>
<tr>
<th>Epuisement (MWj/t)</th>
<th>0</th>
<th>4 000</th>
<th>10 000</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TRI</td>
<td>ICA</td>
<td>TRI</td>
</tr>
<tr>
<td>Ecarts, conduits</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A3</td>
<td>- 5,8</td>
<td>- 4,5</td>
<td>- 4,7</td>
</tr>
<tr>
<td>B4</td>
<td>- 3,8</td>
<td>- 3,8</td>
<td>- 1,9</td>
</tr>
<tr>
<td>B3</td>
<td>4</td>
<td>3,4</td>
<td>0,4</td>
</tr>
<tr>
<td>B2</td>
<td>3</td>
<td>2,5</td>
<td>4</td>
</tr>
<tr>
<td>C3</td>
<td>1,4</td>
<td>1,2</td>
<td>2,3</td>
</tr>
<tr>
<td>C2</td>
<td>3</td>
<td>2,7</td>
<td>2</td>
</tr>
</tbody>
</table>

Tableau II
Ecarts en % (calcul-mesure) / mesure pour l'intégrale axiale des activités.

- 353 -
<table>
<thead>
<tr>
<th>.996</th>
<th>1.003</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 1.10 %</td>
<td>- 2.49 %</td>
</tr>
<tr>
<td>.985</td>
<td>.978</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>1.014</th>
<th>1.097</th>
<th>1.084</th>
<th>.936</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 1.87 %</td>
<td>+ 1.09 %</td>
<td>+ 0.65 %</td>
<td>- 1.82 %</td>
</tr>
<tr>
<td>.995</td>
<td>1.109</td>
<td>1.099</td>
<td>.919</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>.935</th>
<th>1.082</th>
<th>1.096</th>
<th>1.017</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 1.71 %</td>
<td>+ 0.83 %</td>
<td>+ 0.73 %</td>
<td>- 2.46 %</td>
</tr>
<tr>
<td>.919</td>
<td>1.091</td>
<td>1.104</td>
<td>.992</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1.000</th>
<th>.995</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 2.80 %</td>
<td>- 2.21 %</td>
</tr>
<tr>
<td>.970</td>
<td>.973</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>.995</th>
<th>.999</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 2.51 %</td>
<td>- 3.10 %</td>
</tr>
<tr>
<td>.970</td>
<td>.968</td>
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<table>
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<th>1.105</th>
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<tbody>
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<td>- 2.46 %</td>
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<tr>
<td>.985</td>
<td>1.137</td>
<td>1.123</td>
<td>.913</td>
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<table>
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<th>1.117</th>
<th>1.012</th>
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<tbody>
<tr>
<td>- 2.03 %</td>
<td>+ 1.81 %</td>
<td>+ 1.70 %</td>
<td>- 2.86 %</td>
</tr>
<tr>
<td>.913</td>
<td>1.123</td>
<td>1.136</td>
<td>.983</td>
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<table>
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<tr>
<th>.997</th>
<th>.993</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 3.11 %</td>
<td>- 2.62 %</td>
</tr>
<tr>
<td>.966</td>
<td>.967</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>.961</th>
<th>.998</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 1.87 %</td>
<td>- 1.90 %</td>
</tr>
<tr>
<td>.943</td>
<td>.979</td>
</tr>
</tbody>
</table>

<table>
<thead>
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<th>1.145</th>
<th>1.136</th>
<th>.913</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 1.39 %</td>
<td>- 1.83 %</td>
<td>- 1.58 %</td>
<td>- 0.22 %</td>
</tr>
<tr>
<td>.992</td>
<td>1.124</td>
<td>1.118</td>
<td>.911</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>.912</th>
<th>1.134</th>
<th>1.149</th>
<th>1.006</th>
</tr>
</thead>
<tbody>
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<td>- 1.50 %</td>
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</tr>
<tr>
<td>.911</td>
<td>1.117</td>
<td>1.124</td>
<td>.990</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>.995</th>
<th>.957</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 1.81 %</td>
<td>- 1.78 %</td>
</tr>
<tr>
<td>.977</td>
<td>.940</td>
</tr>
</tbody>
</table>

Figure 3 : DENSITE DE PUISSANCE PAR ASSEMBLAGE
COURBES AXIALES D'ACTIVITÉ
CALCULÉE ET MÉSUREE
DES FILS DE CUIVRE
GRAPPE À 1200 MM
BUHOMULLU CYCLE 1 1000 PPM

Figure 1

Résistance à
Calcul ICARE

30  60  90  120  150
Sur les figures 4 à 11, nous avons représenté les activités calculées (par les deux méthodes) et mesurées, pour un conduit situé en périphérie du cœur dans un assemblage contenant une barre et un autre au centre, en début de vie et en fin de vie.

Ces résultats montrent un léger avantage pour le calcul aux différences finies ICARE, mais dans les deux calculs on sous-estime l’activité en périphérie, les écarts étant plus répartis dans le calcul fin.

CONCLUSION

La comparaison des deux méthodes de calcul sur ce cœur de réacteur expérimental, montre que le calcul par la méthode des éléments finis appliqué à des mailles larges, donne des résultats comparables à quelques pourcents près au calcul détaillé crayon par crayon, pour ce qui concerne les densités de puissance, l’efficacité du bore, les mesures internes d’activation ... Les fuites radiales importantes dans ce cœur de faibles dimensions et les nombreuses hétérogénéités rendent la comparaison d’autant plus délicate : l’homogénéisation des poissons ainsi que celle des structures (réflecteurs notamment) dans le calcul à mailles larges doit être faite avec beaucoup de soins.

Le calcul à mailles larges a bien sûr l’avantage d’être beaucoup moins coûteux et permet de ce fait de nombreuses utilisations que nous n’avons pas mentionnées ici : efficacité des barres de contrôle, calculs de suivi de charge et de téléréglage notamment.

Le calcul fin par la méthode de synthèse mononucléaire, permet en revanche d’obtenir directement les densités de puissance et les nombres de noyaux évoluants au niveau des crayons eux-mêmes. Ces informations sont particulièrement nécessaires dans un réacteur expérimental de ce type, puisque le but de l’irradiation est en définitive l’analyse du comportement des crayons ayant subi des variations bien localisées de puissance dues au téléréglage en particulier.

Références


/4/ S. NIZAMUDDIN - Une nouvelle méthode pour le calcul de l’interface cœur-réflecteur dans les réacteurs à eau ordinaire. Rapport SERMA n° 204 T.
COURSES AXIALES D'ACTIVITE CALCULEE ET MEASUREE

DES FILS DE CUIVRE

GRAPPE 9 1200MM

BUXOMAJ/TU CYCLE 1 1000 PPM

ASSEMBLAGE C2

Est-ce ICARE

Figure 6

- 359 -
Courbes axiales d'activité
Calculée et mesurée
des fils de cuivre
Grappes à 1200mm
8U=10880 MW/1U 155 PPM cycle7
Courbes axiales d'activité calculée et mesurée des fils de cuivre grappes à 1200 mm.

BU=10880 MWJ/TU 155 PPM CYCLE 1.
CALCULATION OF POWER DISTRIBUTION IN A BWR CORE

BY A NEW FINITE DIFFERENCE METHOD

Y. Naito

JAPAN ATOMIC ENERGY RESEARCH INSTITUTE

Division of JPDR in JAERI, Tokai-mura, Ibaraki-ken, Japan

A computer code, STEADY-ACE, is developed for analysing core performances of a BWR. The calculational schemes of STEADY-ACE are described, where it is proposed that the calculation of neutron flux in reflector regions is performed analytically without assigning any meshpoints. Using this code, check calculations were carried out. The neutron diffusion calculation method used in STEADY-ACE were confirmed to be as reliable as ordinary finite difference method. Power distributions in a BWR were analysed and compared with experimental data, and not so good results are obtained as expected from the diffusion calculation method.

1. Introduction

Many kinds of methods to calculate nuclear characteristics of power reactor cores have been developed. They are, for instance, flux synthesis, coarse-mesh finite difference, modal expansion and nodal method. The most straightforward and reliable method is the fine-mesh difference approximation. For analysing power reactor cores, it is desirable to calculate the neutron flux by solving the neutron diffusion equation with the fine-mesh difference approximation method. This approach is, however, not always practical for calculations of large nuclear power reactors, especially for BWR core analyses which require power void iteration. The author proposed a new method "Leakage Iterative Method" to make it possible to analyse power reactor cores with a difference approximation method.

We have applied this method to analyse a BWR cores and developed a computer code named as STEADY-ACE, which is composed of two programs DIFFUSION-ACE and HYDRO-ACE. The program DIFFUSION-ACE is a three-dimensional neutron diffusion calculation program with "Leakage Iterative Method." The program HYDRO-ACE is developed by us to deal with multi-channel hydraulics in a BWR core calculation. The advantages of STEADY-ACE are: (1) it solves three-dimensional diffusion equation of two or three energy groups with finite difference approximation to obtain the power distribution; and (2) it includes a thermal-hydraulic model which calculates the flow rate and void fraction distributions, so that the interdependency between the void fraction distribution and the power distribution can be treated accurately.

We have analysed power reactor cores many times by this program and for all cases, iteration schemes were converged without any trouble. Some
results of them will be shown in this report to predict the points of investigations. At first, sample out-put of STEADY-ACE will be shown to exhibit the items of the calculation and convergence schemes. Secondly, the computed results by DIFFUSION-ACE will be compared with those by the CITATION\textsuperscript{5)} code to check the reliability of the Leakage Iterative Method. Thirdly, the power distribution calculation for a BWR core will be presented to evaluate the accuracy and to predict the points of our method. Finally, the flow distribution in a BWR core will be obtained to show the effectiveness of HYDRO-ACE program in STEADY-ACE.

2. Computer Code STEADY-ACE

2.1 Purpose for Development of STEADY-ACE

One of the objectives in the BWR core design is to verify that the power peaking factors do not exceed the limiting value. It is therefore very important to calculate the peaking factors accurately. The difficulty in the calculation of the peaking factors in a BWR core arises from the fact that (1) the power distribution is skewed both horizontally and vertically due to the insertion of the control rods, and (2) the void fraction distribution and the power distribution depend strongly on each other and they cannot be calculated separately. Due to the first fact, three-dimensional calculations are required, and due to the second fact, the iteration is also required between the thermal-hydraulic calculation to get the void fraction distribution and the neutron diffusion equation calculation to obtain the power distribution.

A number of computer programs have been developed for these purposes. The program used frequently is FLARE\textsuperscript{5)} which has an advantage of short computation time but a disadvantage of low accuracy. One of the causes for its low accuracy is that the power distribution calculation is based on the pseudo-diffusion equation using the neutron transport kernel. Another cause is that the flow rate distribution in the flow channels is obtained apriori from a separate thermal hydraulic calculation. The interdependency between the void fraction distribution and the power distribution cannot be treated by FLARE in a satisfactory manner.

A computer program named as STEADY-ACE is developed here to overcome the disadvantages of FLARE. Its recipe is: (1) to solve three-dimensional diffusion equation of two or three energy groups to calculate the power distribution; and (2) to include a thermal-hydraulic model which calculates the flow rate and void fraction distributions in order to treat accurately the interdependency between the void fraction distribution and the power distribution.

The program STEADY-ACE combines the two computer programs; the thermal-hydraulic program HYDRO-ACE and the three-dimensional diffusion equation program DIFFUSION-ACE. The DIFFUSION-ACE adopts a new method called "Leakage Iterative Method" to solve the three-dimensional diffusion equation. This new method is one of the synthesis methods which combine the z-directional one-dimension calculation with the x-y directional two-dimensional calculation. The computation time can be reduced significantly by the "Leakage Iterative Method" without sacrificing the accuracy. The advantage of short computation time in DIFFUSION-ACE makes the void-power iteration in STEADY-ACE practical.

2.2 Reactor Model for STEADY-ACE

The STEADY-ACE simulates a BWR core. The calculation model of STEADY-ACE is explained here using an example for the JPDR-II core. The JPDR is a small BWR located in Tokai Research Establishment of Japan Atomic Energy Research Institute. The reactor has been modified since 1964 to double the power level.
The modified reactor is called as JPDR-II. The major core parameters of JPDR-II are given in Table I. The x–y cross section of the JPDR-II core is illustrated in Fig. 1.

The calculational model of a BWR core for the thermal-hydraulic calculation code HYDRO-ACE is presented first. A BWR core, such as JPDR-II core, consists of parallel channels. As each fuel assembly is enclosed by a channel box, each flow path in a channel box can be separately treated to predict its thermal-hydraulic behaviors. The flow channel is divided into a number of sections based on the flow area and thermal characteristics. The heated zone is separately treated from the unheated zone. The heated zone is further equally divided into blocks. The blocks are numbered sequentially from the bottom to the top. Next, the calculational model of a BWR core for the nuclear calculation code DIFFUSION-ACE is discussed. A BWR core is divided into square lattice cells of fuel bundles. The nuclear cross sections associated with the lattice cells are defined as the homogenized ones over the fuel, cladding, moderator and channel box. The fuel bundle cells are designated by the same number as in the thermal-hydraulic model. The regions outside of the fuel bundles are collectively called as "reflector." The "core" region is further divided into blocks in the same way as mentioned in the thermo-hydraulic model. The size, elevation and identification number of the blocks in the nuclear model should be identical to those in the thermal-hydraulic model. As the blocks of the same identification number are at the same elevation, they form layers with the two horizontal parallel planes. In other words, a block is a parallelepiped defined by a channel and a layer, as shown in Fig. 2.

The program DIFFUSION-ACE solves the three-dimensional diffusion equation by alternatively solving one-dimensional equation for each of the channels and two-dimensional equation for each of the layers. In order to improve the accuracy of calculations, the blocks are further subdivided into meshes, for example, as shown in Fig. 2. The objective of the sub-division into meshes is to make the mesh size comparable to the diffusion length of thermal neutrons. Similarly, a block is subdivided into a few meshes in the x and y directions in the two-dimensional diffusion calculation for each of the layers.

2.3 Basic Equations

The STEADY-ACE is composed of the thermo-hydraulic subprogram HYDRO-ACE and the three-dimensional diffusion equation subprogram DIFFUSION-ACE. The basic equations of the two subprograms and their interface are explained in this section.

2.3.1 Basic Equations in HYDRO-ACE

The HYDRO-ACE calculates the flow rates and the void distributions in the flow channels in the core shroud. The power distributions in the channels are supplied from DIFFUSION-ACE. The flow rates in the flow channels are determined in a way that the pressure differences between the inlets and outlets are equal for all of the flow channels. The pressure differences consist of heat loss, friction loss, expansion/contraction loss, spacer loss and acceleration loss.

\[ \Delta P_I = \Delta P_R + \Delta P_{FR} + \Delta P_{E/C} + \Delta P_{sp} + \Delta P_{acc}. \] (1)

The \( \Delta P_I \) must be same for all flow channels, so that the inlet flow distribution is adjusted iteratively until the total pressure differences of all channels become almost the same values. This iteration is converged and the thermal hydraulic conditions at each block in the core are fixed to the given power distribution which is supplied from DIFFUSION-ACE.

2.3.2 Basic Equations in DIFFUSION-ACE

The DIFFUSION-ACE solves a three-dimensional diffusion equation by com-
Fig. 1  X-Y cross section of JPDR-II core

Fig. 2  Configuration of Channels, Layers, and Blocks.
hiring z-directional one-dimension calculations with x-y-directional two-dimension calculations. A new method called "Leakage Iterative Method" has been developed for this purpose. The method was reported already so we explain here only briefly.

A general diffusion equation is written as

\[ \nabla D \nabla \phi - \Sigma_i \phi + S = 0 \]  \hspace{1cm} (2)

where the notation is conventional.

Integrating Eq. (2) over a block which is assumed to be homogeneous in its nuclear characteristics, we have

\[ D \int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \phi \, dx\,dy\,dz + \int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) \, dx\,dy\,dz + D \int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \left( \frac{\partial^2 \phi}{\partial z^2} \right) \, dx\,dy\,dz - \Sigma_t \int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \phi \, dx\,dy\,dz + \int_{\Delta x} \int_{\Delta y} \int_{\Delta z} S \, dx\,dy\,dz = 0 \]  \hspace{1cm} (3)

where \( \Delta x, \Delta y \) and \( \Delta z \) give the dimensions of the block.

The leakages \( L_{xy} \) and \( L_z \) are written as:

\[ L_{xy} = \frac{D \int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) \, dx\,dy\,dz}{\int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \phi \, dx\,dy\,dz} \]  \hspace{1cm} (4)

\[ L_z = \frac{D \int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \left( \frac{\partial^2 \phi}{\partial z^2} \right) \, dx\,dy\,dz}{\int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \phi \, dx\,dy\,dz} \]  \hspace{1cm} (5)

The flux and the source integrated over a block are respectively given as:

\[ \theta_b = \int_{\Delta x} \int_{\Delta y} \int_{\Delta z} S \, dx\,dy\,dz \]  \hspace{1cm} (6)

Inserting Eqs. (4), (5) and (6) into Eq. (3), we get

\[- (L_{xy} + L_z + \Sigma_t) \phi + \theta_b = 0 \]  \hspace{1cm} (7)

which shows the integrated flux \( \phi_b \) can be easily derived if \( \theta_b, L_{xy}, L_z \) and \( \Sigma_t \) are given. However, the leakage terms \( L_{xy} \) and \( L_z \) are not given a priori but to be derived from the two-dimensional calculations and the one-dimensional calculations, respectively.

Let \( \psi_z, \theta_z, \psi_{xy} \) and \( \theta_{xy} \) be defined as:

\[ \psi_z = \int_{\Delta x} \int_{\Delta y} \phi \, dx\,dy \]  \hspace{1cm} (8)

\[ \theta_z = \int_{\Delta x} \int_{\Delta y} S \, dx\,dy \cdot \psi_{xy} \equiv \int_{\Delta z} \phi \, dz \]  \hspace{1cm} (9)

Inserting Eqs. (8) and (9) into Eq. (3), we have

\[ \frac{\partial^2 \psi_z}{\partial z^2} - (L_{xy} + \Sigma_t) \psi_z + \theta_z = 0 \]  \hspace{1cm} (10)
Fig 3  Schematic diagram of the Leakage Iterative Method.
\[ D \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi_{xy} - \left( L_3 + L_\perp \right) \psi_{xy} + \theta_{xy} = 0 \] (11)

The leakage \( L_{xy} \) and \( L_z \) are obtained from Eqs. (4) and (5) respectively, but \( L_{xy} \) should be given to derive \( L_z \) and \( L_z \) should be given to derive \( L_{xy} \). Therefore, an iterative calculation is necessary to obtain \( L_{xy} \) and \( L_z \). This iterative schematic diagram is shown in Fig. 3. The convergence of the iteration is determined by comparing the following two quantities with each other.

\[ \begin{align*}
(\psi_b)_z &= \int dx \int dy \psi_z\ dx\ dy, \\
(\psi_{b_{xy}})_{xy} &= \int \psi_{xy}\ dz \Delta z.
\end{align*} \] (12)

If \( L_{xy} \) and \( L_z \) have the consistency, the following relation should be satisfied.

\[ \psi_b = (\psi_b)_z = (\psi_{b_{xy}})_{xy}. \] (13)

The neutron balance is thus achieved by the iteration mentioned above, which corresponds to the inner iteration in the finite difference calculation.

The advantage of the Leakage Iterative Method is to allow subdivisions of the blocks into one-dimensional and/or two-dimensional geometry. Use of coarse meshes, such as 1 mesh point in an assembly (1/2 foot width), makes the finite difference method less accurate than desired because the diffusion length of thermal neutrons in light water is less than the mesh width. In the present approach, one-dimensional calculations and two-dimensional calculations are performed separately, and hence the subdivisions of the blocks can provide a desired accuracy in solving the diffusion equation without increasing computation time significantly.

2.3.3 Treatment of Neutron Flux in Reflector Regions

Another feature of DIFFUSION-ACE exists in the treatment of the reflector region. In general, a large number of mesh points is assigned to the reflector region because the thermal neutron flux has a peak in the region, which increases the computation time and computer storage requirement dramatically. In order to avoid assigning a large number of mesh points, a new boundary condition is derived here to obtain the flux analytically. At the boundary between the core and the reflector, the continuities of the neutron current and the neutron flux are assumed. This approach called as "analytical boundary condition" is explained here by using an example of one-dimensional geometry illustrated in Fig. 4. In the reflector regions the one-dimensional diffusion equation is expressed and solved under the following conditions:

\[ \frac{d^2}{dr^2} \phi - k^2 \phi = 0 \quad , \quad \phi(r) = \phi_{Bl} \cdot e^{-kr}. \] (14)

\[ \phi_R = \phi_{Bl}, \quad \text{at} \quad 0 \quad \text{and} \quad \phi_R = 0, \quad \text{at} \quad r \rightarrow \infty \]

where \( \phi_{Bl} \) refers to the boundary shown in Fig. 4.

The continuity of the neutron current at the boundary is expressed as:

\[ (- D_R \frac{d\phi}{dr} |_{r=0} ) = -D_1 \cdot \frac{\phi_I - \phi_{Bl}}{\Delta z_1} \] (15)

where the subscript 1 refers to the first mesh point in the core region.

The one-dimensional diffusion equation is expressed by the following difference equation for the first mesh point in the core region.

\[ D_1 \frac{\phi_I - \phi_{Bl}}{\Delta z_1/2} - D_1' (\phi_2 - \phi_1) + D_1' B^2 \phi_1 \Delta z_1 + \Sigma_{T1} \phi_1 \Delta z_1 = S_1 \Delta z_1. \] (16)

where
Fig. 4  Mesh distribution to calculate one dimensional diffusion equation

Fig. 5  General flow chart of STEADY-ACE
and the subscripts 1 and 2 refer to the first and second mesh points in the core region, respectively.

The approach described above is for the first energy group in the one-dimensional calculation, but the same approach is applied to other energy groups and also the two-dimensional calculation.

2.3.4 Interface between HYDRO-ACE and DIFFUSION-ACE

As mentioned before, STEADY-ACE consists of the thermal-hydraulic part HYDRO-ACE and the three-dimensional neutron diffusion part DIFFUSION-ACE. The interfaces between these two parts are presented here. As the interface from the thermal-hydraulic part into the nuclear part, the output of the thermal-hydraulic calculation is mainly given as the block-wise void fraction within the channel box, for which the input of the nuclear calculation is the block-wise neutron cross sections. The SUBROUTINE CROSS serves as an interface by calculating the block-wise neutron cross sections from the block-wise void volume fraction and thermal power.

The neutron macroscopic cross sections are prepared as quadratic functions of the void fraction within the channel box.

\[ \Sigma_x = (\Sigma_x^0) + (\Sigma_x^1) \cdot a + (\Sigma_x^2) \cdot a^2 \]  

where \( \Sigma_x \) refers to the neutron cross sections, such as absorption cross section, slowing down cross section, diffusion coefficient and emission cross section (product of neutron number per fission and fission cross section): The \( a \) is a void fraction within the channel box, and \( \Sigma_x^0, \Sigma_x^1 \) and \( \Sigma_x^2 \) are fitting constants, which depend upon the thermal power.

The fitting constants are prepared by the multi-group calculations for lattice cells parametrically as a function of void fraction and thermal power. These parametric calculations produce two or three group cross sections homogenized over the lattice cells. A quadratic fitting computer program processes these data into tables of the fitting constants. Then, given the block-wise void fraction and thermal power from the thermal-hydraulic part HYDRO-ACE, the block-wise cross sections are calculated by Eq. (17).

The calculation starts with the initial power distribution guess specified by the user. With this power distribution HYDRO-ACE calculates the void fraction distribution. From the void fraction and thermal power distributions, subroutine CROSS calculates the neutron cross sections for the core region and upper reflector region. Given the cross sections, DIFFUSION-ACE calculates the power distribution. Iterative calculations are performed until the consistency is attained between the power distribution and void fraction distribution. The convergence of the iteration is judged by comparing the power residuals to the convergence criterion specified by the user, where the power residual is defined as:

\[ (R_p)_n = \max_{l,k} \left| \frac{p^n - p^{n-1}}{p^n} \right|_{l,k} \]  

\( n \): iteration index  
| \( l \): channel identification number  
| \( k \): axial block number  
| \( P \): normalized power of the block \((l, k)\)

The flow chart of the calculation is illustrated in Fig. 5.
### DETAILS OF THE 3-RD ASSEMBLY

1. **Coolant Flow**: 10.758 KG/SEC
2. **Variation from Inlet to Exit**

<table>
<thead>
<tr>
<th>Region</th>
<th>Height (m)</th>
<th>Entalphy (KJ/HR)</th>
<th>Quality</th>
<th>Void Fr.</th>
<th>Density (Kg/M³)</th>
<th>MPH</th>
<th>CMFR (Inlet)</th>
<th>CMFR (Outlet)</th>
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</thead>
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<td>310.71</td>
<td>0.0511</td>
<td>4.593</td>
<td>429.71</td>
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<td></td>
<td></td>
</tr>
<tr>
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<td>0.04663</td>
<td>0.4311</td>
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<tr>
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<td>0.04156</td>
<td>0.4071</td>
<td>461.04</td>
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<td>0.2694</td>
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</tbody>
</table>

### DETAILS OF THE 4-TH ASSEMBLY

1. **Channel Heat Product**: 310.56 Kcal/SEC
2. **Rate to Core Ave.**: 1.0359

<table>
<thead>
<tr>
<th>Region</th>
<th>Height (m)</th>
<th>HLat (KJ/HR)</th>
<th>Noul To Chan Ave</th>
<th>Noul To Core Ave</th>
<th>Heat Flux (KJ/HR)</th>
<th>Heat Inft (KJ/HR)</th>
<th>Axisl Heat Distribution Normalized to Channel Ave.</th>
</tr>
</thead>
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<tr>
<td>K-12</td>
<td>3.7900</td>
<td>9.29</td>
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<td>0.3806</td>
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<tr>
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<td>3.6678</td>
<td>16.47</td>
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<td>0.6444</td>
<td>71.53</td>
<td>301.27</td>
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<tr>
<td>K-10</td>
<td>3.5455</td>
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<td>0.5460</td>
<td>0.8967</td>
<td>95.11</td>
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<td>25.86</td>
<td>0.9991</td>
<td>1.0589</td>
<td>122.32</td>
<td>262.91</td>
<td>*</td>
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<tr>
<td>K-8</td>
<td>3.3010</td>
<td>28.63</td>
<td>1.1063</td>
<td>1.1726</td>
<td>124.37</td>
<td>237.05</td>
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<tr>
<td>K-7</td>
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<td>1.5383</td>
<td>163.17</td>
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<td>K-3</td>
<td>2.6908</td>
<td>31.14</td>
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<td>1.2753</td>
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<td>65.43</td>
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<td>K-2</td>
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<td>109.43</td>
<td>37.49</td>
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<td>0.5037</td>
<td>53.42</td>
<td>0.0</td>
<td>*</td>
</tr>
</tbody>
</table>

Fig. 6 Sample out-put of STEADY-ACE
3. Calculational Results

3.1 Sample Out-Put of STEADY-ACE

Test calculation was performed to JPDR-II (Japan Power Demonstration Reactor) whose core data are shown in Table I. The sample out-put is shown in Fig. 6 which shows consistent moderator void and thermal power distribution in a channel for an example. The convergence history of the power-void iteration is shown in Table II, which predicts the iterative scheme is converged smoothly.

3.2 Check Calculation of DIFFUSION-ACE

To check the reliability of the Leakage Iterative Method which is used in DIFFUSION-ACE, computed results by DIFFUSION-ACE were compared with those by the computer code CITATION which was one of the most standard neutron diffusion code with fine mesh finite difference method. One of the results is shown in Fig. 7. In this case, the CITATION code calculated neutron fluxes at the 4 x 4 mesh points in each channel whose cross section was 18cm x 18cm and DIFFUSION-ACE calculated channel-integrated fluxes. Hence, the solid line should be compared with the average of the point fluxes by CITATION. As shown in Fig. 7, axial neutron flux distribution in a channel showed a good agreement with each other.

The above results show that neutron diffusion calculation method which is used in STEADY-ACE is as reliable as ordinary finite difference method.

3.3 Power Distribution in JPDR-II Core

Power distribution in JPDR-II core was estimated by measuring decay γ-rays of Ti-Cu wires in incore monitors. Comparison of the power distributions obtained by measurement and calculation with STEADY-ACE are shown in Figs. 8 and 9. Figure 9 shows the axial power distributions in channels located at (16, 5), (17, 5) and (18, 5) in Fig. 1. The channels (16, 5) and (17, 5) are close to a control rod which is inserted into No.8 block from bottom. In this figure, calculated power distributions near the control rod, are more flattened than measured ones.

This is caused by over estimation of the neutron leakage to the control channel from neighbour channels. Figure 9 shows the heat production rate in JPDR-II core. The heat rate in channels near the reflector is over estimated and the heat rate distribution is more flattened than measured one. The above results suggest that it is very important and difficult to estimate neutron flux distribution near control rods and reflector.

3.4 Coolant Flow Distribution in JPDR-II Core

Four instrumented fuel assemblies (IFA) were loaded in JPDR-II core and coolant flow rates through the IFAs were measured by turbine flow meter attached to inlet and outlet of IFAs as shown in Fig. 10. Calculated coolant flow rates through IFAs were compared with measured data and the results shown in Table III and IV. Table III shows that the calculated results are agreement with measured ones within a few percent error. In Table IV, relations between normalized heat production rate and coolant flow rate are shown. The more heat products in a channel, the less coolant flows through the channel near the rated flow rate (100% flow) and the more coolant flows at less than 80% coolant flow rate. The above coolant flow characteristics in JPDR-II core are obtained both by measurement and by calculation.
Fig. 7  Comparison of Z-Directional Flux.
Fig. 8  Axial power distribution normalized to core average of unity
Fig. 9 Heat Production Rate in JPDR-II Core
4. Conclusions

i) A new three-dimensional neutron diffusion calculation code DIFFUSION-ACE have been developed on the basis of the "Leakage Iterative Method". Computed results by this code were compared with those by CITATION. The results agree well with each other and show that neutron diffusion calculation method which is used in STEADY-ACE is as reliable as ordinary finite difference method.

ii) By linking DIFFUSION-ACE with multi-channel hydraulics code HYDRO-ACE, core performance analysis code STEADY-ACE is developed. With this code, core performances of a small BWR type JPDR are analysed and the results show that the calculated power distribution is more flattened than measured one. This is caused by over estimation of the neutron leakage to a control channel from neighbour channels and by over estimation of the heat production rate in a channel near reflector.

iii) A new method is proposed to calculate the neutron flux in reflector regions analytically. With this method it becomes not necessary to assign mesh points to reflector regions, and computation time and computer storage requirement are decreased dramatically. But not so good computed results were obtained as expected the diffusion calculation method. The measured value itself of heat production rate in a channel near reflector indeed has uncertainty because the channel is far from in-core detectors.

iv) The calculated coolant flow rates through IFAs were compared with measured data and the results showed a good agreement. This predicts that STEADY-ACE is applicable to analyse efficiently coolant flow distribution in a BWR core.

Acknowledgement

The computer code STEADY-ACE is programed by two talented computer engineers, K. Abe who programed the HYDRO-ACE code and M. Maekawa who programed the DIFFUSION-ACE code and linked it to the HYDRO-ACE code. Without their help, this program could not appear in the world. The author wish to thank to them for their works. Thanks are also due to T. Asaoka and S. Matsumura of the Japan Atomic Energy Research Institute for their valuable discussions.

Reference

Fig. 10 JPDR-II Instrumented Fuel Assembly
### TABLE I  JFDR-II core data

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<th>(1) Fuel rod</th>
<th>(3) Control rod</th>
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<td>Pellet diameter</td>
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</tr>
<tr>
<td>Clad outer diameter</td>
<td>12.23 mm</td>
</tr>
<tr>
<td>Fuel effective length</td>
<td>1,467 mm</td>
</tr>
<tr>
<td>Fuel material</td>
<td>UO₂</td>
</tr>
<tr>
<td>Clad material</td>
<td>Zr-2</td>
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<tr>
<td>Fuel density</td>
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</tr>
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</table>

<table>
<thead>
<tr>
<th>(2) Fuel assembly</th>
<th>(4) Poison curtain</th>
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</thead>
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<tr>
<td>Fuel rod array</td>
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</tr>
<tr>
<td>Number of fuel rods per assembly</td>
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<tr>
<td>Fuel rod pitch</td>
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### TABLE II  Convergence history of power-void iteration

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<th>No. of power-void iteration</th>
<th>No. of Outer iteration</th>
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### TABLE III  Comparison of flow rate in IPA channels between calculation and measurement

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<td>5.29</td>
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<td>kg/sec</td>
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<tr>
<td></td>
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<td>%</td>
<td>+1.88</td>
<td>+0.95</td>
<td>-1.16</td>
</tr>
<tr>
<td>IPA HYDRO-ACE</td>
<td># 6</td>
<td>kg/sec</td>
<td>6.65</td>
<td>5.56</td>
<td>4.27</td>
</tr>
<tr>
<td>Error</td>
<td></td>
<td>kg/sec</td>
<td>6.52</td>
<td>5.35</td>
<td>4.27</td>
</tr>
<tr>
<td></td>
<td></td>
<td>%</td>
<td>-1.95</td>
<td>-3.78</td>
<td>-0.0</td>
</tr>
<tr>
<td>IPA HYDRO-ACE</td>
<td># 7</td>
<td>kg/sec</td>
<td>6.50</td>
<td>5.56</td>
<td>4.50</td>
</tr>
<tr>
<td>Error</td>
<td></td>
<td>kg/sec</td>
<td>6.55</td>
<td>5.41</td>
<td>4.35</td>
</tr>
<tr>
<td></td>
<td></td>
<td>%</td>
<td>-0.77</td>
<td>-2.70</td>
<td>-3.33</td>
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</tbody>
</table>

### TABLE IV  Dependency of coolant flow rate on heat production

<table>
<thead>
<tr>
<th>Location of Assembly</th>
<th>Normalized Heat Production Rate in Assembly</th>
<th>Coolant Flow Rate (kg/sec)</th>
<th>Nominal Value (%)</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>100</td>
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<tr>
<td>Calculated by STEADY-ACE</td>
<td></td>
<td></td>
<td>10.90</td>
</tr>
<tr>
<td>(12, 6)</td>
<td>1.349</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(11, 5)</td>
<td>1.003</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(15, 5)</td>
<td>0.508</td>
<td></td>
<td></td>
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<tr>
<td>Measured</td>
<td></td>
<td></td>
<td>10.90</td>
</tr>
<tr>
<td>IPA #4</td>
<td>6.50</td>
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</tr>
<tr>
<td>IPA #5</td>
<td>6.39</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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New Coarse-Mesh Diffusion and Transport Theory Methods for the Efficient Numerical Calculation of Multi-Dimensional Reactor Power Distributions* 

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ABSTRACT 

A nodal diffusion theory method based upon the use of local Green's functions is applied to several static and transient, multidimensional, fast and thermal reactor benchmark and design problems to verify its vastly superior accuracy and computational efficiency. It is demonstrated to be approximately one thousand times faster than conventional fine-mesh methods for comparable accuracies in three-dimensional applications. Two new nodal transport theory methods which are also based upon the use of local Green's functions are developed and tested on one-dimensional one-speed model problems and a one-dimensional eight group heterogeneous-design fast reactor problem to examine their computational efficiencies relative to conventional fine mesh (discrete-SN) methods. They are approximately an order of magnitude faster than the fine-mesh methods for the one-dimensional fast reactor problem studied. 

I. INTRODUCTION 

A set of coarse-mesh computational methods have been developed based upon the use of local Green's functions to convert differential equations in space (the neutron diffusion equation and the neutron transport equation) to sets of coupled local integral equations in space defined on computational-element volumes and surfaces (subdomains and their boundaries). 

Two of these methods,1-6 for coarse-mesh neutron diffusion calculations have already been extensively developed, tested and applied to numerous static and transient benchmark and design problems. The partial current balance method1-3,6,7 (PCBM) is extremely accurate, but due to the large number of variables per node and the related computational costs it has only been applied to one-dimensional and two-dimensional statics problems (even though the computational costs are still much lower6,7 than those required for modern fully-accelerated codes based upon finite difference methods). The nodal Green's function method4-8 (NGFM) is very accurate and very efficient; it therefore 

*This research was supported by the Electric Power Research Institute.
has been applied to a large number of static and transient benchmark and design problems. [It uses straightforward backward differencing of the time derivative of the flux and partial currents to obtain a (stable) implicit solution to the time-dependent equation for the transient problems combined with the reference cross section (or reference Green's function) method to treat feedback.]

The formal development of the nodal Green's function method for steady-state problems is reviewed in Sec. II. The NGFM formalism for time-dependent problems has been reported previously, as has the PCBM formalisms for time-dependent and steady-state problems. Extensive computational results for thermal and fast reactor benchmark and design problems are presented in Sec. III in which these methods are compared with other coarse-mesh methods with the finite element method and with standard finite difference methods.

Two generalizations of the nodal Green's function method which result in different formalisms for the numerical solution of the neutron transport equation on an extremely coarse mesh are also developed for high accuracy, high efficiency computations. The formalisms which lead to these methods, the discrete nodal transport method (DNTM) and the piecewise polynomial nodal transport method (PNTM), are developed in detail for the one-dimensional transport equation in Sec. IV and for the multidimensional transport equation in the Appendix. Computational results of these two methods for one-dimensional one-speed problems and for a one-dimensional eight-group heterogeneous fast reactor problem are presented in Sec. V.

Further developments which are ongoing are briefly described in Sec. VI in which related activities in areas involving other physical problems, viz. heat conduction and fluid flow, are also mentioned. Finally, conclusions based on the salient features of the results are summarized in the closing section.

II. DIFFUSION THEORY: THE NGFM FORMALISM

In this section, we briefly review the formalism for the nodal Green's function method; a more detailed development is given in References 6 and 8. We begin with the time-independent diffusion equation written in standard multigroup form:

\[-\nabla \cdot (r) + \sum_{g'=1}^{G} \left( \frac{1}{\lambda} \chi_g \nu_g f_g(r) + \chi_g S_{gg'}(r) \right) \phi_g(r), r \in V, g=1,...,G. \tag{1} \]

Assuming Cartesian geometry, we partition the reactor configuration \( V \) into an array of \( K \) homogeneous boxes \( V_k \). Integrating Eq. (1) over a box \( V_k \) yields the nodal balance equation, which we write in terms of the face-averaged partial currents:
\[
\sum_{u=x,y,z} \frac{1}{2a_u^k} \left[ J_{\text{out},k}(a_u^k) - J_{\text{in},k}(a_u^k) + J_{\text{out},k}(-a_u^k) - J_{\text{in},k}(-a_u^k) \right] \\
+ \Sigma^k_{\text{r}} \phi^k_{g} = \bar{q}^k_{g}, \quad k=1,\ldots,K, \quad g=1,\ldots,G,
\]

(2)

where the average (or nodal) fluxes and group sources are defined by

\[
\bar{\phi}^k_{g} \equiv \frac{1}{V_k} \int_{V_k} d^3r \phi(r)
\]

and

\[
q^k_{g} = \sum_{g'=1}^{G} \left[ \frac{1}{V_{g'}} \left( \Sigma^{f,k}_{g'} + \Sigma^{s,k}_{g'} \right) \right] \phi^k_{g'},
\]

(3a)

(3b)

respectively, and \(a_u^k, \ u=x,y,z\), denotes the node halfwidths in each direction. The face-averaged outgoing and incoming partial currents across the node surfaces perpendicular to the \(u\)-direction are given by

\[
J_{\text{out},k}(\pm a_u^k) = \left[ \frac{1}{V_{\text{gu}}} \phi^k_{\text{gu}}(u) \mp \frac{1}{2} \left( \frac{\partial}{\partial u} \phi^k_{\text{gu}}(u) \right) \right]_{u=\pm a_u^k},
\]

(4a)

\[
J_{\text{in},k}(\pm a_u^k) = \left[ \frac{1}{V_{\text{gu}}} \phi^k_{\text{gu}}(u) \mp \frac{1}{2} \left( \frac{\partial}{\partial u} \phi^k_{\text{gu}}(u) \right) \right]_{u=\pm a_u^k},
\]

(4b)

where \(\phi^k_{\text{gu}}(u)\) is a partially-integrated flux defined by

\[
\phi^k_{\text{gu}}(u) \equiv \frac{1}{4a_w^k a_v^k} \int_{-a_w^k}^{a_w^k} dw \int_{-a_v^k}^{a_v^k} dv \phi^k_g(u,v,w), \ u=x,y,z, \ \text{w} \neq u.
\]

(5)

Here \(v\) and \(w\) denote the two coordinate directions transverse to the \(u\)-direction; hence \(\phi^k_{\text{gu}}(u)\) \(u=\pm a_u^k\) represents the face-averaged fluxes on the surfaces perpendicular to the \(u\)-direction.

Equation (2) cannot be solved for the nodal fluxes without additional equations relating the surface partial currents to the interior fluxes. These relationships are developed from the set of three one-dimensional equations obtained by integrating Eq. (1) for each box over the two directions transverse to each coordinate direction. The transverse-integrated equations can be written in the form
\[
-d_k^2 \frac{d^2}{du^2} \phi_{gu}^k(u) + \sum_{g} \phi_{gu}^k(u) = q_{gu}^k(u) - L_{gu}^k(u),
\]

\(u=x,y,z, g=1,...,G, k=1,...,K,\)

where the partially-integrated source \(q_{gu}^k(u)\) is defined as in Eq. (5), and

\[
L_{gu}^k(u) \equiv -\frac{1}{4a_w^2 a_v^2} \int_{-a_w}^{a_w} dw \int_{-a_v}^{a_v} dv \int_{-a_w}^{a_w} dw' \int_{-a_v}^{a_v} dv' \frac{\partial^2}{\partial w^2} \delta_{gw}^k(u,v,v') \delta_{gw}^k(u,v,w') + \frac{\partial^2}{\partial v^2} \delta_{gw}^k(u,v,w) .
\]

The term \(L_{gu}^k(u)\) represents the combined \(u\)-dependent net leakage in the two directions transverse to the \(u\)-direction. Using Eqs. (4) the \(u\)-averaged value of the transverse leakage can be written in terms of the face-averaged partial currents in the two transverse directions.

Equation (6) is converted to an integral equation using the Green's function defined for the one-dimensional diffusion-removal operator on the left-hand side of that equation:

\[
-d_k^2 \frac{d^2}{du^2} \phi_{gu}^k(u|u_0) + \sum_{g} \phi_{gu}^k(u|u_0) = \delta(u-u_0),
\]

\(-a_u^k < u, u_0 < +a_u^k, u=x,y,z, g=1,...,G,\)

where \(\delta(u-u_0)\) is the Dirac delta function. [Alternatively, the formalism can be developed in terms of "reference" Green's functions calculated using reference values of the diffusion coefficient and removal cross section. This development thus eliminates the need to recalculate large numbers of different Green's functions frequently during a transient with feedback.] Multiplying Eq. (7) by \(G_{gu}^k(u|u_0),\) Eq. (8) by \(\phi_{gu}^k(u),\) subtracting the results, and then integrating over \(-a_u^k < u < +a_u^k\) yields, after rearrangement,

\[
\phi_{gu}^k(u) = \int_{-a_u^k}^{a_u^k} du_0 \ G_{gu}^k(u|u_0) \left[ Q_{gu}^k(u) - L_{gu}^k(u) \right]
\]

\(+ 2G_{gu}^k(u|a_u^k) \phi_{gu}^k(a_u^k) + 2G_{gu}^k(u|-a_u^k) \phi_{gu}^k(-a_u^k),\)

\(-a_u^k < u < +a_u^k, u=x,y,z, g=1,...,G, k=1,...,K.\)

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Using Eq. (9), an equation for the average outgoing partial currents is readily obtained:

\[ J_{\text{out},k}(\pm a_u^k) = \frac{1}{2} \phi_{\text{gu}}(\pm a_u^k) - J_{\text{in},k}(\pm a_u^k) \]

\[ = \int_{-a_u^k}^{a_u^k} du_x c_{\text{gu}}^k(\pm a_u^k|u_x) \left[ q_{\text{gu}}^k(u_x) - l_{\text{gu}}^k(u_x) \right] \]

\[ + \left[ g_{\text{gu}}^k(a_u^k|-a_u^k) - 1 \right] J_{\text{gu}}^k(\pm a_u^k) + g_{\text{gu}}^k(a_u^k|-a_u^k) J_{\text{gu}}^k(-a_u^k), \]

\[ u=x,y,z, \ g=1,...,G, \ k=1,...,K. \quad (10) \]

Equations (9) and (10) are exact local integral equations for the partially-integrated fluxes and face-averaged partial currents for each computational node. The coupling between nodes is achieved by requiring that the partial currents be continuous across the nodal boundaries.

Equations (9) and (10) are approximated using a local weighted residual procedure in which the partially-integrated group fluxes, group sources, and transverse leakages are expanded in quadratic polynomials. An equation for the expansion coefficients of the partially-integrated fluxes is obtained by substituting the flux, source, and leakage expansions into Eq. (9), weighting with simple polynomials, and then integrating over the \( u \)-direction from \(-a_u^k\) to \(+a_u^k\).

The result can be written in the following matrix form:

\[ \phi_{\text{gu}}^k = \left[ g_{\text{gu}}^k \right] \left( q_{\text{gu}}^k - l_{\text{gu}}^k \right) + 2g_{\text{gu}}^k J_{\text{in},k}(a_u^k) + 2g_{\text{gu}}^k J_{\text{in},k}(-a_u^k), \]

\[ (11) \]

where \( \phi_{\text{gu}}^k \), \( q_{\text{gu}}^k \), and \( l_{\text{gu}}^k \) are column vectors containing the expansion coefficients, \( G_{\text{gu}}^{uu} \) is a 3x3 matrix with entries given as double weighted moments of the Green's function, and the \( g_{\text{gu}}^k \) are column vectors with entries given as simple weighted moments of the Green's function evaluated at the surfaces \( u = \pm a_u^k \).

An equation for the outgoing partial currents is obtained by substituting the source and leakage expansions into Eq. (10):

\[ J_{\text{out},k}(\pm a_u^k) = \left[ a_{\text{gu}}^T \right] \left( q_{\text{gu}}^k - l_{\text{gu}}^k \right) + g_{\text{gu}}^k J_{\text{in},k}(a_u^k) + G_{\text{gu}}^k J_{\text{in},k}(-a_u^k), \]

\[ \text{(12)} \]

where \( G_{\text{gu}}^{uu} \) is a column vector, and the reflection \( R_{\text{gu}}^k \) and transmission \( T_{\text{gu}}^k \) coefficients are defined by

\[ R_{\text{gu}}^k \equiv G_{\text{gu}}^k(a_u^k|-a_u^k) - 1 \quad (13a) \]

\[ T_{\text{gu}}^k \equiv G_{\text{gu}}^k(a_u^k|-a_u^k). \quad (13b) \]
Explicit expressions for the elements of the matrices appearing in Eqs. (11) and (12) are given in Appendix C of Reference 6.

The expansion coefficients for the transverse leakage are computed using the quadratic approximation introduced in the context of the nodal expansion method19 and later implemented in other recently developed nodal schemes. In calculating these coefficients, it is assumed that the quadratic polynomial also extends over the two nodes k− and k+ adjacent to the kth node in the minus and plus u-direction. The average values \( \overline{L}_{gu}^{k−} \), \( \overline{L}_{gu}^{k+} \), and \( L_{gu}^{k+} \) of the u-dependent transverse leakages in these three nodes can be calculated in terms of the average partial currents on the faces parallel to the u-direction. These three average leakages thus uniquely determine the coefficients in the quadratic expansion: the leading coefficient is simply the average leakage \( L_{gu}^{k} \) in the center node, while the two remaining coefficients are calculated by requiring that the quadratic polynomial yield the proper average values \( \overline{L}_{gu}^{k−} \) and \( L_{gu}^{k+} \) when integrated separately over each of the adjacent nodes, i.e.

\[
\frac{1}{2a_u} \int_{-a_u-2a_u}^{-a_u} du \ L_{gu}^{k−}(u) \equiv \overline{L}_{gu}^{k−}
\]

\[
\frac{1}{2a_u} \int_{+a_u}^{+a_u+2a_u} du \ L_{gu}^{k+}(u) \equiv L_{gu}^{k+}
\]

For nodes adjacent to an outer reactor boundary, the quadratic coefficients are calculated such that the transverse leakage at the reactor boundary is identically zero.

The steady-state eigenvalue problem is solved using a fission source iteration procedure. At each outer iteration, the one-dimensional partial current equations, Eq. (10), are solved using a single Gauss-Seidel iteration on each x-, y-, and z-line of the three-dimensional mesh. The transverse leakage contribution to the effective group source is updated using the most recently calculated values for the partial currents. The expansion coefficients for the partially-integrated fluxes are updated using Eq. (9), and are normalized to the nodal fluxes calculated from Eq. (3). This procedure is repeated for each energy group. The outer iterations are accelerated using a coarse-mesh rebalance technique and asymptotic source extrapolation.20

For transient problems, the time-dependent equations are discretized using a "time-integrated" approximation to the delayed neutron precursor equations in combination with a fully implicit approximation21 to the remaining equations for the nodal fluxes, flux expansion coefficients, and the partial currents.
III. DIFFUSION THEORY: NUMERICAL RESULTS FOR THERMAL AND FAST REACTOR PROBLEMS

The nodal Green's function method (NGFM) developed in the previous section has been applied to a large number of steady-state and transient reactor calculations. In this section, we present results for three two-group light water reactor problems and for an eight-group heterogeneous-design fast reactor.

The Two-Dimensional Biblis PWR Test Problem

The Biblis test problem\(^6,22\) is representative of an actual operating pressurized water reactor (PWR) with a "checkerboard" fuel loading. The multi-zone core contains seven different types of fuel assemblies with dimensions of 23.1226 cm. This problem is highly non-separable; hence it represents a severe challenge to any coarse-mesh method. The PCBM and NGFM results for this problem are summarized in Table I. Here \(\varepsilon_{\text{max}}\) is the maximum error in the assembly-averaged power densities. The execution times are for the CYBER 175 computer. These results exhibit the rapid convergence of the NGFM to the reference solution as the mesh spacing is decreased. We note that even for this very difficult problem, the results obtained using the NGFM on the assembly-size mesh are very accurate. Those obtained using the PCBM on this mesh are even more accurate; however this latter method requires substantially more computing time.

<table>
<thead>
<tr>
<th>Method</th>
<th>Mesh Spacing (cm), Nodes per Assembly</th>
<th>Eigenvalue</th>
<th>(\varepsilon_{\text{max}}) (%)</th>
<th>Execution Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NGFM</td>
<td>23.1226, (1x1)</td>
<td>1.025248</td>
<td>1.7</td>
<td>1.9</td>
</tr>
<tr>
<td>NGFM</td>
<td>11.5672, (2x2)</td>
<td>1.025112</td>
<td>0.15</td>
<td>5.0</td>
</tr>
<tr>
<td>NGFM</td>
<td>5.7806, (4x4)</td>
<td>1.025103</td>
<td>0.03</td>
<td>15.2</td>
</tr>
<tr>
<td>PCBM</td>
<td>23.1226, (1x1)</td>
<td>1.025044</td>
<td>0.60</td>
<td>12.8</td>
</tr>
</tbody>
</table>

Reference\(^a\) 1.025103

\(^a\)Reference solution: 3.8537 cm (6x6) NGFM Calculation

The Three-Dimensional IAEA Benchmark Problem

The well-known IAEA benchmark problem\(^16\) is a simplified two- or three-dimensional model of a pressurized water reactor. The two-zone core consists of 177 fuel assemblies with dimensions of 20 cm on a side and is reflected radially and axially by 20 cm of water. Nine fully-inserted control rods and four partially-inserted control rods are each represented as a smeared
absorber within a single homogenized fuel assembly. Results for the three-dimensional IAEA benchmark problem are compared in Table II in which it can be seen that the maximum error in the assembly powers for the NGFM calculation is smaller than that for the other calculations. The 20 cm NGFM calculation is more accurate than the 1.67 cm finite difference result; yet it required only 1 CPU minute compared to the 6 CPU hours for the finite difference calculation. Taking into consideration the fact that the computer on which the finite difference calculation was done is twice as fast as the one on which the NGFM calculation was done, the fact that the finite difference calculation was done using the fully converged solution on the next coarser spatial mesh as a starting guess, and the fact that the results of the finite difference calculation are less accurate than those of the NGFM calculation, it appears that for comparable practical accuracy requirements, the NGFM is about 1000 times as fast as conventional finite-difference methods for this three-dimensional thermal reactor problem. Table II also shows that the NGFM is also considerably more efficient than the finite element method for this problem.

### TABLE II

Comparison of Results for the Three-Dimensional IAEA Benchmark Problem

<table>
<thead>
<tr>
<th>Method</th>
<th>Reference $\epsilon_{\text{max}}$</th>
<th>Execution Times(s)</th>
<th>Computer</th>
<th>Symmetry</th>
<th>Point-wise Convergence</th>
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</thead>
<tbody>
<tr>
<td>Analytic Method (QUANDRY)</td>
<td>10.11</td>
<td>0.7</td>
<td>29</td>
<td>IBM 370/168</td>
<td>1/8 core</td>
</tr>
<tr>
<td>Finite Difference Method</td>
<td></td>
<td></td>
<td></td>
<td>IBM 370/195</td>
<td>1/4 core</td>
</tr>
<tr>
<td>(VENTURE )</td>
<td>16</td>
<td>2.1</td>
<td>21,600</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Finite Element Method</td>
<td></td>
<td></td>
<td></td>
<td>IBM 370/195</td>
<td>1/8 core</td>
</tr>
<tr>
<td>(FEM3D )</td>
<td>16</td>
<td>4.0</td>
<td>82,800</td>
<td>B-6700</td>
<td></td>
</tr>
<tr>
<td>Nodal Expansion Method</td>
<td>12.13</td>
<td>0.9</td>
<td>50</td>
<td>CDC 6600</td>
<td>1/8 core</td>
</tr>
<tr>
<td>Nodal Green's Fuction</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Method</td>
<td>4.6</td>
<td>0.4</td>
<td>62</td>
<td>CYBER 175</td>
<td>1/4 core</td>
</tr>
<tr>
<td>NODLEG Method</td>
<td>14</td>
<td>1.0</td>
<td>672</td>
<td>CDC 6500</td>
<td>1/4 core</td>
</tr>
</tbody>
</table>

The Three-Dimensional LMW Kinetics Test Problem

This problem, originally introduced by Langenbuch, Maurer, and Werner16 (LMW), represents an operational transient in a model light water reactor with assembly dimensions of 20 cm. The transient is initiated by withdrawing a bank of four partially-inserted control rods at a rate of 3 cm/s over $0 \leq t \leq 26.7$ s. A second bank of control rods is inserted at the same rate over $7.5 \leq t \leq 47.5$ s. The transient is followed for 60 s.
The NGFM and CUBBOX\textsuperscript{15} results shown in Table III were obtained using a uniform 20 cm mesh spacing with various time stepsizes. These results demonstrate that for comparable temporal truncation errors, the time steps which can be used with the fully implicit NGFM are roughly ten times larger than those which can be used in the alternating direction method\textsuperscript{15} used in the CUBBOX code. Hence, although CUBBOX requires less execution time than the NGFM when both methods use a time step of 1.0 s, it is clear that the NGFM solution is considerably more accurate. For comparable temporal accuracy (e.g. NGFM with $\Delta t = 10$ s, CUBBOX with $\Delta t = 1.0$ s) the execution times (30 s and 45 s, respectively) are also comparable. It is apparent from the results in Table III that the NGFM and CUBBOX solutions do not converge to the same solution in the limit as the time step size goes to zero. This behavior is due to the differences in the usual errors resulting from the respective spatial approximations to the diffusion equation, as well as to the differences in the representation of a control rod which is partially inserted into a mesh box. While the CUBBOX method represents the partially-inserted rod explicitly, the present formulation of the NGFM requires that the cross sections be spatially constant within a mesh box. Hence the NGFM code computes a single constant cross section for the partially-rodded box by flux weighting the cross sections in the controlled and un-controlled regions of the box. It is likely that this difference in the treatment of the partially-rodded box represents the dominant contribution to the 5\% difference in the temporally-converged NGFM and CUBBOX mean power densities at $t = 30.0$ s.

Two-Dimensional Heterogeneous-Design Fast Reactor Problems

The NGFM has also been applied to the determination of $k_{\text{eff}}$ and the power distribution in a beginning-of-life, no-control, radially heterogeneous 1000 MWe LMFBR design\textsuperscript{23}. The two-dimensional hexagonal fuel assembly representation of this core\textsuperscript{24} is shown in Fig. 1. Because the NGFM is presently limited to Cartesian geometries, the equivalent x-y layout shown in Fig. 2 was developed by retaining the assembly pitches in the x-direction and adjusting the assembly widths in the y-direction so that their areas were preserved. The original hexagonal layout was calculated\textsuperscript{25} using the DIF2D finite-difference code\textsuperscript{26}. The x-y layout has been calculated\textsuperscript{24} using the NGFM with nodes that were equal in height to an assembly y-dimension and equal in width to one half of an assembly x-dimension, and it was also calculated\textsuperscript{27} using the two-dimensional option of the DIF3D finite-difference code.\textsuperscript{28} The NGFM eigenvalue was $k_{\text{eff}} = 0.99784$, and the calculated two-dimensional power distribution along the y-axis is plotted in Fig. 3. Four DIF3D calculations\textsuperscript{27} were done using a sequence of spatial meshes: the same mesh (1x1) as was used in the NGFM calculations, one-half that mesh in each direction (2x2), one-quarter in each direction (4x4), and one-eighth in each direction (8x8). The eigenvalue errors in the NGFM 1x1 calculation and the DIF3D 8x8 calculation were $2.2 \times 10^{-4}$ and $1.0 \times 10^{-4}$, respectively. However, the NGFM calculation required 51 s on the University of Illinois CYBER 175 whereas the DIF3D calculation required 764 s on the ANL IBM 370/195 which is
Fig. 1: Original hexagonal lay-out of beginning-of-life, no control, radially heterogeneous 1000 MWe LMFBR core.
Fig 2: Equivalent x-y lay-out of radially heterogeneous 1000 MWe LMFBR core.
Fig. 3: Power distribution by assembly along the y-axis of the equivalent x-y core calculated using the two-dimensional diffusion theory nodal Green's function method (NGFM) ($k_{eff}=0.99784$). [The ordinate must be multiplied by 0.075647 to obtain power fractions in per cent.]
approximately twice as fast. Hence the NGFM is about 30 times as fast as a highly efficient finite difference code for a comparable accuracy requirement for this rather substantial design problem. Actually a fairer comparison would be between the NGFM 1x1 calculation and a DIF3D 6x6 calculation. Although a DIF3D 6x6 calculation was not done, it is reasonable to expect that such a calculation would have an accuracy of $1.8 \times 10^{-4}$ and would require a computing time of ~400 s; hence, the NGFM is about 15 times more efficient than the DIF3D finite difference code.

Comparison of Results for the Three-Dimensional LMW Kinetics Test Problem

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*Execution times (CYBER 175):* 30 s for $\Delta t = 10.0$ s 37 s for $\Delta t = 5.0$ s 83 s for $\Delta t = 2.0$ s 131 s for $\Delta t = 1.0$ s

*Execution time (IBM 360/91):* 45 s for $\Delta t = 1.0$ s
IV. TRANSPORT THEORY: THE ONE-DIMENSIONAL DNTM AND PNTM FORMALISMS

In this section, we develop the formalism for the discrete nodal transport method (DNTM) and the polynomial nodal transport method (PNTM) in slab geometry. These methods draw on ideas originally proposed several years ago, and more recently applied to the solution at the Boltzmann equation for rarefied gas dynamics. They are also related to some of the ideas which are utilized in a recently developed thermal reactor cell homogenization code. The extension of both the DNTM and PNTM to multidimensional (Cartesian) geometries is discussed in the Appendix.

As in the NGFM development, we partition the spatial domain into $K$ homogeneous nodes and then write the transport equation in multigroup form for the $k$-th node:

$$\mu \frac{\partial}{\partial x} \psi_g^k(x, \mu) + \sum_g \Sigma_g^T \psi_g(x, \mu) = a_k^x S^k_g(x, \mu), \quad -1 < x < 1,$$

$$k = 1, \ldots, K, \quad g = 1, \ldots, G,$$  \hspace{1cm} (14)

where the dimensionless variables $x$ and $\Sigma_g^T$ are written in units of the node half-width $a_k^x$. We consider only isotropic scattering, although the extension to general anisotropic scattering is straightforward. Hence, in the absence of external sources, the group source term is

$$S^k_g(x) = \frac{1}{2} \sum_{g' = 1}^G \left( \frac{\Sigma_{g'} k}{\Sigma_{g'} g' k} \right) \phi_g^{k'}(x),$$  \hspace{1cm} (15)

where $\psi_g(x)$ is the scalar flux. Equation (14) is converted to two coupled local integral equations using the adjoint Green's function for the adjoint streaming-removal operator. This procedure is equivalent to simply integrating Equation (14) separately for $\mu > 0$ and $\mu < 0$ over the $k$-th node. The resulting integral equations are

$$\psi^+_g(x, \mu) = a_x^x \int_{-1}^x dx_0 \frac{1}{\mu} e^{-\Sigma_g^T (x-x_0)/\mu} S^+_g(x_0) + \psi^+_g(-1, \mu) e^{-\Sigma_g^T (1)/\mu},$$  \hspace{1cm} (16)

$$\psi^-_g(x, \mu) = a_x^x \int_{-1}^x dx_0 \frac{1}{|\mu|} e^{-\Sigma_g^T (x-x_0)/|\mu|} S^-g(x_0) + \psi^-_g(1, \mu) e^{-\Sigma_g^T (1)/|\mu|},$$  \hspace{1cm} (17)

where the node index $k$ has been omitted and

$$\psi^+_g(x, \mu) = \left\{ \begin{array}{ll} \psi^+_g(x, \mu), & \mu > 0 \\ 0, & \mu < 0 \end{array} \right.$$  \hspace{1cm} (18)
The two necessary additional equations for the surface angular fluxes $\psi_g^+(1,\mu)$ and $\psi_g^-(1,\mu)$ are obtained by evaluating Eqs. (16) and (17) at $x=+1$ and $x=-1$, respectively:

$$
\psi_g^+(1,\mu) = a_x \int_{-1}^{1} dx_0 \left( \frac{1}{\mu} e^{-\Sigma_T^+(1-x_0)/\mu} S_g^+(x_0) \right) + \psi_g^-(1,\mu)e^{-2\Sigma_T^+/\mu} 
$$

(18)

$$
\psi_g^-(1,\mu) = a_x \int_{-1}^{1} dx_0 \left( \frac{1}{\mu} e^{\Sigma_T^-(1+x_0)/\mu} S_g^-(x_0) \right) + \psi_g^+(1,\mu)e^{2\Sigma_T^-/\mu} 
$$

(19)

Equations (16)-(19) form the basis for both the DNTM and the PNTM. Following the application of the respective approximation procedures, the approximate forms of Eqs. (16) and (17) are used to construct the spatial shape at the flux (and hence the shape of the source) in the interior of the node; this source shape is then used in the approximate forms of Eqs. (18) and (19) to calculate the angular fluxes at the nodal surfaces. The nodes are coupled by requiring that the angular fluxes be continuous across the nodal interfaces.

The Discrete Nodal Transport Method (DNTM)

The discrete nodal transport method (DNTM) is obtained by solving Eqs. (16) - (19) along discrete ordinates which can be chosen as the standard Gauss-Legendre points. If $N$ is the number of ordinates, we refer to this approach as a $DN_N$ approximation. (We use $DN_N$ rather than $SN_N$ in order to avoid confusion with the standard discrete $SN_N$ methods in which the spatial approximations are quite different than those used in the DNTM.) The space-dependence of the fluxes for each ordinate $\mu_n$, and the group sources, are expanded in Legendre polynomials in each node

$$
\psi_g^+(x,\mu_n) = \sum_{j=0}^{J} \frac{2j+1}{2} \psi_g^+(\mu_n) P_j(x), \mu_n > 0 \quad \left\{ \begin{array}{c} -1 \leq x \leq 1 \end{array} \right. 
$$

(20a)

$$
S_g(x) = \sum_{j=0}^{J} \frac{2j+1}{2} S_g P_j(x) 
$$

(20b)

The source expansion coefficients, $S_{gj}$, are related to the expansion coefficients for the scalar flux via Eq. (15). An equation for the $\psi_{gj}(\mu_n)$ is obtained by substituting Eqs. (20) into Eq. (16), weighting with $P_i(x)$, $i=0, ..., J$, and then integrating over $x$ from -1 to +1. The result is

$$
\psi_g^+(\mu_n) = \left[ c_{gxx}^+(\mu_n) \right] S_g + G_{g}^x(\mu_n) \psi_{g}^-(1,\mu_n), \quad \mu_n > 0, 
$$

(21)

- 397 -
where \( \psi_g(\mu_n) \) and \( S_g \) are column vectors of expansion coefficients, and the entries of the \( J \times J \) matrix \( [G_{g}^{xx}(\mu_n)] \) and the vector \( G_{g}^{xx}(\mu_n) \) are

\[
\left[ G_{g}^{xx}(\mu_n) \right]_{ij} = \frac{2j+1}{2} a_x \int_{-1}^{1} dx P_i(x) \int_{-1}^{1} dx \frac{1}{\mu_n} e^{-\Sigma(x-x_0)/\mu_n} p_j(x_0)
\]

(22a)

\[
\left[ G_{g}^{xx}(\mu_n) \right]_i = \int_{-1}^{1} dx P_i(x) e^{-\Sigma(x+1)/\mu_n}
\]

(22b)

(Here we have dropped the superscript and subscript on the total cross section \( \Sigma_g \).) Substituting Eq. (20b) into Eq. (18) yields

\[
\psi_g^+(1,\mu_n) = [G_g^{xx}(\mu_n)]^T S_g + T_g(\mu_n) \psi_g^+(-1,\mu_n), \quad \mu_n > 0,
\]

(23)

where the entries of the column vector \( [G_g^{xx}(\mu_n)] \) are defined by

\[
\left[ G_g^{xx}(\mu_n) \right]_j = \frac{2j+1}{2} a_x \int_{-1}^{1} dx e^{-\Sigma(x-x_0)/\mu_n} p_j(x_0)
\]

(24a)

and the transmission coefficient along ordinate \( \mu_n \) is given by

\[
T_g(\mu_n) \equiv e^{-2\Sigma/\mu_n}
\]

(24b)

Analogous equations for \( \psi_g(-\mu_n) \) and \( \psi_g(-1,\mu_n), \mu_n < 0 \), are developed by substituting the appropriate expansions into Eqs. (17) and (19).

The approximate equations are solved via a standard inner (in-group scattering) and outer (fission source) iteration procedure which utilizes directed sweeps through the space-angle mesh analogous to those employed in standard explicit \( S_n \) calculations. Both the inner and the outer iterations are accelerated using coarse-mesh rebalancing.

The Polynomial Nodal Transport Method (PNTM)

Piecewise polynomial expansions in angle can be used instead of projection onto discrete ordinates to approximate the angular dependence in Eqs. (16)-(19). To do this, the angular domain \(-1 \leq \mu \leq +1\) is partitioned into \( M \) (\( M \) even) mesh cells or angular elements such that \( \Delta \mu_m \equiv [\mu_m, \mu_{m+1}] \). Letting \( \bar{\mu}_m \equiv \frac{1}{2} (\mu_m + \mu_{m+1}) \) and \( \delta \mu_m \equiv \frac{1}{2} (\mu_{m+1} - \mu_m) \), we write Eqs. (16) and (18) for \( 0 < \mu < \Delta \mu_m \) and then make the following local expansions in Legendre polynomials:
\[
\psi^+_g(x, \mu) = \sum_{j=0}^{J} \frac{2j+1}{2} \sum_{n=0}^{2n+1} \psi^+_{gjn} P^n_j(x) P^n_m(\frac{\mu-\bar{\mu}}{\delta\mu}), \quad -1 < x < 1
\]
\[
\psi^+_{\pm}(\pm\mu, \mu) = \sum_{n=0}^{NS} \frac{2n+1}{2} \psi^+_{g(n)}(\pm1) P^n_m(\frac{\mu-\bar{\mu}}{\delta\mu}), \quad 0 < \mu < \Delta\mu_m
\]

where the angular subscripts on \( \mu_m \) and \( \delta\mu_m \) have been suppressed, and \( NV \) and \( NS \) are the orders of the angular expansions used within the spatial node and on the nodal surfaces, respectively. For the case of isotropic scattering considered here, only the coefficients \( \psi^+_{g0} \) are required in order to construct the group source; the higher order angular coefficients are needed only if the angular distribution of the flux within the node is desired at the end of the calculation. The arguments of the Legendre polynomials in angle are chosen in order to preserve orthogonality over the partial range \( \mu_m < \mu < \mu_m+1 \). We refer to an angular approximation using \( M \) angular nodes with an order \( N = NS \) angular expansion on the nodal surfaces as the \( MP_N \) approximation. Hence the \( 2P_N \) approximation is simply a double \( P \) expansion of the surface angular flux.

The expansion coefficients shown in Eqs. (25) are determined using a local weighted residual procedure. Substituting Eq. (25) and (20b) into Eq. (16), and then operating on the result with

\[
\int_{-1}^{1} \int_{-1}^{1} dx \ P^n_j(x) \int_{-1}^{1} d\mu \ P^n_m(\frac{\mu-\bar{\mu}}{\delta\mu}), \quad i=0, \ldots, J, \quad \ell=0, \ldots, NV,
\]

yields

\[
\psi^+_g = \begin{bmatrix} \ell = 1 \\ \ell = 0 \end{bmatrix} F_{g}^{\ell x} S_g + \begin{bmatrix} \ell = 1 \\ \ell = 0 \end{bmatrix} \psi^+_{g(-1)},
\]

where \( \psi^+_g, S_g, \) and \( \psi^+_{g(-1)} \) are column vectors with lengths \( J+NV, J, \) and \( NS, \) respectively. The matrix [\( F_{g}^{\ell x} \)] has dimensions \( (J+NV) \times J \) and its entries are defined by

\[
\left[ F_{g}^{\ell x} \right]_{ij} = \frac{a}{\delta \mu} \frac{2j+1}{2} \int_{-1}^{1} dx \ P^n_i(x) \int_{-1}^{1} dx_0 \ P^n_j(x_0) \int_{-1}^{1} d\mu \ P^n_m(\frac{\mu-\bar{\mu}}{\delta\mu})
\]

\[
\cdot \left[ 1 + \Sigma(x-x_0)/\mu \right], \quad i,j=0, \ldots, J, \quad \ell=0, \ldots, NV.
\]

The matrix [\( F_{g}^{\ell x} \)] has dimensions of \( (J+NV) \times NS, \) and its entries are defined by

\[
\left[ F_{g}^{\ell x} \right]_{i\ell n} = \frac{1}{\delta \mu} \frac{2n+1}{2} \int_{-1}^{1} dx \ P^n_i(x) \int_{-1}^{1} d\mu \ P^n_m(\frac{\mu-\bar{\mu}}{\delta\mu}) e^{-\Sigma(x+1)/\mu}
\]

\[
\cdot \left[ \ell = 1 \\ \ell = 0 \right], \quad i=0, \ldots, J, \quad \ell=0, \ldots, NV, \quad n=0, \ldots, JS.
\]
Substituting Eqs. (25b) and (20b) into Eq. (18), and operating on the result with
\[
\int_{\mu_m}^{\mu_{m+1}} d\mu \, p_{\xi} \frac{(\mu - \mu)}{(\delta \mu)} \cdot , \quad \xi = 0, \ldots, \text{NS},
\]
yields
\[
\psi_1^+(1) = \left[ F_x^g \right] s_g + \left[ T_g \right] \psi_1^+(-1) .
\]  \hspace{1cm} (28)

Here \([F_x^g]\) is a matrix with dimensions \(
\text{NS} \times \text{J}\), and entries defined by
\[
\left[ F_x^g \right]_{\xi j} = \frac{a}{\delta \mu} \left( \frac{2n+1}{2} \right) \int_{\mu_m}^{\mu_{m+1}} d\mu \, p_{\xi} \frac{(\mu - \mu)}{(\delta \mu)} \int_{-1}^{1} dx_0 \, p_j(x_0) \frac{1}{\mu} e^{-\Sigma(1-x_0)/\mu}
\]
\[
\xi = 0, \ldots, \text{NS}, \quad j = 0, \ldots, \text{J} . \]  \hspace{1cm} (29a)

Finally the transmission matrix \([T_g]\) has dimensions \(
\text{NS} \times \text{NS}\), and entries given by
\[
\left[ T_g \right]_{\xi n} = \frac{1}{\delta \mu} \left( \frac{2n+1}{2} \right) \int_{\mu_m}^{\mu_{m+1}} d\mu \, p_{\xi} \frac{(\mu - \mu)}{(\delta \mu)} p_n \frac{(\mu - \mu)}{(\delta \mu)} e^{-2\Sigma/\mu}
\]
\[
\xi = 0, \ldots, \text{NS}, \quad n = 0, \ldots, \text{NS} . \]  \hspace{1cm} (29b)

An analogous procedure is followed in approximating Eqs. (17) and (19).

All the matrix elements in Eqs. (27) and (29) are evaluated analytically in terms of the exponential integral functions
\[
E_n(x) \equiv \int_0^1 d\mu \, \mu^{n-2} e^{-x/\mu} .
\]

The PNTM equations developed here are solved using an iterative procedure similar to that used to solve the DNTM equations. Since both methods are explicit, neither the discrete angular fluxes in the DNTM, nor the angular flux expansion coefficients in the PNTM need be stored during the calculation.
V. TRANSPORT THEORY: NUMERICAL RESULTS FOR ONE-DIMENSIONAL MODEL AND FAST REACTOR PROBLEMS

In this section, we present numerical results obtained for two one-dimensional one-group model problems and for a one-dimensional eight group heterogeneous-design fast reactor.

One-Group Critical Slab Problems

Table IV gives the values of \( c \), the number of secondary neutrons per collision for criticality, calculated for two one-dimensional slabs using the DNTM and PNTM. These results were obtained using a quadratic expansion of the interior fluxes. The convergence of each method is studied by simultaneously refining the spatial mesh and the angular approximation. These results show that the \( 2P_2 \) approximation (i.e. a double \( P_2 \) expansion of the surface angular fluxes) with 2 spatial nodes is of comparable accuracy to the \( D_{16} \) calculation with 16 spatial nodes. The very high accuracy of the PNTM is evident in the results for the 1 mean free path (mfp) slab; here the \( 16P_2 \) calculation with 16 spatial nodes is nearly 4 orders of magnitude more accurate than the \( D_{16} \) calculation with 16 spatial nodes.

\[
\begin{array}{|c|c|c|c|c|}
\hline
\text{Number of Spatial Nodes} & \text{Angular Approximation} & \text{1 mfp Slab} & \text{10 mfp Slab} \\
 & & \text{c} & \text{Error} & \text{c} & \text{Error} \\
\hline
2 & D_2 & 1.88663519 & 1.68 \times 10^{-1} & 1.02651894 & 1.60 \times 10^{-2} \\
4 & D_4 & 1.68567280 & 4.35 \times 10^{-2} & 1.02503150 & 1.48 \times 10^{-4} \\
8 & D_8 & 1.62686654 & 7.11 \times 10^{-3} & 1.02491152 & 3.14 \times 10^{-5} \\
16 & D_{16} & 1.61733470 & 1.21 \times 10^{-3} & 1.02488693 & 7.38 \times 10^{-6} \\
\hline
2 & 2P_2 & 1.61568679 & 1.91 \times 10^{-4} & 1.02488820 & 8.62 \times 10^{-6} \\
4 & 4P_2 & 1.61546214 & 5.18 \times 10^{-5} & 1.02488104 & 1.63 \times 10^{-6} \\
8 & 8P_2 & 1.61536750 & -6.83 \times 10^{-6} & 1.02488010 & 7.12 \times 10^{-7} \\
16 & 16P_2 & 1.61537809 & 2.67 \times 10^{-7} & 1.02487954 & 1.66 \times 10^{-7} \\
\hline
\end{array}
\]

\( ^a\)Exact Eigenvalues\(^32\): 1.61537852 - 1.02487937 -

\( ^b\)With quadratic expansions of node-interior spatial fluxes.
Multi-Region One-Group Model Problem

The geometry in this problem is a one-dimensional slab with four regions of different composition. The cross sections and source strengths are shown in Fig. 4. The left boundary condition is reflecting and the right boundary condition is vacuum. This problem has proven to be a severe test of standard diamond difference schemes. The solutions plotted in Fig. 4 were obtained using the D8 angular approximation with 40 and 8 spatial nodes. The spatial distribution of the flux within the node is calculated by simply evaluating the quadratic expansion used to approximate the interior fluxes. The 8-spatial-node calculation deviates from the fine-mesh calculation only in the third node (2 < x < 3 cm), where the single quadratic representation of the flux cannot accurately reproduce the severe flux gradients near the surfaces of the node. Both solutions compare well with other published solutions to this problem and also to a 2P2 PNTM calculation. The 8-node D8 calculation using coarse-mesh rebalance acceleration on the same mesh required 15 iterations and 0.04 s on a CYBER 175 computer in order to achieve $10^{-6}$ pointwise convergence.

One-Dimensional (Theta-Homogenized) Heterogeneous-Design Fast Reactor Problem

The one-dimensional fast reactor problem studied here was obtained by theta-homogenizing the hexagonal layout shown in Fig. 1, and then treating the resulting cylindrical problem in slab geometry. In Table V(a), we compare results obtained via the DNTM with those obtained via the widely-used discrete ordinates code ANISN and those obtained via ILLSN (Illinois $S_N$), a special purpose discrete $S_N$ program with the same acceleration schemes used in the DNTM program. The DNTM calculations were done using a quadratic expansion of the node-interior fluxes. Since both methods, the DNTM and the two discrete $S_N$ codes, used two angular quadrature points, the results in Table V(a) serve as a comparison of the spatial convergence of the two methods. All execution times are for the CYBER 175. The 4 nodes-per-assembly DNTM eigenvalue (and the zero-mesh-size extrapolated ILLSN eigenvalue which agrees with it) was taken as the reference (spatially-converged) eigenvalue. (Due to incomplete iterative convergence, the ANISN eigenvalues are low by $\sim 2 \times 10^{-5}$. ) The errors in the DNTM calculations using 1 and 2 nodes per assembly with respect to this reference eigenvalue are $2.9 \times 10^{-5}$ and $2. \times 10^{-6}$, respectively, while the error in the ANISN calculation with 20 nodes per assembly is $4.0 \times 10^{-5}$. Hence the DNTM is 100 times faster (2.7 s vs. 263.3 s) than ANISN for comparable eigenvalue errors ($2.9 \times 10^{-5}$ vs. $4.0 \times 10^{-5}$).

The spatial and angular convergence of the DNTM and PNTM are compared in Table V(b). For the DNTM, the D16 approximation with 2 nodes per assembly is required in order to reduce the eigenvalue error to $< 1.0 \times 10^{-5}$. (The $< 1.0 \times 10^{-5}$ error in the D8 calculation with 1 node per assembly results from a fortuitous cancellation of the error components due to the spatial and angular approximations.) Eigenvalue convergence to within $1.0 \times 10^{-5}$ is achieved with the PNTM using 2 nodes per assembly with the 2P2 angular approximation. These DNTM and PNTM calculations required 19.6 s and 7.7 s, respectively; hence, for
Fig. 4. Scalar Flux for the One-Group Multi-Region Model Problem.
comparable accuracy, the PNTM is roughly twice as fast as the DNTM for this problem. Furthermore, in view of the results of the comparison between the DNTM and the ANISN and ILLSN calculations, it is also likely that for comparable accuracy, the PNTM is at least 200 times faster than ANISN and 12 times faster than ILLSN.

Table V
Transport Theory Results for the One-Dimensional (Theta-Homogenized) Heterogeneous-Design Fast Reactor Problem

<table>
<thead>
<tr>
<th>Number of Nodes Per Assembly</th>
<th>DNTM(S2) k-eff</th>
<th>CPU(s)</th>
<th>ANISN(D2) k-eff</th>
<th>CPU(s)</th>
<th>ILLSN(S2) k-eff</th>
<th>CPU(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.998144</td>
<td>2.7</td>
<td>0.996086</td>
<td>28.7</td>
<td>0.996108</td>
<td>1.9</td>
</tr>
<tr>
<td>2</td>
<td>0.998117</td>
<td>3.7</td>
<td>0.997584</td>
<td>36.3</td>
<td>0.997605</td>
<td>3.7</td>
</tr>
<tr>
<td>4</td>
<td>0.998115</td>
<td>8.6</td>
<td>0.997966</td>
<td>75.3</td>
<td>0.997987</td>
<td>6.9</td>
</tr>
<tr>
<td>8</td>
<td>0.998013</td>
<td>102.1</td>
<td>0.998033</td>
<td>8.8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.998075</td>
<td>263.3</td>
<td>0.998095</td>
<td>16.5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Due to incomplete iterative convergence, the ANISN eigenvalues are low by -2x10^-5.

b) DNTM and PNTM Results

<table>
<thead>
<tr>
<th>Number of Nodes Per Assembly</th>
<th>Angular Approximation</th>
<th>k-eff</th>
<th>Error</th>
<th>CPU(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>D₂</td>
<td>0.998144</td>
<td>-3.0x10^-3</td>
<td>2.7</td>
</tr>
<tr>
<td>1</td>
<td>D₄</td>
<td>1.001072</td>
<td>-1.2x10^-4</td>
<td>3.3</td>
</tr>
<tr>
<td>1</td>
<td>D₈</td>
<td>1.001199</td>
<td>&lt;1.0x10^-5</td>
<td>5.4</td>
</tr>
<tr>
<td>1</td>
<td>D₁₆</td>
<td>1.001213</td>
<td>2.4x10^-5</td>
<td>9.5</td>
</tr>
<tr>
<td>1</td>
<td>D₁₆</td>
<td>1.001213</td>
<td>2.4x10^-5</td>
<td>9.5</td>
</tr>
<tr>
<td>2</td>
<td>D₁₆</td>
<td>1.001185</td>
<td>&lt;1.0x10^-5</td>
<td>19.6</td>
</tr>
<tr>
<td>4</td>
<td>D₁₆</td>
<td>1.001183</td>
<td>&lt;1.0x10^-5</td>
<td>40.0</td>
</tr>
<tr>
<td>1</td>
<td>2P₁</td>
<td>1.001126</td>
<td>-6.4x10^-5</td>
<td>3.3</td>
</tr>
<tr>
<td>1</td>
<td>2P₂</td>
<td>1.001218</td>
<td>2.8x10^-5</td>
<td>3.9</td>
</tr>
<tr>
<td>1</td>
<td>4P₁</td>
<td>1.001212</td>
<td>2.2x10^-5</td>
<td>5.4</td>
</tr>
<tr>
<td>1</td>
<td>4P₂</td>
<td>1.001218</td>
<td>2.8x10^-5</td>
<td>6.7</td>
</tr>
<tr>
<td>1</td>
<td>2P₂</td>
<td>1.001218</td>
<td>2.8x10^-5</td>
<td>3.9</td>
</tr>
<tr>
<td>2</td>
<td>2P₂</td>
<td>1.001191</td>
<td>&lt;1.0x10^-5</td>
<td>7.7</td>
</tr>
<tr>
<td>4</td>
<td>2P₂</td>
<td>1.001193</td>
<td>&lt;1.0x10^-5</td>
<td>15.5</td>
</tr>
</tbody>
</table>

Reference 1.00119
VI. FURTHER DEVELOPMENTS AND RELATED ACTIVITIES

The multidimensional version of the DNTM developed in the Appendix is presently being implemented for two-dimensional calculations and will be tested soon on simple model problems and on large heterogeneous fast reactor problems. After that, the multidimensional version of the PNTM which is also developed in the Appendix will be implemented and tested. Because the anticipated superiority of the PNTM over the DNTM has been verified by the results presented in Section V for one-dimensional applications, it is further anticipated that it will be superior in two- and three-dimensional applications. Nevertheless, the DNTM is being implemented first because this is less difficult; however it is expected that it will be superseded by the PNTM for both one- and multidimensional applications.

Two new coarse-mesh methods\textsuperscript{35} for neutron diffusion calculations which are related to the PCBM and the NGFM have also been developed and are presently being implemented to determine whether the fact that they have fewer variables per computational element will in fact permit them to be even more efficient than the PCBM and the NGFM. Rather than using one Green's function with boundary conditions of the third kind to convert the differential equations to sets of coupled local integral equations as in the development of the PCBM and NGFM, these "hybrid" methods, the HPCBM and the HNGFM, both use two different Green's functions in their formalisms, one subject to Dirichlet boundary conditions and the other subject to Neumann boundary conditions. Because of this, the new formalisms are developed in terms of fluxes defined on the volumes of the computational elements and net currents rather than partial currents defined on the surfaces of the elements; this results in fewer variables per element and therefore in potentially greater computational efficiency. The details of the formalisms of these two newly-developed methods have been completed and they are presently being implemented.\textsuperscript{36} Ultimately the HNGFM will be developed as both a standard zeroth-order modern nodal method and also as a higher-order\textsuperscript{7} modern nodal method from which the fluxes in the interiors of the computational nodes can be reconstructed and for which transverse (quadratic) fits using three nodes to obtain leakages are unnecessary. A new combined coarse-mesh method in space-time\textsuperscript{37} based upon the application of ideas used in the NGFM to space and time variables simultaneously has also been developed in order to increase the computational time step used in reactor dynamics calculations, and it is presently being implemented. Variational methods have been developed\textsuperscript{38} for the construction of the matrix elements which are required in multidimensional applications of the PCBM and the HPCBM so that the values of these matrix elements can be efficiently calculated when irregular elements such as hexagonal elements are used. The variational
principles have been developed for computational elements of arbitrary geometry and they are now being tested numerically (compared with the exact analytical numerical values) for rectangular elements.

Finally, in addition to these further developments, related coarse-mesh methods development activities in the areas of heat conduction and fluid flow have been completed. Space and space-time local Green's function methods (LGFM) have been developed for the solution of the steady-state\textsuperscript{39,40} and time-dependent\textsuperscript{41,40} heat conduction equation, applied to one-dimensional and two-dimensional test problems and compared with finite difference methods. Related, but significantly different new coarse-mesh methods have also been developed for the fluid flow (Navier-Stokes) equations by utilizing Green's tensors\textsuperscript{42,40} (LGTM) rather than Green's functions, and applied to the (two-dimensional) Stokes' flow, inlet-flow, and driven-cavity problems as test problems.\textsuperscript{40}

VII. SUMMARY

Two new coarse-mesh methods for multidimensional diffusion theory calculations of reactor power distributions, the partial current balance method (PCBM) and the nodal Green's function method (NGFM), have been reviewed with emphasis on the latter, more practical one. Extensive numerical results from recent applications of these methods to model problems and multidimensional benchmark problems and from the present applications to multidimensional benchmark problems and design problems have explicitly demonstrated their superior computational efficiencies when compared with conventional fine-mesh methods based on finite-difference techniques and finite-element techniques. For thermal reactor applications the NGFM leads to computational efficiencies which are superior by approximately a factor of 10 (in computing time for comparable practical accuracy requirements) for each dimension involved in the multidimensional problem, viz. a factor of -10 improvement for one-dimensional calculations, -100 for two-dimensional calculations, and -1000 for three-dimensional calculations. Although the finite difference calculations for the two-dimensional eight group heterogeneous fast reactor design problem studied are not complete it is clear that a factor of at least 30 in computing speed over a high-efficiency finite-difference code for comparable accuracy requirements is achieved in addition to substantial computer core storage gains. We anticipate that these gains may be even more impressive when the study of the convergence of the finite-difference calculations is completed. The practical implications of these superior computational efficiencies for the calculation of multidimensional power ratings in operating reactors are clear. It is likely that these and/or other modern coarse-mesh methods will supply the technical basis from which a new capability for calculations of detailed power rating distributions will emerge to begin a new era in power reactor calculations.

Two new coarse-mesh methods for the numerical solution of the transport equation have also been developed here and verified by computational tests on one-dimensional model problems and a one-dimensional eight group heterogeneous-
design fast reactor problem. Both new methods, the discrete nodal transport method (DNTM) and the piecewise polynomial nodal transport method (PNTM) were shown to yield accurate solutions for the elementary model problems which are generally considered difficult tests for transport theory computational methods. (In fact, these elementary problems are not particularly difficult tests for these new methods because these methods yield extremely accurate solutions in vacuum regions and strongly absorbing regions which represent the most difficult computational challenges for most other methods. This is because the Green's functions utilized in the newly developed methods are in fact the exact analytical solutions for neutron transport through pure absorbing and vacuum regions.) After establishing the high accuracy for the one-dimensional one-speed "difficult" elementary model problems, the DNTM and PNTM were applied to a one-dimensional eight-group heterogeneous design fast reactor model and compared with the conventional fine-mesh finite-difference (discrete-$S_N$) transport theory code ANISN. The results of these calculations showed that the DNTM and PNTM were faster than ANISN for comparable accuracy requirements by factors of 100 and 200 respectively.

The improved computational efficiencies achieved by the diffusion theory coarse-mesh NGFM for multidimensional thermal reactor power rating distributions [a factor of ~10 per dimension] combined with the results of the initial one-dimensional applications of the two (discrete, polynomial) new coarse-mesh transport theory methods [a factor of (~100, ~200) compared with ANISN and (~6, ~12) compared with ILLSN] lead us to be optimistic with respect to our applications of these new methods to two- and three-dimensional transport problems.

ACKNOWLEDGEMENTS

Mr. Abderrafig Ougouag is gratefully acknowledged for his contributions to the one-dimensional DNTM and ANISN calculations and to the two-dimensional DNTM calculations of the heterogeneous-design fast reactor. Drs. Y. Orechwa, C. Adams and K. Dertime are also gratefully acknowledged for supplying us with the results of their DIF20 calculations for the heterogeneous-design fast reactor.

Note added: Important related references\textsuperscript{a,b} were called to our attention\textsuperscript{c} shortly after the Meeting. Those references\textsuperscript{a,b} report nodal transport methods which are closely related to the PNTM. Like the PNTM, they use polynomial expansions in space and angle, and they also use the local integral equation on the node surfaces to determine the outgoing angular fluxes. The major difference is that those methods, as reported,\textsuperscript{a,b} determine the expansion coefficients of the node-interior flux via moments of the differential form of the transport equation, whereas the PNTM uses a local integral equation for this purpose. Another difference is that those methods use half-range angular expansions for the surface angular fluxes whereas the PNTM uses more general fractional-range angular expansions for these quantities.

\textsuperscript{a} C. Maeder, "OP1, a Transport Program in x-y Geometry Based on Function Expansions in Angle and Space", EIR-Bericht Nr 290, Swiss Federal Institute for Reactor Research, 1979.


\textsuperscript{c} C. Maeder, personal communication, November 30, 1979.
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36. A. M. Ougouag, unpublished University of Illinois research.

37. T. M. Sullivan, unpublished University of Illinois research.

38. O. M. B. Dieter, unpublished University of Illinois research.


APPENDIX. THE MULTIDIMENSIONAL DNTM AND PNTM FORMALISMS

The discrete nodal transport method (DNTM) and the polynomial nodal transport method (PNTM) developed in Sec. IV for one-dimensional slab geometry can be directly extended to multidimensional Cartesian geometries by first reducing the multidimensional transport equation to coupled one-dimensional equations using techniques analogous to those applied in Sec. II to the multidimensional diffusion equation. The two-dimensional transport equation in $x$-$y$ geometry is

$$
\frac{\mu}{a_x} \frac{\partial}{\partial x} \psi^k_g(x,y,\mu,\eta) + \frac{\nu}{a_y} \frac{\partial}{\partial y} \psi^k_g(x,y,\mu,\eta) + \Sigma^k_g \psi^k_g(x,y,\mu,\eta) = S^k_g(x,y,\mu,\eta)
$$

$$(x,y) \in V_k, \quad -1 < x < +1, \quad -1 < y < +1, \quad k=1, \ldots, K, \quad g=1, \ldots, G,$$  \hspace{1cm} (A-1)

where the dimensionless (local) variables $x$ and $y$ are written in terms of the node half-widths $a_x$ and $a_y$. Integrating Eq. (A-1) over $y$ from $-1$ to $+1$ yields the $x$-dependent equation

$$
\frac{\mu}{a_x} \frac{\partial}{\partial x} \psi^k_{gx}(x,\mu,\eta) + \Sigma^k_{gx} \psi^k_{gx}(x,\mu,\eta) = S^k_{gx}(x,\mu,\eta) - L^k_{gx}(x,\mu,\eta),
$$

\hspace{1cm} (A-2)

where $\psi^k_{gx}$ and $S^k_{gx}$ are partially-integrated angular fluxes and sources, e.g.,

$$
\psi^k_{gx}(x,\mu,\eta) = \frac{1}{2} \int_{-1}^{1} dy \, \psi^k_g(x,y,\mu,\eta),
$$

\hspace{1cm} (A-3a)

and the transverse leakage term takes the form

$$
L^k_{gx}(x,\mu,\eta) = \frac{1}{2a_y} \int_{-1}^{1} dy \, \eta [\psi^k_g(x,1,\mu,\eta) - \psi^k_g(x,-1,\mu,\eta)].
$$

\hspace{1cm} (A-3b)

The one-dimensional equation, Eq. (A-2), is then solved separately for $\mu<0$ and $\mu>0$ as in Sec. IV. For $\mu>0$, this yields

$$
\psi^+_{gx}(x,\mu,\eta) = a_x \int_{-1}^{1} dx_0 \frac{1}{\mu} e^{-\Sigma(x-x_0)/\mu} \left\{ S^+_x(x_0,\mu,\eta) - L^+_gx(x_0,\mu,\eta) \right\} + \psi^+_{gx}(-1,\mu,\eta) e^{-\Sigma(+1)/\mu},
$$

\hspace{1cm} (A-4)
where \( \Sigma = \int_{-1}^{1} k_{a} \, d \chi \), the half-range fluxes are defined by,

\[
\psi_{g \chi}^{+}(x, \mu, \eta) = \begin{cases} 
\psi_{g \chi}^{+}(x, \mu, \eta), & \mu > 0 \\
0, & \mu < 0
\end{cases}
\]

and the half-range sources and transverse leakages are analogously defined.

Evaluating Eq. (A-4) at \( x = 1 \) yields the following equation for the average outgoing angular flux on the right surface of the two-dimensional node:

\[
\psi_{g \chi}^{+}(1, \mu, \eta) = a_{\chi} \int_{-1}^{1} dx_{0} \frac{1}{\mu} e^{-\Sigma(1-x_{0})/\mu} \left\{ \psi_{g \chi}^{+}(x_{0}, \mu, \eta) - L_{g \chi}^{+}(x_{0}, \mu, \eta) \right\}
\]

\[+ \psi_{g \chi}^{-}(-1, \mu, \eta) e^{-\Sigma(x+1)/\mu}.\]

As in Sec. III, analogous equations for \( \psi_{g \chi}^{-}(x, \mu, \eta) \) and \( \psi_{g \chi}^{-}(-1, \mu, \eta) \) are also developed. Finally, four additional equations are derived for the \( y \)-dependent partially-integrated fluxes by integrating Eq. (A-1) over \( x \) from \(-1\) to \(+1\). Thus a total of eight coupled equations must be solved in the two-dimensional case (and twelve in the three-dimensional case).

The spatial dependence of the one-dimensional partially-integrated fluxes and sources in the interior of the node are expanded in Legendre polynomials as in Sec. IV. Analogous to the diffusion theory NGFM, the space-dependent transverse leakage is approximated by a quadratic polynomial with coefficients given in terms of the average (angle-dependent) leakages in adjacent nodes.

The angular dependence is approximated by either projecting onto discrete ordinates (DNTM) or by employing low-order spherical harmonics (PNTM) defined on the sub-domains of the surface of the unit sphere. The calculation of the DNTM matrix elements is straightforward since it involves only the evaluation of simple exponential functions; although the calculation of the PNTM matrix elements is somewhat more complicated, for a low-order (\( N=1 \)) spherical harmonics approximation on each angular subdomain all the required matrix elements have been written explicitly in terms of \( E_{n} \)-functions and a single more complicated integral of a transcendental function. Although the discrete ordinate DNTM approach is more straightforward, it will not be free of the ray effects which often occur in standard multidimensional \( S_{N} \) calculations. The PNTM appears particularly attractive because of its potential for eliminating ray effects, and also because of its high accuracy and very rapid angular convergence as demonstrated in the one-dimensional PNTM results presented in Sec. V.
ON THE FEASIBILITY OF USING PARALLEL MICROPROCESSORS FOR THE CALCULATION OF 3-DIMENSIONAL RATING DISTRIBUTIONS IN OPERATING REACTORS

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ABSTRACT

A Parallel Microprocessor (PMP) is a collection of independent Microprocessors (MP), each capable of performing a separate task. While each MP may be slow, a collection of 100 of them rivals the speed of today's medium-sized computers. The feasibility of using a PMP to calculate 3-dimensional rating distributions was investigated. The results indicate that a stand-alone PMP using current technology could serve as a reactor simulator at a nuclear power station.

INTRODUCTION

A Parallel Microprocessor (PMP) is a collection of independent Microprocessors (MP), each capable of performing a separate complex computational task. This is in contrast to vector or array processors where each processor must perform the same simple computation on each element of the array or vector. Prototype PMPs have been built and demonstrated /1/ but none are commercially available today. Further, existing PMPs lack the error detection and correction features necessary for a production computer. However, this situation will change rapidly within the next two years. Reliable low-cost PMPs will be available and their performance will rival today's large scientific computers.

The PMP will find many applications in the nuclear industry. One application is to use a dedicated PMP at a nuclear power station to compute 3-dimensional rating distributions, burnup, and control rod worths. The purpose of this paper is to demonstrate the feasibility of using a PMP for this application.

PMP ORGANIZATION

The components of a PMP are illustrated in Figure 1. Several organizations of these components are possible. A very simple organization is described here.

Each MP is constructed on a single printed circuit board. Each MP is a complete processor containing a Central Processor Unit (CPU) and Random Access Memory (RAM). A typical CPU is the Z-80 with a cycle time of 250 nanoseconds (ns). Typical RAM size is 16-32K bytes, but 64K is currently practical. The Z-80 does not perform floating point calculations so that a separate Arithmetic Processing Unit (APU) is required. A typical APU is the Am 9511 which will perform a 32 bit floating multiply in about 40 microseconds (µs). A small (1-2K byte) Read-Only Memory (ROM) contains a simple operating system.
FIGURE 1. TYPICAL PARALLEL MICRO-PROCESSOR ORGANIZATION

RAM - Random Access Memory
CPU - Central Processor Unit
APU - Arithmetic Processor Unit
ROM - Read-Only Memory
BUF - Bus Buffer Memory
Figure 1 shows 8 MP boards plugged into a common printed circuit board called the mother board. The mother board contains a bus which connects each of the MP boards in parallel. A buffer (2-4K RAM) is used to interface the MP to the bus. A typical arrangement is to have 16 MP boards mounted on a single mother board and installed in a rack-mounted chassis containing a power supply. A group of 8 such units mounted in a single rack is a PMP with 128 MPs. The buses from each unit are connected together with a flat ribbon cable terminated at a Programmable Interface (PI).

The PMP as described above is used as a peripheral device attached to a standard minicomputer (Mini) via a cable. The PI allows the PMP to be interfaced to a wide variety of minicomputers.

**PMP OPERATION**

The PMP is completely controlled by the Mini. Each MP is a slave computer using programs and data sent to it by the Mini. We will briefly review this operation.

Programs are written in FORTRAN using all of the terminal, printer, and disk storage facilities of the Mini. If the Mini is interfaced to a large computer, then programs and data could originate there. Special compilers called cross-compilers translate the FORTRAN into the object program for the CPU and APU of the MP. This object program is transmitted from the Mini to one (or every) MP where it is stored in RAM. Note that each MP can have a different program or all MPs can have a copy of the same program.

Data is also transmitted from the Mini to each MP where it is stored in RAM. The Mini then directs each MP to begin execution using the stored program and data. Each MP places status information in its buffer which can be read by the Mini. The Mini can either wait for a MP to complete execution or it can interrupt the execution. Results of the computation can be transmitted from the MP to the Mini where they are stored in memory and/or on disk.

Note that the operation of each MP is completely controlled by the Mini and is independent of the operation of any other MP. In the PMP organization described here, the individual MPs "talk" only to the Mini and not to each other. Other PMP organizations /2/ allow the MPs to "talk" to each other and exchange data. These organizations tend to be specific to the application and are not considered here.

**PMP PERFORMANCE AND COST**

The RAM in each MP is large enough (16-64K) to hold a substantial program and its data. If we assume that an iterative calculation is being done, then calculations can be done almost continually with only minor interruptions for data exchange between the MP and the Mini. With these assumptions we can estimate the computational power of the MP. The estimates are based on the time required to evaluate the FORTRAN statement \( A(N)=B(N)+C(N)*D(N) \) which is counted as 2 floating point operations. Assuming a Z-80 CPU and Am 9511 APU running at 4 MHz, each MP can perform 0.009 MFLOPS (Million Floating Point Operations/Second). A PMP with 128 MPs would be rated at 1.2 MFLOPS.

Measurements on an IBM 360/195 yield a speed of 4.6 MFLOPS. This corresponds to a speed of approximately 2.3 MFLOPS for a CDC 6600. We then obtain the following ratio of speeds:

\[
\begin{align*}
\text{[IBM 360/195]/[1-Am 9511]} &= 500 \\
\text{[CDC 6600]/[1-Am 9511]} &= 250 \\
\text{[IBM 360/195]/[128-Am 9511]} &= 4 \\
\text{[CDC 6600]/[128-Am 9511]} &= 2
\end{align*}
\]
In practice it will not be possible to obtain the full speed of the MP. A realistic estimate is that each MP can be kept busy 50% of the time, so that a factor of 2 should be applied to the above ratios.

MP costs depend strongly on time and volume. In reasonable quantities the cost today of a 32K RAM MP with a Z-80 and AM 9511 would be about $2000. Probably this cost can be reduced to about $1000 within the next two years. Therefore, a PMP with 64 MPs would cost about $60K. Adding $40K for a Mini, the total cost would be $100K. The next generation of MP will be much faster (perhaps by a factor of 10) with only a small increase in cost.

CODE STRUCTURE

It is clear that we must structure our codes in a different way to run on a PMP. The computations must be organized to run in parallel instead of in sequence as they do on single processor computers. The computations must be organized into independent tasks where possible, and weakly dependent tasks otherwise. Fortunately this is relatively easy to do for most scientific calculations since they generally solve equations by iteration in some multidimensional phase space. The general approach is to divide the full phase space into subspaces and assign each subspace to a MP. The boundary conditions for a subspace depend on the solution in neighbor subspaces. Therefore the Mini must periodically update boundary conditions. The solution strategy is then for each MP to iterate on the solution within a subspace using fixed boundary conditions and for the Mini to iterate the boundary conditions. We use the Nodal Diffusion Theory method in this paper to illustrate this approach. The PMP can also be used for other types of reactor calculations as follows:

- Each MP follows neutron histories in a space-energy region. Neutrons leaving a region are transferred by the Mini to the appropriate MP for the region entered.
- Each MP performs a lattice physics calculation for one cell of the lattice.
- Each MP iterates the thermal-hydraulic solution at one node of a reactor system. The Mini exchanges boundary conditions and controls the time advancement.

NODAL DIFFUSION THEORY

Nodal Diffusion Theory (NDT) is a fast and accurate method for computing rating distributions in 3D Light Water Reactors. NDT has been applied to the 3D IAEA benchmark problem /3/ by several investigators. This problem is used here as an example. A quarter core calculation is done with a 9x9x19 node array for the x,y,z dimensions. The x,y layout is shown in Figure 2a. A full core calculation is done with a 17x17x19 node array. Two neutron energy groups are used.

The NDT method calculates an average flux in each group and node by iteration of the NDT equations. These equations are similar to response matrix equations in that they relate volume average flux in a node and surface average currents leaving the node to surface average currents entering the node. The equations are usually formulated as coarse-mesh finite-different equations with leakage coefficients determined by fine-structure calculations within the node. From an iteration point of view there are seven quantities per node and group to be determined, the volume average flux plus the six leakage coefficients.

The best computing time reported /4/ for the 3D IAEA benchmark problem is 1.0 min on a CDC 6600. This time is for a 1/8 core problem. The results presented in /5/ can be used to scale this time for large problems. We obtain the estimate of 1.4 min for the 1/4 core problem and 5.0 min for the full core problem.
FIGURE 2. EXAMPLE OF SPATIAL SUBDIVISION
The NDT node array can be partitioned into sub-arrays each of which will be placed in one MP of a PMP. One possible partitioning is to use a 3x3x3 node array in each MP. This partitioning is illustrated in 2D by the heavy lines in Figure 2a. Each MP would iterate on the 3x3x3=27 nodes (actually 2x7x27=378 unknowns) using known entering surface currents as illustrated in Figure 2b. Quadratic interpolation is used in the NDT method to estimate the spatial distribution of surface currents. If there are N nodes on a 1D surface, then N+2 entering surface currents are needed. The entering surface currents are illustrated by the arrows in Figure 2b.

As each MP iterates the solution using the fixed entering surface currents, new estimates of the exiting surface currents are produced. These are illustrated in Figure 2c. The exiting surface currents produced by one MP become the entering surface currents used by the other MPs iterating on neighboring node arrays. The Mini has the job of collecting exiting surface currents from the individual MPs and distributing them as entering surface currents to the appropriate MPs.

The basic solution strategy can be summarized as follows. Each MP iterates on the solution within a sub-region of the reactor using the best current estimate of the neutron currents entering that sub-region and predicts neutron currents output from each MP as input to other MPs. The process continues until the solution converges.

The basic solution strategy can be enhanced using some form of coarse-mesh rebalancing. Each MP would be treated as a coarse-mesh node and would produce appropriate coarse-mesh coefficients corresponding to the current solution. The Mini would collect these coefficients and solve the coarse-mesh equations. Alternatively, these coefficients could be sent to a MP programmed to solve the coarse-mesh equations.

Many details of the iteration strategy have yet to be determined. We do not have any experience in using a PMP for this type of problem. One very important question is the time sequence of events. On a serial computer we would perform several iterations on a fine solution, then perform a coarse-mesh rebalance, and repeat these two steps until the solution converged. On a PMP can we perform these two steps in parallel? Can we update the boundary surface currents continually or only periodically? Which strategies guarantee stability?

PMP strategies can be simulated on serial computers so that these questions can be answered without actually having a PMP. For the purposes here we assume that the actual efficiency of a PMP is 50%. This could result from using a continual update strategy requiring twice as many iterations as on a serial computer. Alternatively it could also result from using a periodic update strategy in which each MP is working usefully only half the time.

SIZE AND TIME ESTIMATES

The node array assigned to each MP was illustrated as a 3x3x3 array in Figure 2. Several additional node arrays are listed in Table I. The MP memory requirements were calculated and listed in Table I for each node array. The size of the iteration program in each MP is estimated /5/ to be about 6K bytes. We observe from Table I that the MP memory requirements are modest (13-35K bytes). Further, the surface data (2-4K bytes) is small enough to be resident in the MP buffer. This last observation could strongly affect the choice of iteration strategy.
TABLE I. MP MEMORY REQUIREMENTS (K BYTES)

<table>
<thead>
<tr>
<th>Node Array/MP</th>
<th>3x3x3</th>
<th>3x3x5</th>
<th>3x3x7</th>
<th>4x4x5</th>
<th>5x5x5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nodes/MP</td>
<td>27</td>
<td>45</td>
<td>63</td>
<td>80</td>
<td>125</td>
</tr>
<tr>
<td>Volume Data</td>
<td>5.3</td>
<td>8.8</td>
<td>12.3</td>
<td>15.6</td>
<td>24.4</td>
</tr>
<tr>
<td>Surface Data</td>
<td>1.6</td>
<td>2.1</td>
<td>2.6</td>
<td>2.8</td>
<td>4.3</td>
</tr>
<tr>
<td>Program</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
</tr>
<tr>
<td>Total</td>
<td>12.9</td>
<td>16.9</td>
<td>20.9</td>
<td>24.4</td>
<td>34.7</td>
</tr>
</tbody>
</table>

Tables II and III list the computing time estimates for each node array choice. For example, a 3x3x3 node array requires a 3x3x7 array of MPs to solve a 9x9x19 node quarter core problem. A total of 63 MPs would be required. The CDC 6600 computing time is estimated at 1.4 min. The ratio of CDC 6600 time to single MP time is 250. This leads to a minimum PMP time of 1.4x250/63=6 min. Since we estimate the PMP efficiency at 50%, the estimated PMP time is 12 min.

TABLE II. ESTIMATES FOR A QUARTER CORE CALCULATION

<table>
<thead>
<tr>
<th>Node Array</th>
<th>3x3x3</th>
<th>3x3x5</th>
<th>3x3x7</th>
<th>4x4x5</th>
<th>5x5x5</th>
</tr>
</thead>
<tbody>
<tr>
<td>MP Array</td>
<td>3x3x7</td>
<td>3x3x4</td>
<td>3x3x3</td>
<td>3x3x4</td>
<td>2x2x4</td>
</tr>
<tr>
<td>Number of MPs</td>
<td>63</td>
<td>36</td>
<td>27</td>
<td>36</td>
<td>16</td>
</tr>
<tr>
<td>Min. Time (Min)</td>
<td>6</td>
<td>10</td>
<td>13</td>
<td>10</td>
<td>22</td>
</tr>
<tr>
<td>Est. Time (Min)</td>
<td>12</td>
<td>20</td>
<td>26</td>
<td>20</td>
<td>44</td>
</tr>
</tbody>
</table>

TABLE III. ESTIMATES FOR A FULL CORE CALCULATION

<table>
<thead>
<tr>
<th>Node Array</th>
<th>3x3x3</th>
<th>3x3x5</th>
<th>3x3x7</th>
<th>4x4x5</th>
<th>5x5x5</th>
</tr>
</thead>
<tbody>
<tr>
<td>MP Array</td>
<td>6x6x7</td>
<td>6x6x4</td>
<td>6x6x3</td>
<td>5x5x4</td>
<td>4x4x4</td>
</tr>
<tr>
<td>Number of MPs</td>
<td>252</td>
<td>144</td>
<td>108</td>
<td>100</td>
<td>64</td>
</tr>
<tr>
<td>Min. Time (Min)</td>
<td>5</td>
<td>9</td>
<td>12</td>
<td>13</td>
<td>20</td>
</tr>
<tr>
<td>Est. Time (Min)</td>
<td>10</td>
<td>18</td>
<td>24</td>
<td>26</td>
<td>40</td>
</tr>
</tbody>
</table>

We observe from Tables II and III that a 3D rating distribution can be computed on a PMP in a very reasonable amount of real time. For example, a full core calculation on a PMP with 64 MPs (estimated to cost $100K) is estimated to take 40 min. A larger PMP with 108 MPs would reduce the time to 24 min.

CONCLUSION

We conclude that 3D full core rating distributions can be computed on a PMP in times ranging from 24-40 minutes using existing MP technology. PMPs of this type would cost in the range of $100-200K. It would be practical to have a PMP dedicated to reactor simulation at each operating reactor. We believe the above estimates of cost and performance are conservative and reflect today's proven technology.
ACKNOWLEDGMENT

This work was done while the author was on leave-of-absence from the E. I. du Pont de Nemours & Company. The author expresses his appreciation to Dr. W. Werner (GRS) for introducing him to the PMP concept. A part of this work was done while the author was a guest scientist at EIR (Switzerland) and at Winfrith (England).

REFERENCES


/2/ International Conference on Parallel Processing, Bellaire, Michigan, USA, April 22-25, 1978, Pages 18-23.


Summary of the Session 5

A. Kavenoky

Five reports had been presented during this last session of the meeting dealing with PWR, BWR, LMFBR, numerical methods and new data processing systems.

The first paper was devoted to the follow-up of the fuel testing reactor CAP: the calculations had been performed using a 3D finite difference synthesis method providing approximate cell by cell power distributions and using a 3D finite element calculation. The assembly power distribution obtained by these two methods are in good agreement (the discrepancy is always lower than 3%); comparisons with experimental results were presented for axial power distributions.

The subject of the next paper was the calculation of the power distribution for a BWR; the computer code described is divided into two parts. The first one provides a 3D diffusion calculation based on a new numerical technique named "Leakage Iterative Methods" which seems to be closely related to an alternating direction methods. The thermohydraulic feedbacks are taken into account to obtain the steady state of a BWR. Experimental comparison with an operating reactor are provided; they show a good general agreement but some significant discrepancies.

The third paper had presented a fundamental approach to coarse mesh calculation for diffusion and transport calculations; in the framework of the nodal method a new and very promising technique named the Nodal Green's function method is presented. With this technique the 1D diffusion equations to be solved are transformed into integral equations, the kernel of which is the Green's function. Numerical results compared this method to standard calculations and show large savings in computing time; the last part of this paper was devoted to a new nodal method for the transport equation it is described as the "Discrete Nodal Transport Method". This method is based on approximation of the interface angular fluxes: numerical results on benchmark problems show the benefits of this method.

The next paper has dealt with LMFBR diffusion calculations; the first part of this report was a comparison of three numerical methods for the 3D calculation of a rectangular geometry experiment: conventional finite differences, Kaplan synthesis and finite element. This comparison was in favour of the finite element method which gives a better accuracy for a given computing time. In the second part of this paper the same comparison was performed for the 2D geometry of Super Phenix, but the results are only provisional.

The last report of the session was devoted on the feasibility of using parallel microprocessors for the calculation of 3D power distributions. First, the paper had introduced the concept of parallel microprocessors and had estimated that this device using 128 microprocessors may perform at half the speed of a CDC 6600. The structure of this new computing device is well fitted for the solution of nodal diffusion equation. Finally the author had estimated that 3D full core rating distribution can be computed on this device in times ranging from 24-40 minutes. The author had said that it would be practical to have this device at each operating reactor.
This session had shown that the computing methods for the solution of the diffusion are not yet completely defined: very promising attempts are performed to enhance its efficiency: nodal and finite element methods are achieving very good performance; in the near future the new types of computing devices and mainly microprocessors may completely change the habits of reactor physicists.
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LISTE DES PARTICIPANTS
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APPENDIX

Abstracts of Computer Programmes mentioned at this Meeting

APPENDICE

Résumé des programmes de calcul mentionnés lors de cette réunion
Name of Program: MERCATOR
Laboratory: Electrobel, Belgium
Computer language: FORTRAN
Computer used: Siemens

General Description:
PWR Core Simulation

Code Status:
This code is ready for production. It is not a modified version of a previous code. It has been verified by comparison with experiment to a limited extent. Further experiment is needed to verify some part of it. This code has not been used or tested by any other organisation.

Availability:
This code is not available through any computer program library. There are restrictions on its distribution. Conditions for obtaining this code have to be negotiated.

Reference document: NEARCP-L-228

The scientist responsible for this program is:
Mr. M. Melice
Electrobel
1 Place du Trône
B-1000 BRUSSELS
Belgium
Name of Program: TRILUX Nodal System
Laboratory: Belgonucléaire, Belgium

General Description:
In-core fuel management studies using a one-group nodal coupling

Code Status:
The code is ready for production. It is a modified version of TRILUX, which was originated at GUNF and is modified by MICROLUX. It has been extensively verified by comparison with experiment, and no further experiment is needed. This code has been used and tested by GUNF.

Availability:
This code is not available through any computer program library, as there are restrictions on its distribution. This is a commercial code, however, and the conditions under which it can be obtained have to be negotiated. The contact person is:

Mr. Leon Bindler
Liaison Officer
Belgonucléaire
25 rue du Champ de Mars
RAL, Belgium.

Related or equivalent codes are SIMULATE and FLAME-3.
The scientist responsible for this program is Albert Charlier.
Name of Program: HEXBU-3D

Laboratory: Technical Research Centre of Finland

Computer language: FORTRAN V

Computer used: UNIVAC 1108

Computer resources required: 64 K words of core memory

General Description:

3-D two-group diffusion problem with feedback effects and fuel burnup for a hexagonal fuel assembly geometry. Appl: Loviisa 1 & 2 (VVER-440).

Code Status:

This code is ready for production. It is not a modified version of a previous code. It has been verified by comparison with experiment to a limited extent, and further experiment would be needed to verify some part of it, in which case in-core measurements and reactivity measurements from Loviisa 1 & 2 would be needed.

Availability:

This code is not available through any computer program library. There are restrictions on its distribution. It is a commercial code and the conditions under which it can be obtained are undefined as yet.

Reference documents: E. Kaloinen, R. Teräsvirta: "HEXBU-3D, a Three-Dimensional PWR-Simulator Program for Hexagonal Fuel Assemblies", Technical Research Centre of Finland (to be published). Related or equivalent codes: HEXBU (2D)

The scientist responsible for this program:

Mr. P. Siltanen
Imatran Voima Oy
P.O. Box 138
SF-00101 HELSINKI 10
Finland

Additional Information:


Name of Program: COSTAR
Laboratory: FRAMATOME, Courbevoie, France
Computer language: FORTRAN
Computer used: CDC 7600
Computer resources required: Variable

General Description:
1D x 2D x 3D synthesis. Peaking factor FQ and hot channel factor PDH under normal, transient and abnormal conditions. 3D pointwise power distribution.

Code Status:
This code is ready for production. It is not a modified version of a previous code. It has been verified by comparison with experiment to a limited extent, and further experiments are planned.

Availability:
This code is not available through any computer program library. It is not available since it is part of a modular system of design codes and cannot be used without data provided by the 1D, 2D and 3D diffusion codes used in FRAMATOME design, none of which are available. This is a commercial code.
Name of Program: POLESTAR-2F/3F
Laboratory: Power Reactor and Nuclear Fuel Development Corporation, Japan.
Computer language: FORTRAN
Computer used: CDC 6600

General Description:
2 and 3 dimensional power mapping and refuelling analysis by coarse mesh, one group approximation.

Code Status:
This code is ready for production. It is not a modified version of a previous code. It has been verified by comparison with experiment to a limited extent. Further experiment is needed to verify some parts of the code, in which case power mapping data from operation of HWR-Fugen would be needed. This code has not been used nor tested by any other organisation.

Availability:
This code is not available through any computer program library, and there are restrictions on its distribution. It is a commercial code and can be obtained by individual negotiation. The contact person is:

Mr. T. Haga
Heavy Water Reactor Development Project
Power Reactor and Nuclear Fuel Development Corporation
9-13, 1-chome, Akasaka, Minato-ku
TOKYO
Japan

Mr. T. Haga is also the scientist responsible for this program.

Additional Information:
This program may be used for analysis of any pressure tube type HWRs.
Name of Program: BWRSIM
Laboratory: N.V. KEMA
Computer language: FORTRAN
Computer used: CDC 6400/CDC 6600/CYBER 175/CDC 7600/IBM 370/168/ VAX 11-780
Computer resources required: 40 K 60 bits - CDC-words (ca. 2000 nodal points)

General Description:
BWRSIM calculates a nodal power distribution for a three dimensional XYZ core geometry.
Options: control and positioning - EOC-prediction - core follow - control rod burnup - axial flux profiles.

Code Status:
The code is ready for production. It is not a modified version of a previous code. To a limited extent it has been verified by comparison with experiment, and some further experiment is needed to verify some part of the code. The data needed for this are: Y-scan/measured flux profiles/rod burnup. This code has not been tested elsewhere.

Availability:
This code is not available through any computer program library as there are restrictions on its distribution. This is a commercial code, however, and can be obtained by mutual agreement. The contact person is:

Mr. G.J. Duin
N.V. KEMA
Utrechseweg 310
ARNHEM
The Netherlands

Reference documents are: BWRSIM, een fortran IV programma ter simulatie von een kokend water reactor; and NV KEMA 5939-77.

The scientists responsible for this program are: G.J. Duin, J.C. Bruggink and W.J. Oosterkamp.
Name of Program: RECORD/PRESTO

Laboratory: Institutt for Atomenergi, Norway

Computer language: FORTRAN

Computer used: CDC CYBER-74 (see below also)

Computer resources required: RECORD, CM = 115 000
PRESTO, CM = 220 000

General Description:
Analysis and simulation of operating LWR cores using 3-D 2-group diffusion theory.

Code Status:
The code is ready for production. It is not a modified version of a previous code. It has been extensively verified by comparison with experiment, and has been used and tested by: Bernische Kraftwerke, Bern, Switzerland; Kernkraftwerk Philippsburg, Germany; Carolina Power and Light Corporation, USA; NUCLEONOR, Spain.

Availability:
This code is not available through any computer program library although there are no restrictions on its distribution. It is commercially available through:

Scandpower A/S
Box 3
2007 Kjeller
Norway


The scientists responsible for the programs are: T. Skardhamar for RECORD, and S. Børresen for PRESTO.

Additional Information:
RECORD and PRESTO are components of the FMS (Fuel Management System) Code Package. The codes are applicable to both PWR and BWR calculations. The PRESTO formalism is also used in the 3-D transient analysis program, RAMONA-III. The PRESTO Program has been implemented on the following computers: CDC-CYBER-74, CDC-6600, IBM-370/168, UNIVAC-1110, NCR-8450.
Name of Program: CITATION-TRACA

Laboratory: ETSII-UPM and JEN; Madrid (Spain)

Computer language: FORTRAN-V

Computer used: UNIVAC-1100/80

Computer resources required: 42 K words + core memory for problem-dependent data

General Description:

2-D and 3-D diffusion theory calculation by finite differences with criticality searches and burnup.

Code Status:

This code is ready for production. It is a modified version of CITATION which originated at ORNL. There have been minor adaptations. It has to a limited extent been verified by comparison with experiment. Further experiments are needed; data required are 3-D detailed power distributions at different conditions of operating reactors. The code has been used by ORNL and many other laboratories.

Availability:

This code is available through the NEA Data Bank. It is not a commercial code and there are no restrictions on distribution.


Related or equivalent codes: PENELOPE (ref. JEN-300) for interfaced feedback of macroscopic cross sections dependent on local conditions.

The scientist responsible for this program:

Ms Carol AHNERT
Teoria y Calculo de Reactores; Junta de Energia Nuclear Avda. Complutense 12; Madrid-3, Spain
Name of Program: PENELLOPE

Laboratory: ETSII-UPM and JEN; Madrid (Spain)

Computer language: FORTRAN-V

Computer used: UNIVAC-1100/80

Computer resources required: 50 K words

General Description:

Interfaced feedback of macroscopic cross sections dependent on local conditions for CITATION-TRACA and VENTURE-TRACA.

Code Status:

This code will be ready for production in a few months. It is not a modified version of another code. It has been verified by comparison with experiment to a limited extent. Further experiments are needed and the data required are 3-D power density distributions at different conditions of operating reactors. This code has not been used or tested by another organisation.

Availability:

This code is not available through any computer program library. There are no restrictions on its distribution and it can be obtained by contacting:

Dr. G. Velarde
Catedra de Fisica Nuclear
ETS Ingenieros Industriales; Univ. Politecnica
Gutierrez Abascal, 2, Madrid-6, Spain

It is not a commercial code.


Related or equivalent codes: CITATION-TRACA and VENTURE-TRACA for interfaced coupling.

The scientist responsible for this program:

Ms. Carol AHNERT
Teoria y Calculo de Reactores; Junta de Energia Nuclear
Avda. Complutense, 12; Madrid-3, Spain

Additional Information:

PENELLOPE is being improved and verified further for application to core analysis of 900 Mwe PWR's.
Name of Program: SIMULA-3
Laboratory: ETSII-UPM and JEN, Madrid (Spain)
Computer language: FORTRAN-V
Computer used: UNIVAC-1100/80
Computer resources required: 30 K words + core memory for problem dependent data

General Description:
3-D nodal simulator of the FLARE type for PWR and BWR core calculations including nuclear and thermohydraulic feedback.

Code Status:
This code will be ready for production in a few months. It is a modified version of NUTRIX which originated at NUS Corp. (USA) and several improvements have been incorporated. It has to a limited extent been verified by comparison with experiment. Some further experiments are needed and data required are 3-D assembly-wise power distributions at different conditions of operating reactors. This code has been used by the NUS Corporation and other organisations.

Availability:
This code is not available through any computer program library. There are no restrictions on its distribution and it can be obtained by contacting:

Dr. G. Velarde
Catedra de Fisica Nuclear
ETS Ingenieros Industriales; Univ. Politecnica
Gutierrez Abascal, 2; Madrid-6, Spain

It is not a commercial code. Reference documents: JEN-250, G. Velarde et al., Junta de Energia Nuclear, Madrid (1972). Related or equivalent codes: MELON-3 (ref. JEN-312) for calculation of $K_{\infty}$ and $\mu^2$ correlations including effects of control, density, Doppler, Xenon, Boron and burnup. ROLLO-3 (ref. JEN-312) for calculation of transport kernel parameters and albedo that best fit to reference power distributions.

The scientist responsible for this program:
Dr. Jose M. Aragones
Teoria y Calculo de Reactores; Junta de Energia Nuclear
Avda. Complutense 12, Madrid-3, Spain

Additional Information:
SIMULA-3 and auxiliary programs MELON-3 and ROLLO-3, are being improved and verified for application to core performance analysis of 900 Mwe PWR's.
Name of Program: VENTURE-TRACA

Laboratory: ETSII-UPM and JEN; Madrid (Spain)

Computer language: FORTRAN-V

Computer used: UNIVAC-1100/80

Computer resources required: 40 K words + core memory for problem dependent data.

General Description:

2-D and 3-D neutron diffusion calculation by finite differences with criticality searches.

Code Status:

This code will be ready for production in a few months. It is a modified version of the code VENTURE which originated at ORNL. It has been modified by a new memory allocation and direct I/O. It has not yet been verified by comparison with experiment and further experiments are needed. Data required are 3-D detailed power density distributions at different conditions of operating reactors. This code has been used by ORNL and many other laboratories.

Availability:

This code is not available through any computer program library. There are no restrictions on its distribution and it can be obtained by contacting:

Dr. G. Velarde
Cátedra de Física Nuclear
ETS Ingenieros Industriales; Univ. Politecnica
Gutierrez Abascal 2, Madrid-6, Spain


Related or equivalent codes: PENELLOPE (ref. JEN-300) for interfaced feedback of macroscopic cross sections dependent on local conditions.

The scientist responsible for this program:

Ms. Carol Ahnert
Teoría y Calculo de Reactores; Junta de Energía Nuclear
Avda. Complutense 12; Madrid-3, Spain

Additional Information:

Complete new routines for dynamic memory allocation and efficient direct I/O have been developed in UNIVAC Assembler language, reducing overhead and clock times to about 1/10 of original FORTRAN direct access I/O. In preliminary calculations VENTURE-TRACA required about one half of both memory and total time used by CITATION-TRACA for large 3-D problems (one group, all space contained data management).
Name of Program: CASMO
Laboratory: Studsvik Energiteknik A.B.
Computer Language: FORTRAN
Computer used: CDC, also running on IBM and UNIVAC
Computer resources required: About 215,000 (Octal) 64-bit words of core memory.

General Description:
Cell and Assembly Spectrum Depletion Code for LWR.

Code Status:
The code is ready for production and has been extensively verified by comparison with experiment. No further experiment is needed. This code has been used and tested by the Swedish and U.S. power utilities and EPRI.

Availability:
This code is not available through any computer program library. It is a commercial code, and license agreements are offered for its use. The contact person is:

Eric Hellstrand or Kim Ekberg
Studsvik Energiteknik A.B.
61182 NYKÖPING
Sweden

Information on reference documents is available on request from either of the contact persons.

The scientists responsible for this program are: Åke Ahlin, Malte Edenius and Hans Häggbom, all of Studsvik Energiteknik A.B.
Name of Program: SIMULATE
Laboratory: Studsvik Energiteknik A.B.
Computer language: FORTRAN
Computer used: CDC, also running on IBM
Computer resources required: Problem dependent.

General Description:
3-D nodal BWR and PWR simulation.

Code Status:
This code is ready for production. It is not a modified version of a previous code. It has been extensively verified by comparison to operating reactors, and further verification is in progress. This code has been used and tested by the US power utilities, EPRI.

Availability:
This is a commercial code. There are restrictions on its distribution. License agreements are offered for its use. The contact person is:
Eric Hellstrand or Kim Ekberg
Studsvik Energiteknik A.B.
61182 NYKÖPING
Sweden

Information on reference documents is available on request from either of the contact persons.

The scientist responsible for this program is: Dr. D.M. Ver Planck of the Yankee Atomic Electric Co.
Name of Program: SILWER

Laboratory: Swiss Federal Institute for Reactor Research, 5303 Würenlingen, Switzerland

Computer language: FORTRAN

Computer used: CDC 6500

Computer resources required: Disc storage device

General Description:

3-Dimensional distributions of burnup, power, fuel and water temperature, water density and isotopic contents in a light water reactor.

Code Status:

This code will not be ready for production until some time in 1980. It is not a modified version of a previous code. It has been verified by comparison with experiment to a limited extent, but further experiment is needed to verify some part of it. In this case burnup data (experimental results are available) would be necessary.

Availability:

This code is not available through any computer program library, and there are restrictions on its distribution. It is a commercial code and can be purchased from EIR or obtained under bilateral agreement.

Reference documents are: C. Maeder, CONF-780401, p. 121 (1978); C. Maeder, K. K. Poskoles, J.-M. Paratte, H.C. Honeck and G. Varaci, "Calculations with the EIR Light Water Reactor Code System", NEA/CF-P-OCDE Meeting, Paris, November 1979. Related or equivalent codes are: ENDF/ Boxer: prepares a multigroup library from ENDF/B data; and BOXER: creates average cross sections per fuel element which are used in the data library of SILWER.

The scientist responsible for this program is:

Dr. C. Maeder
Swiss Federal Institute for Reactor Research
5303 WÜRENLINGEN
Switzerland
Name of Program: JOSHUA
Laboratory: AEE, Winfrith, United Kingdom
Computer language: FORTRAN
Computer used: IBM 370
Computer resources required: Problem dependent core size - typically 400 k bytes.

General Description:
3-D 2-group coarse mesh diffusion with thermal hydraulic feedback, depletion and fuel management. Used mainly in core-follow calculations.

Code Status:
The code is ready for production. It is not a modified version of a previous code. It has been verified extensively by comparison with SGRWR and LWR, and no further experiment is needed to verify it. This code has also been used and tested by NDK, Switzerland.

Availability:
This code is not available through any computer program library as at present there are restrictions on its distribution, but these may soon be lifted. This is a commercial code at present.
Reference documents are: UKAEA Reports AEEW-R1165 and AEEW-R1186. Related or equivalent codes are: LWRWIMS or WIMSD4.
The scientist responsible for this program is:

Mr. M.J. Both
A.E.E. Winfrith
Dorchester, Dorset
United Kingdom
Name of Program: LWR-WIMS

Laboratory: AE&E, Winfrith, United Kingdom

Computer language: FORTRAN

Computer used: IBM 370

Computer resources required: Problem dependent. Most calculations will run in 700 K bytes.

General Description:

Multigroup flux calculation and depletion in LWR cells with few-group cell average cross section output for JOSHUA.

Code Status:

The code is ready for production. It is not a modified version of a previous code but uses many techniques common to other 'WIMS' codes. It has been extensively verified by comparison with experiment, but those parts dealing with boron and control rod worths need further experiment for verification purposes. This code has been used and tested by several other organisations in the United Kingdom and Europe.

Availability:

This code is not available through any computer program library as there are restrictions on its distribution. It is a commercial code, and the terms under which it can be obtained can be agreed by discussion with:

Dr. I.H. Gibson
A.E.E. Winfrith
Dorchester, Dorset
United Kingdom.

Reference document: UKAEA Report - AEEW-R785. Related or equivalent codes are WIMSD, WIMSE and JOSHUA.

The scientist responsible for this program is: Dr. M.J. Halsall, A.E.E. Winfrith, Dorchester.

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Name of Program: DIF3D

Laboratory: Argonne National Laboratory, USA.

Computer language: FORTRAN-IV (IBM Assembler for random access IO)

Computer used: Any IBM OS system, CDC 7600, CRAY-I

Computer resources required: Typically uses 40 logical units of disk storage, random access IO for certain data management options, requires 50,000 words of core.

General Description:
Solves the 1-, 2-, and 3-dimensional, multigroup, steady-state neutron diffusion equation. Real and adjoint solutions, eigenvalue and distributed fixed source.

Code Status:
This code is ready for production; it is not a modified version of a previous code. It has been extensively verified by comparison with experiment and no further experiment is needed to it. This code has been used and tested by Los Alamos Scientific Laboratory and by the Nuclear Energy Division of General Electric, San José.

Availability:
This code will be available through NESC as from September 1980. There are no restrictions on its distribution. It is not a commercial code.

Reference documents are: D.R. Ferguson, K.L. Derstine, "Optimized Iteration Strategies for Fast Reactor Finite Difference Diffusion Theory Codes", NSAE 64, 593-604 (1977). Related or equivalent codes are: VENTURE, CITATION, DIF2D and 3DB.

The scientist responsible for this program is:
Keith L. Derstine
Applied Physics Division
Argonne National Laboratory
ARGONNE, Illinois 60439
United States of America

Additional Information:
DIF3D employed a dynamic three level data storage hierarchy system in order to utilise available auxiliary storage involving relatively slow extended core memory and random access and sequential disc storage. For any problem, a certain minimum amount of core memory is required; this amount is dependent on problem size. In general, increasing the core memory improves overall system performance.

The solution strategy employs an outer (fission source) iteration accelerated by the Chebyshev semi-iterative method; the within group flux (inner) iteration employs line successive overrelaxation to solve the mesh-centered finite-difference diffusion equations.

Special features include: anisotropic diffusion coefficients, blackness theory regions, orthogonal and triangular geometries, mixed or periodic boundary conditions. Upscattering is permitted, although the primary application is fast reactor problems.
Name of Program: SIMULATE
Laboratory: Electric Power Research Institute (EPRI)
Computer language: FORTRAN
Computer used: IBM 360/370; Amdahl; CDC 6600, CYBER 7600
Computer resources required: Flexible with problem and resources available to user. Can utilise either fast core or external storage consistent with problem size.

General Description:
3-dimensional neutronic simulation of reactor core with selection of nodal methods; thermal-hydraulics included.

Code Status:
The code is ready for production. It is not a modified version of a previous code. It has been extensively verified by comparison with experiment; further comparisons are being carried out, and it is being continually tested. No further experiments are needed. This code has been used and tested by many U.S. utilities.

Availability:
This code is available through the Electric Power Software Centre, EPRI. There are some restrictions on the distribution of this code, but it is generally available under information exchange agreements with EPRI. It is a commercial code. The contact person is:

Dr. Burt A. Zolotar
Electric Power Research Institute
3412 Hillview Avenue
P.O. Box 10412
Palo Alto, California 94303
United States of America

Reference documents are: Computer Code Manual and Procedures Manual, both distributed with the code. Numerous articles on this code exist in open literature; see ANS transactions. This code uses published methodologies from code suches as PRESTO, ROCS and FLARE.

The scientist responsible for this program is Dr. Burt A. Zolotar of EPRI.
Name of Program: VENTURE-II and related codes
Laboratory: ORNL, Oak Ridge, Tennessee, USA.
Computer language: Mostly FORTRAN
Computer used: IBM
Computer resources required: Usual for major computers; large memory desirable

General Description:
1, 2, 3 dimensional, multi-group diffusion theory approximation to neutron transport in common geometries (and a simple $P_1$ approximation).

Code Status:
This code is ready for production. It is a modified version of VENTURE I which originated at ORNL. The procedures were modified extensively. The code has been widely verified by comparison with experiment, but further experiment is needed for any new applications. In such a case, data on microscopic cross sections would be needed. This code has been used and tested by several other organisations.

Availability:
This code is available through the RSIC computer program library, and there are no restrictions on its distribution. It is not a commercial code.

The scientists responsible for this program are: D.R. Voudy and T.B. Fowler.

Additional Information:
Version III is in use at ORNL with extended capability including a temperature correlation on microscopic cross sections on the local zone reference temperature, and procedures to resolve the dominant harmonic for sensitivity and stability analysis - and the companion burnup code BURNER. Until resolution of exchange agreements, these are limited to USA use. Separately, fuel management capability is in use and will become available, unlimited distribution (developed under thermal reactor project funding).
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