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New methods in transport theory, (part of a coordinated programme on methods in neutron transport theory

FINAL REPORT FOR THE PERIOD

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FINAL REPORT

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TITLE

New Methods in transport theory

RESEARCH INSTITUTION

Boris Kidrič Institute of Nuclear Sciences, Beograd-Vinča, Yugoslavia.

PRINCIPAL SCIENTIFIC INVESTIGATOR

D.Stefanović

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SCIENTIFIC BACKGROUND AND SCOPE OF PROJECT

Neutron transport theory is the basis for development of reactor theory and reactor calculational methods. It has to be acknoledged that recent applications of these disciplines have influenced cosiderably the development of power reactor concepts and technology. However, these achievements were implemented in a rather heuristic way, since the satisfaction of design demands were of utmost importance. Often this kind of approach turns to be very restrictive and not adequate even rather typical reactor applications.

Many aspects and techniques of reactor theory and calculations ought to be reevaluated and/or reformulated on the more sound physical and mathematical foundations. At the same time, new reactor concept and operational demands give rise to more sophisticated and complex design requirements. These new requirements can be met only by the development of new design techniques, which in the case of rector neutronic calculation lead directly to the advanced transport theory

methods. In addition, the rapid development of computer technology opens new opportunities for applications of advanced transport theory in practical calculations.

RESULTS OBTAINED

(I) ANALYTICAL SOLUTION OF THE NEUTRON SLOWING DOWN TRANSPORT EQUATION AND EXTENSION OF THIS SOLUTION TO INCLUDE THE ENERGY DEPENDENCE OF THE ANISOTROPY OF THE NEUTRON SCATTERING.

The research activity was concentrated on the problem of solving neutron slowing down equation for the case of anisotropic scattering of neutrons. The differential scattering cross section is expanded into an approximative series via Legendre polynomials. Coefficients of the expansion have been determined on the basis of the experimental data concerning the scattering anisotropy taken from the literature. The assumption was that the scattering anisotropy was independent of neutron energy. An analytical procedure for solving the problem has been applied. The results of this approach are Green functions describing neutron slowing down.

The problem of neutron slowing down in an infinit medium with the energy dependent anisotropy of elastic scattering has been solved and discussed in papers /5/, /6/, /7/ and /19/. The scattering cross section is represented by the expansion via Legendre polynomials with energy dependent coefficients. This made it possible to develop a procedure of matrix degeneration of the kernel of the integral slowing down equation and the transforming of such an equation to a differential equation giving Green slowing down functions and also collision density of fission neutrons.

The results for neutron slowing down are obtained with energy dependent and independent anisotropies of scattering in P_o, P_1 and P_2 approximations.

(I) NUMERICAL SOLUTION OF THE FAST AND RESONANCE NEUTRON TRANSPORT EQUATION FOR THE CASE OF MIXTURE OF SCATTERERS AND INCLUDING THE INELASTIC SCATTERING EFFECTS.

The space-angle-lethargy dependence of epithermal neutron flux in a cylindrical reactor lattice cell was described by a system of P_3 spherical harmonics (SH) formalism and a combined analytical-numerical procedure to solve these equations was proposed.

The matrix formulation of the P_3 SH equations was introduced, with the vector of the SH flux moments as the unknown, space and lethargy dependent vector function. The numerical procedure, based on the fine discretization of lethargy variable, was first proposed for describing the lethargy dependence of the flux moments in purely slowing-down region. In order to account for the fast-fission and inelastic-scattering effects, this was later extended to the energy region by introducing a convenient iterative scheme.

For several successive lethargy points an exact analytical solution was derived for the space dependence of the SH flux moments. This exact solution, existing only in highly unrealistic situations and of no practical interest, was then used to formulate and to examine a new procedure for determining an approximate analytical solution for the vector of unknown SH flux moments. The procedure was based on the convenient approximation of the RHS of the SH matrix differential equation and was proved to be very efficient.

The space dependence of the SH flux moments at succesive lethargy points was formulated in the form of recurrence relations, suitable for computational use. For lethargy values arround the strong resonanc an asymtotic expression for the space dependence of the SH flux moments was derived. Finally, a matrix formalism was proposed to solve a system algebraic equations stating the continuity and boundary conditions of the SH flux moments. Accounting for the particular, block-bidiagonal form of the coefficient matrix, this procedure was proved to be more efficient than standard (for instance Gauss

elimination) methods, especially when iterative treatment and many lethargy points were required /1/.

Substituting the lethargy transfer integral by its finite-difference from, the system of matrix integro-differential equations for the vector of the SH flux moments was reduced to the system of matrix ordinary differential equations, which could be solved eiter by successive elimination or by an iteration technique. The choice of the lethargy step for numerical integration over lethargy has now been studied in detail, particularly for the case of slowing-down in a mixture of different scatterers. The convergence of the method in respect to the lethargy step has been examined. Also, the convergence of the iterative procedure has been studied in connection with treating the inelastic scattering and fast fission effects.

The proposed method resulted into a set of recurrence relations for the space dependence of the SH flux moments at succesive lethargy points. These relations are linear combination of the modified Bessel functions of the first and second kind, the coefficients being the unknown integration constants, which have to be determined by solving system of algebraic equations stating the interface and the boundary conditions. However, large arguments of the Bessel functions, caused by the extreme cross-section values in the resonance region, head to machine overflow or underflow. The new expression for the space dependence of the neutron flux moments have been derived in terms of the functions which are defined so to have the values of approximately the some order of magnitude for all possible values of the arguments.

The program SPLET, written in FORTRAN IV for CDC 3600 computer, can produce the space-lethargy distribution of epithermal neutrons in a cylindrical reactor lattice cell, as detailed, as the neutron cross-section are available for the materials of interest /9/. An efficient routine has now been written for generating the given of data, for the given isotope and at the given lethargy, from the KEDAK nuclear data tape /8/.

(III) IMPROVEMENT OF THE EXISTING FORMALISMS FOR TREATING THE SCATTERING OF NEUTRONS ON WATER MOLECULES.

The Van Hove expression of the differential scattering cross-section, in the form of Fourier transform of the correlation function, has been expanded over Legandre polynomials. The obtained expression show that the scattering kernel may be written as a Fourier transform of the spherically symetrical correlation function. By the proposed procedure, and using the Nelkin's formalism to derive the width function which appears in the correlation function of the gaussian form, an analytical expression of the scattering kernel has been obtained. This expression takes the form of a sum over all excitation modes of molecules.

A similar method has also been used to derive the total neutron cross section. It has been shown that this quantity can be represented as a Fourier transform of a function related with the correlation function. Hence, all methods developed for the determination of the correlation function may directly be used to obtain the scattering kernel and the total neutron cross-section.

In the case when the correlation function has the gaussian form, a simple expression for the total neutron cross section has been obtained. It has been proved numerically that this expression is advantageous when compared to the standard expressions for the total cross-section, which all require the double integration /2/.

(IV) MODAL ANALYSIS IN TRANSPORT THEORY

Identifying modal analysis as the Galerkin (projection) method, general conditions for modal technique applications have been investigated. It is shown that under some very general restrictions on the performance index the Galerkin method is applicable to the Hamilton-Jacobi canonical equations. Using the Keldish theory of operator families, the conditions for completness of the eigen-vectors of the Hamilton-Jacobi operator

are established. If these vectors are used as expanding functions in the Galerkin method a rather simple algorithm for computing the optimal control law can be obrained. An iterative variational method for the solution of an eigenvelue problem has been developed enabling on-line implementation of the overall optimization algorithm through a two-level control system. Reactor models for a power control system and a flux distribution control system synthesis are particularly investigated. The methods are illustrated in a simple example of a slab reactor /3/.

(V) INVERS PROBLEMS IN TRANSPORT THEORY

The use of a low-resolution neutron spectrometry apears to be very suitable in certain applications. However, the problems arising in the interpretation of the measured data often limit the accuracy or even preclude the application of such methods. In the present study the unfolding of neutron energy spectra using low-resolution data has been investigated and developments both in techniques and methodology are reported. A theoretical study of the properties of the activation equation has been performed and its close relationchip with the Fredholm integral equation is established. It is pointed out that such a problem is mathematically incorrectly posed and does not allow for a direct solution. Thus, the inherent instabilities of the unfolding procedure are explained.

The method of regularization, devised for the approximate solution of the operator equation of the first kind, is applied to solution of the activation equation. It is shown that instead of solving the activation equation using direct methods, a solution should be sought by minimizing the so called additive functional. The choice of the regularizing part of the additive functional has been discussed thoroughly.

A use of a simple theoretical model reflecting the basic physics of the problem has been proposed for the construction of the regularizing functional. Various underlying numerical techniques have been examined and associated computer programs have been written.

The proposed unfolding method was tested in a series of numerical experiments and measurements of thermal-neutron spectra in some of the lattices of a heavy water-natural uranium zero power reactor. A use of the filtered foil technique is investigated and the results are reported. In addition, the unfolding of some literature results obtained using photographic emulsions, proton-recoil proportional counters, Bonner spheres, and threshold detectors has been performed using the proposed method /4/.

(VI) EVALUATION OF AN ADVANCED LEVEL DISTRIBUTION FUNCTION, IMPROVEMENT OF THE STANDARD FORMALISM FOR TREATING THE INELASTIC SCATTERING AND DEVELOPMENT OF A CLUSTER NUCLEAR MODEL FOR THESE EVALUATIONS.

A rigorous method for describing fast neutron inelastic cross-sections has been developed by ising generalized Faddeev-Yakubovsky equations of many-particle non-relativistic quantum mechanics. However, a direct use of Faddeev-Yakupovsky equations in the case of a great number of nucleons seems to be dificult. For this reason a strong cluster nuclear model has been proposed, i.e. the nucleus has been described as a system of several strong clusters, by means of their binding energies. The interaction potentials between chosen clusters have been derived directly from Faddeev-Yakupovsky equations taking account of the spin and isospin. TEaddFaddeev-Yakupovsky equations have been reduced to a few-particle equation which can be solved easily. From derived equations it is possible to obtain S-matrix elements, nuclear binding energies or nuclear spectral functions, and fast neutron inelastic and elastic cross-sections /10/, /11/.

Explicit equation have been written for the case of fast neutron scattering by ^{6}Li. To assess the validity of the proposed model, a computer program for calculating fast neutron cross-sections has been developed following standard Hauser-Feshbach theory /12/, /13/.

(VII) NEUTRON TRANSPORT TREATMENT IN SPACE POINT ENERGY GROUPS FOR CRITICALITY CALCULATION OF A REACTOR CORE.

The presented theorethical and computing methods, based on combining analytical and numerical approaches, resulted in reasonably accurate models with reduced computing time and capacity requirements. In particular, the polynomial expansions, energy dependent boundary conditions, discretization of variables and pontryagin's method were used. Special consideration was devoted to the space-energy neutron flux distribution in the lattice cell, to the material buckling in mixed lattice and to the optimization of the reactor core configuration. The comparaisons with the experimental results obtained by the Yugoslav research reactors RA and RB were performed /20/.

The lattice cells of a power reactor are very complex, both in geometry and composition. Therefore it is not possible to obtain exact analytical solutions of the Boltzmann equation for these cases. Accurate numerical transport theory approaches (as higher order S_n, P_n, C_n and also Monte Carlo) are mostly employed to calculate some special effects and to examine the soundness of various physical approximations, thus supplying accurate results for comparison with simpler methods. On the other hand, the difusion theory methods cannot be applied, due to the strong absobing properties and the relatively small size (compared to the mean free path) of the lattice cell components. An effective approach to overcome these difficulties is the use of collision probability methods based on integral transport theory. The chapter 3. of the reference /21/ containes the new developments in integral transport theory and their application to lattice cell calculation, performed within the frame of this research contract.

(VIII) DEVELOPMENT OF THE MONTE CARLO SAMPLING SCHEME FROM THE NEUTRON TRANSPORT EQUATION.

The usual diffusion theory approximations are not valid in a real reactor cell due to severe local inhomogeneties. For calculating mean neutron flux over the space zones in the reactor cell two main subject have been studied: Monte Carlo forward sampling schemes for neutron transport; peculiarities of the reactor cell mean flux calculation and selection of the convenient Monte Carlo method.

The method Monte Carlo was also used for treating of the light water lattice cell. Both the problem of taking into account the anisotropy of elastic scattering cross-section and the problem of fuel assembly composition has been considered /14/, /15/, /16/.

L. Cveljanovic

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Lattice cell burnup calculation,
A series of invited lectures at the IAEA Review Course at Mol, Belgium, 7.-18. Oktober 1974. (Chapter 3).

STATEMENT OF PROJECT EXPENDITURES

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Title of Project: New methods in transport theory
Institute where research is being carried out:
Boris Kidrič Institute of Nuclear Sciences, Belgrad-Vinča
Chief scientific investigator: Dr Dušan Stefanović
Time period covered: 1 August 1972. - 1 August 1975.

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Expendable Supplies (computer cards, and magnetic tapes)..	US $	8.000
Computer costs	US $	28.000
Travel	US $	1.400
TOTAL:	US $	178.400

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