

THEORETICAL METHODS FOR
DETERMINATION OF CORE PARAMETERS
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Abstract—Résumé—Аннотация—Resumen

THEORETICAL METHODS FOR DETERMINATION OF CORE PARAMETERS IN URANIUM-PLUTONIUM LATTICES.

The prediction of plutonium production in power reactors depends essentially on how the change of neutron energy spectra in a reactor cell during burn-up is determined. In the epithermal region, where the build-up of plutonium occurs, the slowing down effects are particularly important, whereas, on the other hand, the thermal neutron spectrum is strongly influenced by the low-lying plutonium resonances. For accurate analysis, multi-group numerical methods are required, which, applied to burn-up prediction, are extremely laborious and time consuming even for large computers. This paper contains a comprehensive review of the methods of core parameter determination in the uranium-plutonium lattices developed in Yugoslavia during the last few years. Faced with the problem of using small computers, the authors had to find new approaches combining physical evidence and mathematical elegance. The main feature of these approaches is the tendency to proceed with analytical treatment as far as possible and then to include suitable numerical improvements. With this philosophy, which is generally overlooked when using large computers, fast and reasonably accurate methods were developed. The methods include original means for adequate treatment of neutron spectra and cell geometry effects, especially suitable for U-Pu systems. In particular, procedures based on the energy dependent boundary conditions, the discrete energy representation, the improved collision probabilities and the Green function slowing down solutions were developed and applied. Results obtained with these methods are presented and compared with those of the experiments and those obtained with other methods.

METHODES THEORIQUES DE DETERMINATION DES PARAMETRES DE COEUR DE RESEAUX URANIUM-PLUTONIUM.

La prévision théorique de la production de plutonium dans un réacteur de puissance est essentiellement fonction de la façon dont on détermine la variation du spectre de neutrons dans la cellule de réacteur au cours de l'irradiation du combustible. Dans la région des neutrons épithermiques, où le plutonium est produit, les effets de ralentissement sont particulièrement importants, tandis que les résonances basses du plutonium influent fortement sur le spectre des neutrons thermiques. Pour une analyse précise, on doit faire appel aux méthodes numériques multi-groupes qui deviennent extrêmement laborieuses et prennent beaucoup de temps lorsqu'on calcule le taux d'irradiation, même à l'aide de grands ordinateurs. Le mémoire étudie de manière approfondie les méthodes élaborées en Yougoslavie au cours de ces dernières années pour le calcul des paramètres de cœur d'un réseau uranium-plutonium. Ne disposant que de petits ordinateurs, les auteurs ont cherché à trouver de nouvelles méthodes combinant les données physiques disponibles et des moyens mathématiques appropriés. La caractéristique principale de ces méthodes est de pousser le traitement analytique le plus loin possible et d'y inclure des améliorations numériques pertinentes. Grâce à cette tactique, généralement négligée par les utilisateurs des grands ordinateurs, des méthodes rapides et suffisamment précises ont pu être élaborées. Celles-ci, particulièrement adaptées aux systèmes U-Pu, contiennent des techniques originales pour le traitement de l'influence du spectre de neutrons et de la géométrie des cellules. Les méthodes élaborées portent notamment sur les conditions aux limites variant avec l'énergie, la représentation discontinue de l'énergie, les probabilités de choc améliorées et le calcul du ralentissement à l'aide des fonctions de Green. Les résultats obtenus par ces méthodes sont présentés et comparés avec l'expérience et avec les résultats obtenus à l'aide d'autres méthodes.

ТЕОРЕТИЧЕСКИЕ МЕТОДЫ ОПРЕДЕЛЕНИЯ ПАРАМЕТРОВ АКТИВНОЙ ЗОНЫ, СОСТОЯЩЕЙ ИЗ УРАН-ПЛУТОНИЕВЫХ РЕШЕТОК.

Расчет производства плутония в энергетических реакторах существенно зависит от того, как изменяется энергетический спектр нейтронов в ячейке реактора в процессе выго-

рапия. Накопление плутония идет, в основном, в эпитепловой области энергий, где особенно важны эффекты замедления, тогда как, с другой стороны, резонансы плутония в области низких энергий оказывают заметное влияние на тепловой спектр. Для точного анализа требуется использовать многогрупповые численные методы расчетов, которые в применении к расчетам выгорания особенно трудоемки и занимают много времени даже при работе на крупных электронно-вычислительных машинах. Доклад содержит всеобъемлющий обзор методов определения параметров активной зоны, состоящей из уран-плутониевых решеток. Указанные методы были разработаны в Югославии за последние несколько лет. Оказавшись перед фактом использования небольших вычислительных машин, авторы должны были искать новые пути решения, сочетающие физическую наглядность и математическое изящество. Основная особенность этих решений — аналитическая обработка результатов с использованием соответствующих усовершенствований численных методов расчета. В результате были разработаны сравнительно нетрудоемкие методы, обеспечивающие разумную точность расчета. Разработаны оригинальные методы обработки нейтронных спектров и эффектов геометрии ячейки, в основном применительно к уран-плутониевым системам. В частности, были разработаны и применены методики с использованием энергетической зависимости граничных условий; дискретного энергетического представления, решения функции Грина для процесса замедления. Приводятся результаты, полученные с использованием разработанных методов. Эти результаты сравниваются с экспериментальными данными и результатами других методов.

MÉTODOS TEÓRICOS PARA LA DETERMINACIÓN DE LOS PARÁMETROS DEL NÚCLEO EN RETÍCULOS DE URANIO-PLUTONIO.

La predicción de la producción de plutonio en los reactores de potencia depende esencialmente de cómo se determine la variación del espectro energético en una celda del mismo durante la irradiación del combustible. En la región epitérmica en la que tiene lugar la acumulación del plutonio, son particularmente importantes los efectos de la moderación, mientras que por otra parte el espectro neutrónico térmico se ve considerablemente influido por las resonancias bajas del plutonio. Para un análisis preciso se necesitan métodos numéricos en multigrupos, los cuales, cuando se aplican a la predicción del grado de quemado, son extremadamente laboriosos y consumen mucho tiempo incluso para máquinas calculadoras grandes. Esta memoria contiene una amplia reseña de los métodos desarrollados en Yugoslavia durante los recientes últimos años para la determinación de parámetros del núcleo en retículos de uranio-plutonio. Enfrentados con el problema que supone contar únicamente con máquinas calculadoras pequeñas, fue preciso que los autores encontraran nuevos métodos en los que la evidencia física se combina con la elegancia matemática. La característica principal de estos métodos es la tendencia a seguir un procedimiento analítico hasta donde sea posible para introducir entonces adecuados recursos numéricos. Siguiendo esta línea de pensamiento, que generalmente se pasa por alto cuando se utilizan máquinas calculadoras grandes, se desarrollaron métodos rápidos y de precisión razonable. Los métodos utilizados comprenden técnicas originales para tratar convenientemente los espectros neutrónicos y efectos de la geometría de la celda, y son especialmente idóneos para sistemas U-Pu. En particular fueron desarrollados y aplicados procedimientos basados en las condiciones de contorno dependientes de la energía, la representación discreta de la energía, las probabilidades de colisión mejoradas y el cálculo de la moderación mediante funciones de Green. Se presentan los resultados obtenidos con estos métodos y se comparan con los de la experimentación y con los que resultan de aplicar otros métodos.

1. INTRODUCTION

The prediction of plutonium production in power reactors depends essentially on how the change of neutron energy spectra in a reactor cell during burn-up is determined. In the epithermal region, where the build-up of plutonium occurs, the slowing down effects are particularly important, while, on the other hand, the thermal-neutron spectrum is strongly influenced by the low-lying plutonium resonances. For accurate analysis, multi-group numerical methods are required, which, applied to burn-up prediction, are extremely laborious and time-consuming even for large computers.

There are several plutonium recycling modes, and the decision on which is best for the specific reactor in which plutonium is to be used depends primarily on the detailed nuclear design studies. However, it is usually the case that calculational schemes, used successfully for core parameter determination in UO_2 or metallic uranium lattices, result in systematic discrepancies, when extended and applied to U-Pu lattices, so that semi-empirical nuclear data adjustments are necessary. These discrepancies are especially sensitive to the changes in ^{240}Pu concentration and the lattice pitch, i.e. to thermalization and transport effects.

As is known, plutonium cores, compared with uranium cores, are expected to show improved stability and transient characteristics, because they have more negative Doppler and moderator temperature coefficients due to plutonium resonances, increased resonance absorption and spectrum shift. On the other hand, the control-rod efficiency is reduced as a result of thermal flux reduction, which necessitates an increased number of control rods. Moreover, there is a reactivity penalty caused by intensified resonance effects and yield of fission product poisons. Because of all these effects, more elaborate methods are required for U-Pu lattice calculation, especially for prediction of adequate reactivity and power distribution control.

This paper contains a comprehensive review of the methods for core parameter determination in U-Pu lattices developed in Yugoslavia during the last few years. Faced with the problem of using small computers, the authors had to look for new approaches combining physical evidence and mathematical elegance. The main feature of these approaches is the tendency to proceed with analytical treatment as far as possible and then to include suitable numerical improvements. With this philosophy, which is often overlooked when using large computers, fast and reasonably accurate methods have been obtained. They contain original developments for adequate treatment of neutron spectra, cell geometry and core composition effects, especially suitable for U-Pu systems.

2. LATTICE CELLS

2.1. Thermal-neutron region

Thermal-neutron spectra in plutonium-containing reactor lattice cells are strongly influenced by the 0.297-eV resonance of ^{239}Pu and the 1.055-eV resonance of ^{240}Pu . To treat adequately both thermalization and resonance effects, detailed multi-group calculation is usually required. In the course of Swedish-Yugoslav co-operation, a new idea was developed [1] to replace the standard multi-group method by discrete representation of the neutron spectra according to the Gaussian quadrature scheme. The accuracy of the plutonium reaction rate integration was improved by introducing different integration variables in different parts of the thermal-energy region and clustering the integration points around the plutonium resonance [2]. Furthermore, the convergence of the method, as regards the number of integration points, was improved by splitting the flux under the energy transfer integral into a Maxwellian part and a hardening part with an energy dependent amplitude [3]. When the preliminary guess of the hardening function is good, this approach can be fairly efficient, since only the interpolation in the hardening function amplitude is to be performed.

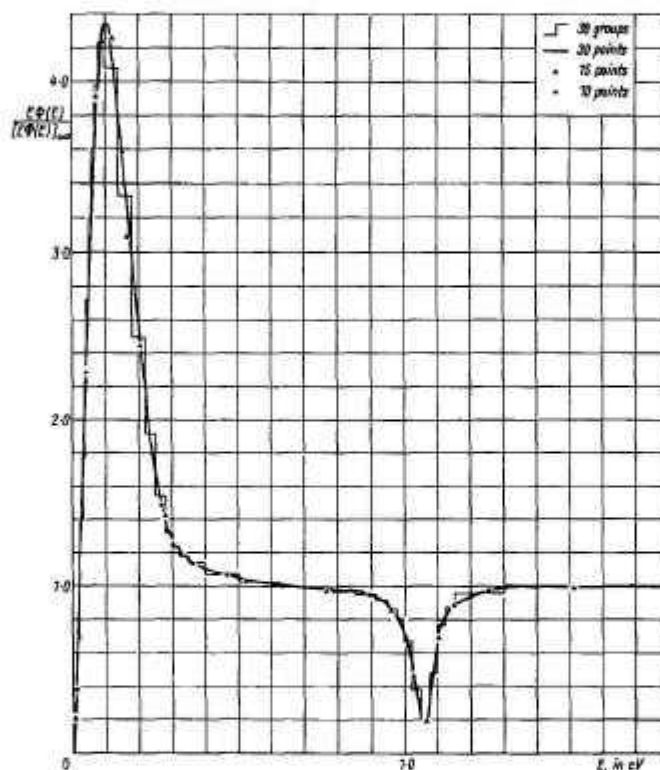


FIG. 1. Thermal-neutron spectrum in fuel of a two-region reactor cell: fuel radius, 0.75 cm; cell radius, 2.25 cm; temperature, 500 °K; ^{239}Pu and ^{240}Pu enrichment, 0.1%.

A system of multi-point equations, formally identical to multi-group equations, was derived [4]. The applicability of the energy point method for heterogeneous systems was examined by combining it with the collision probability technique. The routines PIN and SOMAT [5] were written for calculating thermal neutron spectra and reaction rates in a two-zone Wigner-Seitz cell. Both multi-point and multi-group calculations were performed for a number of different cases, the typical examples being illustrated by Figs 1 and 2. The number of energy points needed to achieve the pre-assigned accuracy of reaction rate integration was shown to be considerably lower than the corresponding number of energy groups.

To study the thermalization effects in a reactor lattice cell, the P_3 approximation of the spherical harmonics method was extensively used and a method was suggested for efficient solution of multi-group or multi-point P_3 equations [6]. A computer program, MULTI, was developed [7] to calculate the space and energy distribution of thermal neutrons in a multi-zone cylindrical lattice cell, using either the multi-group data calculated by program SIGMA or the multi-point data computed by program CAMP [8].

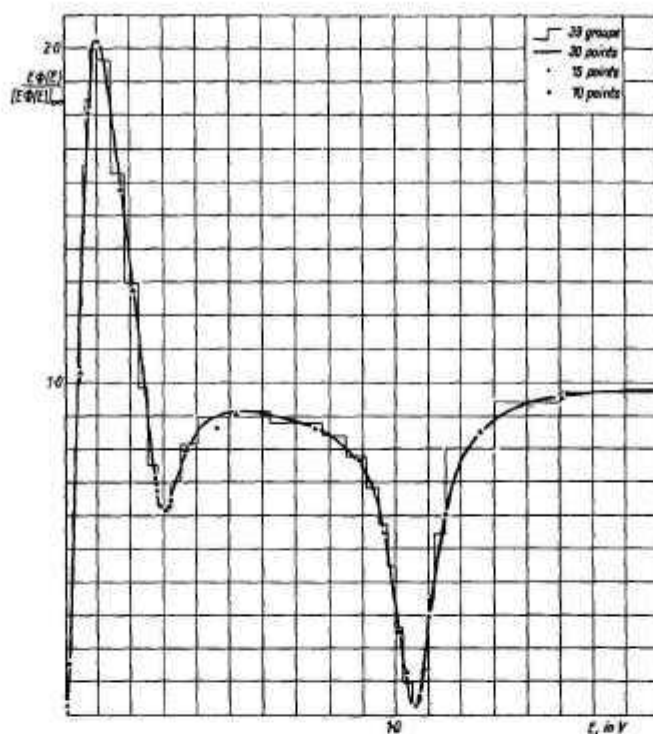


FIG. 2. Thermal-neutron spectrum in fuel of a two-region reactor cell: fuel radius, 0.75 cm; cell radius, 3 cm; temperature, 500 °K; ^{239}Pu and ^{240}Pu enrichment, 0.5%.

In the program CAMP, a procedure was developed for the point scattering matrix construction based on the Lagrange interpolation scheme. Instead of splitting the neutron flux under the energy transfer integral into the Maxwellian part and hardening part, it was approximated by a third degree polynomial with coefficients depending on the flux values at the four neighbouring integration points. The total balance condition is satisfied through the iterative procedure of solving the system of multi-point P_3 equations, which makes this approach much simpler and more straightforward than that suggested in Ref. [1].

Another improvement of the point method was obtained by more exact integration of neutron absorption. Instead of using the Maxwellian amplitude [1] or the iterative procedure applied in Ref. [8], the neutron balance condition was obtained by a more convenient distribution of energy points. The slightly increased thermal energy interval was divided into four sub-intervals according to the physical properties of U and Pu isotopes and a suitable integration procedure was proposed for each interval. The same integration functions were used for determination of scattering matrices.

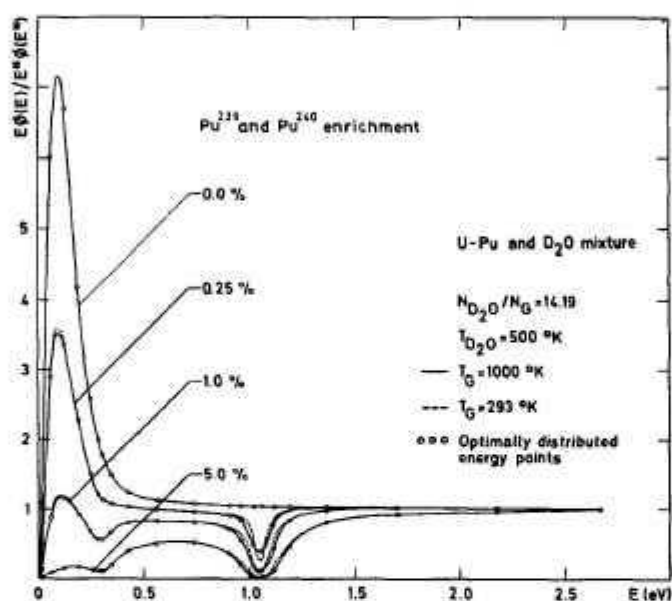


FIG. 3. Neutron energy spectra for different plutonium enrichments.

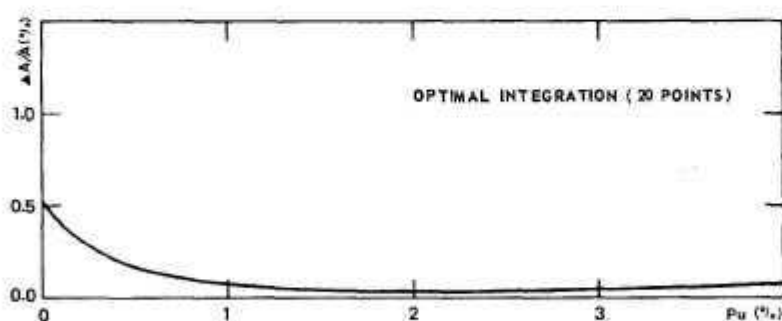


FIG. 4. Accuracy of the reaction rate calculation as function of the plutonium concentration.

The Doppler broadening of Pu resonances was also taken into account. In this procedure, a thermalization program PLUTON was developed and some of the results obtained are presented in Figs 3 and 4.

To take into account the space variation of the thermal flux inside the cell, an investigation was carried out on connecting the collision probability treatment with the energy point method. Starting from a collision probability study for concentric cylindrical zones [9], a corresponding space point method (based on the combination of analytical and numerical approaches) was developed [10]. For every chosen space point, the integral transport equation was written and the flux between the points was interpolated by a

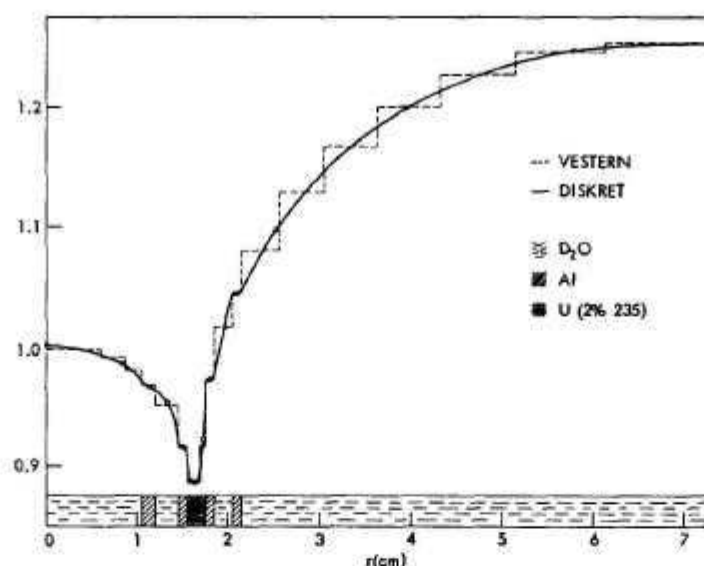


FIG. 5. Thermal-neutron flux distribution in RA reactor cell (VESTERN and DISKRET computer programs).

series in even powers of the radius. The system of linear algebraic equations obtained gives the flux at the desired points. In Fig. 5 some of the results obtained by the method described are compared with the standard collision probability treatment. The application of the method to multi-group calculations is straightforward, as shown in Ref. [11]. The method is also adapted to cluster-type fuel elements [12].

Another rapid and reasonably accurate procedure suitable for Pu lattice calculation is the program ANTER, based on the analytical method for calculating neutron thermalization [13, 14]. In this method, use is made of the energy-dependent boundary conditions combined with the collision probability technique in the fuel and the Laguerre polynomial expansion in the moderator [15]. In many burn-up programs, for instance in the Swedish BOP and the Yugoslav TER [16], the one-velocity ABH procedure [17] is used for disadvantage factor calculation. The accuracy of such programs may be improved by the substitution of ABH by ANTER, since the latter has been shown to give considerably better results [18]. Some comparisons of both methods with the THERMOS procedure and experiments can be seen in Fig. 6.

2.2. Resonance neutron region

In treating the resonance effects in a reactor cell, the usual assumptions are: a spatially flat flux in every cell zone and an asymptotic $1/E$ spectrum between the resonances. As a result, a number of semi-empirical corrections are necessary. In addition, an adequate connection with the usually

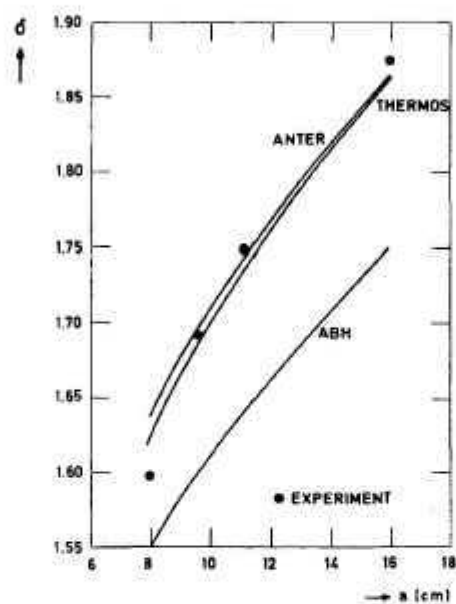
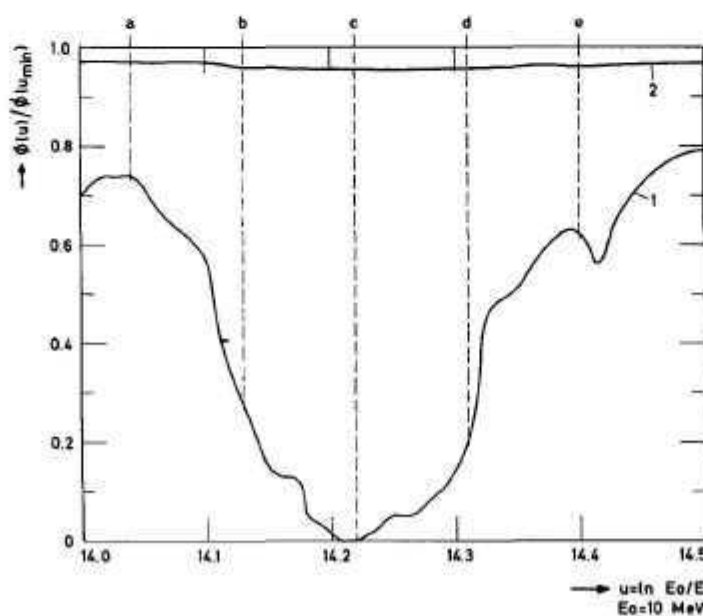


FIG. 6. Cell disadvantage factors for different lattice pitches of RB reactor cell.

FIG. 7. Lethargy distribution of the average flux in fuel (1) and the average flux in moderator (2) in the vicinity of the 6.7-eV resonance of ^{238}U .

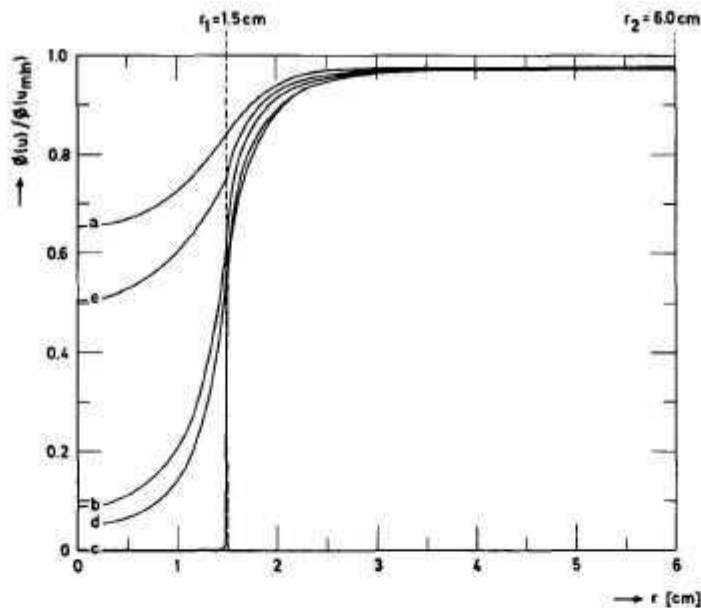


FIG. 8. Space distribution of resonance-neutron flux for the energies denoted by a-e in Fig. 7.

detailed treatment of the thermal neutron region is impossible. Moreover, more rigorous treatment of the resonance region is particularly important for adequate Pu build-up prediction.

To overcome these shortcomings, a new procedure was developed to solve the space-, lethargy- and angle-dependent transport equation for resonance neutrons. In the resonance region, the neutron scattering is isotropic, but, since the values of cross-sections in different zones of a reactor cell are widely different, the neutron flux near the zone boundaries becomes very anisotropic. For this reason, the P_3 approximation of the spherical harmonics method was applied, resulting in a system of integro-differential equations with a difference kernel depending on lethargy and space. Combining the analytical and numerical procedures, the expressions are obtained for the space and energy distributions of resonance neutrons in a multi-zone reactor cell [19]. The accuracy is limited practically only by input cross-section data, and the computing time is relatively short, so that it is convenient for incorporation in burn-up programs. Some results for resonance-neutron flux distributions in the centre of a fuel element and at its surface are shown in Figs 7 and 8. To investigate in detail the effects of ^{238}U resonances (where the build-up of plutonium occurs) the flux distributions near a giant 6.7-eV resonance and the corresponding space and lethargy distribution in a cell are calculated and presented in Figs 9 and 10, respectively.

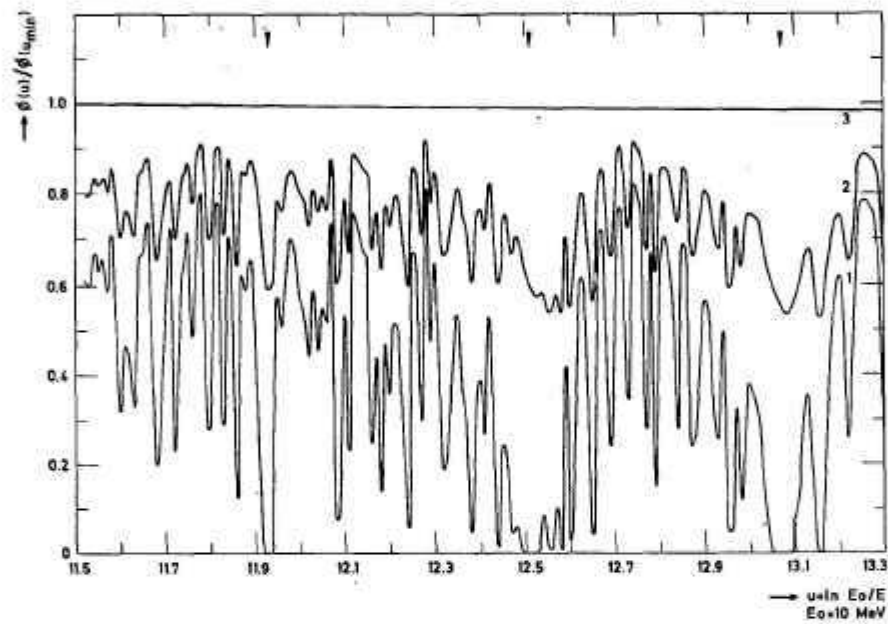


FIG. 9. Lethargy distribution of resonance-neutron flux in the centre of fuel element (1), at the surface of fuel element (2) and at the surface of the cell (3), in the interval 10 eV - 100 eV.

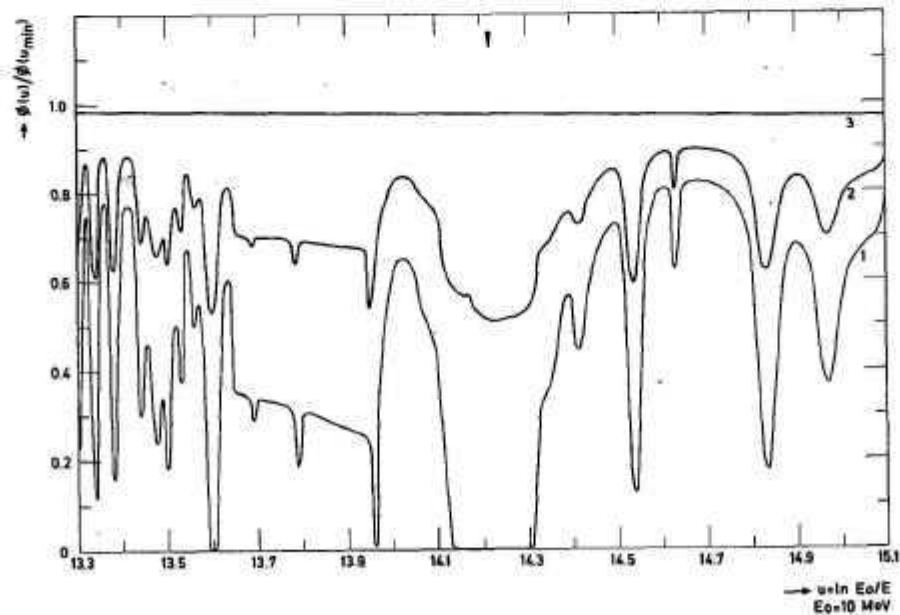


FIG. 10. Lethargy distribution of resonance-neutron flux in the centre of fuel element (1), at the surface of fuel element (2) and at the surface of the cell (3), in the interval 1 eV - 10 eV.

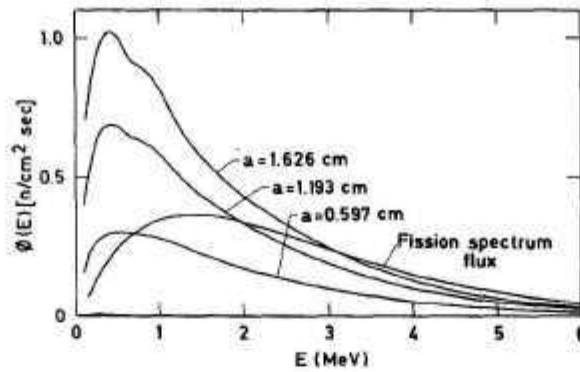


FIG. 11. Energy distribution of the fast-neutron flux in a natural uranium fuel element.

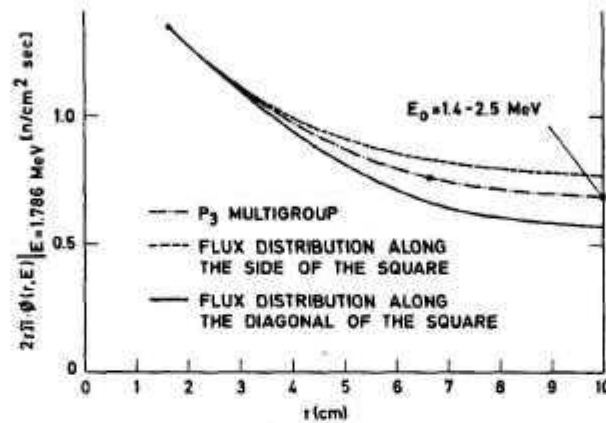


FIG. 12. Space distribution of the fast-neutron flux in the moderator of a natural uranium - D_2O cell, taking into account anisotropic elastic scattering: rod diameter, 1.626 cm; lattice pitch, 17.7 cm.

2.3. Fast-neutron region

The fast region is relevant to the problem of Pu build-up, mostly through supplying adequate sources for resonance neutrons. Here the problem of fast-neutron transport and slowing down becomes important. An exact analytical method for solving the problem of the slowing down of fast neutrons was developed recently [20]. The solution of the slowing down equation was obtained indirectly, by detailed consideration of the neutron slowing-down process. By representing the collision density by a sum of collisions with different prior histories and substituting Green functions by Dirac delta functions, the problem was reduced to determination of neutron scattering functions. These functions were determined by factorization in lethargies (in treating the inelastic scattering) as well as by expansions in cosine of the scattering angle (in treating the elastic scattering). The expression obtained for collision density is valid for arbitrary dependence of cross-sections on energy and angle.

With the Green function technique, the method was applied to a reactor lattice cell [21]. The space energy distribution of fast neutrons in a reactor cell was also determined by the multi-group P_3 procedure with the modified MULTI program [22], as well as by the multi-group collision probability procedure [11]. Some of the results obtained by these methods are displayed in Figs 11 and 12.

3. REACTOR CORE

3.1. Material buckling

U-Pu lattices represent a typical example of the so-called mixed lattices, which contain different types of fuel. In the equilibrium state, by continuous fuel exchange, fuel elements of different uranium and plutonium compositions are uniformly arranged in the reactor lattice. In some cases, e.g. in a reactor with steam superheating, fuel elements of different geometries and compositions are uniformly arranged in the lattice from the very beginning of the operation. To solve the criticality problem, elaborate methods are required, such as the heterogeneous method or the numerical three-dimensional calculation of the reactor core.

When treating the long-term fuel composition changes to determine the maximum fuel burn-up, it is necessary to solve the criticality problem many times, so that application of the above-mentioned methods is laborious and time consuming, even for large-capacity computers. Since fuel elements of different nuclear compositions are uniformly arranged over the whole reactor lattice, it is possible to define the material buckling for a uniformly mixed lattice and to reduce a criticality problem to a problem of finding the roots of the two-group critical equation.

With two types of fuel element, the validity of the definition of the material buckling for the mixed reactor core was experimentally investigated on the Yugoslav heavy-water zero-power reactor RB [23]. Some of the results are presented in Fig. 13. The validity of the adopted simple definition of the material buckling for mixed reactor core, as linearly dependent on the configuration factor, was confirmed.

3.2. Criticality

To be able to establish the best national fuel management policy, special efforts were devoted to the development of fast and reasonably accurate methods for overall reactor core calculation. In addition to the already mentioned burn-up program TER, a criticality program, REDIR, was developed [24]. Galanin's method of effective boundary conditions was used with a two-group calculated effective reflector thickness. The program calculates radial and axial macroparameters and fuel-element burn-up. To calculate U-Pu lattices, suitable averaging procedures have been included. The validity of the assumptions involved in the program was checked by the Feinberg-Galanin heterogeneous method applied in the criticality program HETERO [25], as well as by the experiments described in Section 3.1.

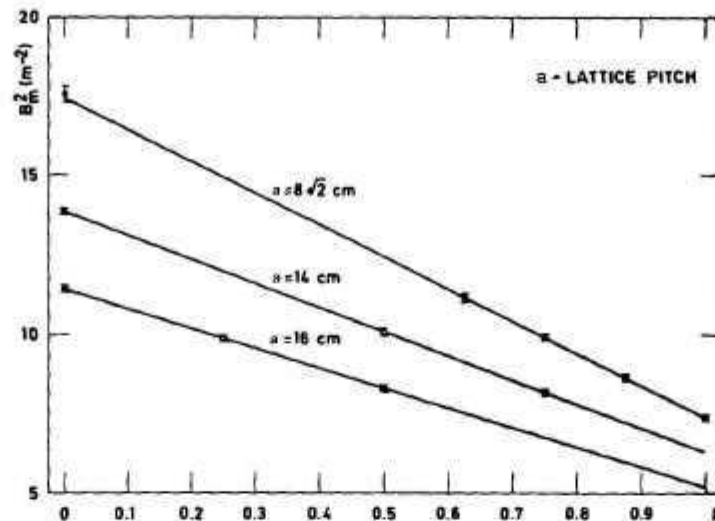


FIG. 13. Material buckling for reactor lattices composed of two types of uniformly arranged fuel elements as function of fraction factor k .

The criticality programs developed were used to study the different refuelling schemes with or without plutonium recycling. Some results of these investigations, including the recommendations for countries with rather small nuclear power programs, are presented in Refs [26] and [27].

3.3. Optimization of core configuration

In designing nuclear reactors and in operating them, a series of problems of variational nature is encountered. The extreme of a physical magnitude is always sought, e.g. minimum critical mass, minimum critical dimensions, maximum reactor power, maximum neutron flux, minimum poisoning after reactor shutdown, minimum time of reactor shutdown, and the like. The function that is varied depends on the nature of the problem investigated. This may be the space distribution of fuel or absorber concentration, the neutron flux, the reactor power, etc. For constructional, thermic, or other reasons, this function is always limited, making these kinds of variational problem non-classical, so that Pontryagin's maximum principle or Bellman's dynamic programming have to be applied.

In the case of U-Pu lattices, the particularly relevant problems are based on the possibility of varying the space distribution of fuel concentration. The shortcoming of all existing solutions is that this distribution is assumed in advance. Here, a direct approach to this problem is defined: to determine the space distribution of fuel concentration in the reactor core directly from the extreme of a desired physical magnitude, satisfying the thermic restrictions.

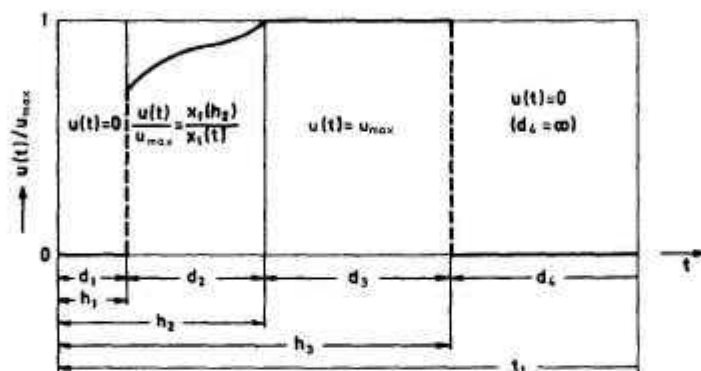


FIG. 14. Optimal core configuration for high-flux reactor.

The mathematical formulation of the above problem is given in Ref. [28] and some applications to the optimization of reactor core configuration are presented in Ref. [29]. For example, the optimal fuel configuration of the reactor core, obtained in the case of a high-flux reactor, consists of a reflector in its centre, a zone of constant (permissible) power density, a zone of constant (maximum) fuel concentration, and a peripheral reflector of infinite thickness (Fig. 14).

The choice of an adequate model of the process in the optimization procedure developed plays an important role. The model presented here is based on the two-group diffusion theory of neutrons, and is given for arbitrary core geometry. However, the same optimization procedure is also applicable with the multi-group diffusion model.

In a similar way, with a corresponding model of the process, numerous problems in reactor kinetics and the control of U-Pu cores can be solved.

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