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THE NEUTRON PHYSICS CONSTANTS BANK OF THE I.V. KURCHATOV INSTITUTE OF ATOMIC ENERGY

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ABSTRACT

This paper describes the structure and contents of a neutron physics constants bank consisting of libraries, service programs and data preparation codes for reactor calculations. Use of the bank makes the constants fully accessible to users.

In the field of reactor calculation wide use is made of various libraries of neutron physics constants, which describe the interaction between neutrons and nuclei. The principal libraries have been linked up to form a bank (see table). All the libraries are magnetically recorded in the same way, use identical software, and permit the use of a single system for preparing the constants for reactor calculation codes. Hence these libraries, when all put together, can be called a bank.

All of the libraries in the bank, along with their software, are recorded on a collectively-used disk, available to all computer users in the form of a print-out and also in non-readable form as a recording. The bank also contains a number of programs for preparing reactor constants.

The authors of the bank's software took as their starting point the fact that reactor program users must have free access to the source data contained in constants libraries. In other words, it must be made possible for information to be drawn without difficulty from the libraries, for it to be printed out and, if necessary, corrected.

All the libraries are magnetically recorded on disks in the form of texts. The recording unit is an 80-symbol card. The libraries have various information recording formats, but the information is always arranged hierarchically (for example, in the case of multigroup constants, by nuclide,

group and section). Each card bears a number showing the hierarchy and the exact location of the card in the library.

For the purposes of library work information recorded in textual form permits the use of a text processing system which has long been used on all types of computer. In the case of the BEhSM-6 computer this takes the form of an editor program which is part of the standard software. The editor program's capabilities are increased by incorporating extra commands. It is, in particular, possible to extract information located in various parts of the library but linked by a common characteristic (for example, in the case of a multigroup library, the mean group cross-sections of the elements of all or of particular groups).

The TEKDA [1] software for library work makes it possible: to create a temporary library containing only the information required for a particular calculation; to alter and add to the information held in the temporary library; to extract and print out reference information on the composition of the permanent and temporary libraries; to read the library material in the form of programs in FORTRAN.

In this way it is possible, in the course of calculation, to change the source data at will, while at the same time ensuring that the main library remains intact. The editing system is particularly suitable for matching the constants.

A further advantage of libraries recorded in textual form is their ease of adaptation to different types of computer. However, the textual recording of numerical information has a disadvantage in that extra time must be spent on re-encoding. Therefore, for mass operational computation it is advisable to set up a working library and to record it on a magnetic disk in non-format form. The format of a working library must be geared to a specific program.

Libraries recorded in textual form we shall henceforth refer to as base libraries, as opposed to non-format working libraries.

The BNAB constants system

This is the basic system for fast reactor calculations. The latest version, BNAB-78 [2], is recorded in the bank. It contains the resonance parameters of the main fissile and source isotopes, calculated using a generalized subgroup approach [3]. This permits the resulting constants system also to be used for calculations relating to heterogeneous thermal reactors. The BNAB constants are recorded in the bank in a format specially devised for this purpose, called TEMBR [4]. It is closely related to the well-known ENDF/B [5] format, but it also takes account of the specific nature of multigroup constants.

The MARS [6] program has been written for the preparation of macroscopic reactor constants. It uses the same algorithms as are used in the ARAMAKO-2F [7] program, which is recommended by the authors of the BNAB library. The MARS program is arranged in the form of a module, and the results of work conducted with it are recorded on an external carrier. The recording is built up from separate records, each of which contains precisely determined items of information of the same kind. The records are given names for location and counting purposes. There are search and readout programs which outwardly imitate direct access. The working library of the MARS program is also recorded in the TEMBR format. It differs from the base library in its data hierarchy, which is arranged: group - section - material. The information required may thus be read in the course of a single viewing of the library. The editor program BINED has been written to service the working library, and makes it possible to select any information required from the library and to put together a temporary working library, which may, if necessary, be modified.

There is a large family of reactor programs for use mainly in fast reactor calculation. The fast reactor constants are prepared by means of the ARAMAKO-2F [7] or MIM [8] programs. In order to include them in the bank, the

Name of library; country or organization; year established	Contents	Constant preparation programs
ENDF/B: IV - full V - partial USA, 1974, 1979	Evaluated data on all neutron-nuclei interaction characteristics (0.005 eV $\leq E \leq$ 20 MeV)	MINX, GRUKON, NEDAM
ENDF - LLL USA, 1976		
UKNDL, United Kingdom, 1971		
BNAB, FEhI[*], 1978	26-group constant system for reactor and shielding calculation	MARS, ARAMAKO-2F, MIM
KORT, IAEh[**], 1980	Constants for thermal reactor calculation	TERMAC
LIPAR, IAEh, 1983	Evaluated resolved resonance parameters	CROSS

[*] FEhI: Institute of Physics and Power Engineering.

[**] IAEh: Institute of Atomic Energy.

LONT[*] program, written for ARAMAKO, and the TITOBI[*] program, written for MIM, prepare working libraries for these programs. It should be noted that the working libraries, formulated by the authors of the ARAMAKO program and obtained from the bank's library through the LONT program, naturally coincide. The chief advantage of the bank is that it makes constants fully accessible to the user. The same is true for the MIM program.

[*] The LONT program was written by E.A. Makarova, and the TITOBI program by B.A. Stukalov.

Constants for thermal reactors

Reactor calculation requirements in the field of neutron thermalization are supplied by the KORT [9] library. In it are recorded the general characteristics of the nuclei (mass, lifetime, etc.), thermal cross-sections, the energy dependence of cross-sections below 5 eV (where this energy dependence is not subject to the 1/v law), and the number of secondary fission neutrons. The same library contains the oscillation frequency spectrum for atoms of the main reactor moderators. This permits calculation of the differential elastic and non-elastic scattering cross-sections, taking into account the chemical bond and thermal motion of the atoms. For this purpose the bank contains the NEWRAS [10] and ELCOHR [11] programs.

The bank's libraries may be linked to reactor programs through the TERMAC [12] constant preparation program, which prepares and records onto an external carrier either the microscopic partial cross-sections and scattering matrices in a given energy scale (working library), or the macroscopic cross-sections according to a given medium composition.

The resolved resonance energy field

Precision calculations of resonance absorption are provided by the CROSS program package, which has come about through development of the CROS [13] program described earlier. It consists of the LIPAR library of resonance parameters, the CROSN cross-section calculation program and service subprograms.

The LIPAR-3 version of the resonance parameters library contains data on 66 isotopes. It replaces the less complete and partially obsolete LIPAR-1 [13] version.

The CROSN program on resonance parameters is used to calculate cross-sections at one energy point for a given list of isotopes, along with their concentrations and temperatures. The same algorithm is used as when evaluating the parameters of a specific nucleus. The thermal motion of the

nuclei is taken into account, as is resonance and potential scattering interference and, if necessary, resonance interference. The calculation data are obtained from the LIPAR working library. The program for setting up the CROSN program is also included in the package, and the user may add to or change the data. The service programs permit cross-section calculation, depending for this on the ENDF/B evaluated neutron data library.

REFERENCES

[1] CHISTYAKOVA, V.A., YUDKEVICH, M.S., A system for storing, editing and using data libraries on the BEhSM-6 computer [in Russian], Preprint No. 3046, Inst. of Atomic Energy, Moscow (1978).

[2] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for reactor and shielding calculation [in Russian], Ehnergoizdat, Moscow (1981).

[3] TEBIN, V.V., YUDKEVICH, M.S., Sub-group parameters in the resolved resonance region [in Russian], Preprint No. 3955/5, Inst. of Atomic Energy, Moscow (1981).

[4] OSIPOV, V.K., CHISTYAKOVA, V.A., YUDKEVICH, M.S., TEMBR - a format for the textual recording of multigroup constant libraries for reactor and shielding calculation [in Russian], Voprosy Atomnoj Nauki i Tekhniki, Ser. Fizika i Tekhnika Yadernykh Reaktorov 8 (21) (1982) 62.

[5] Data format and procedures for the evaluated nuclear data file, BNL-NCS-50496 (ENDF-102) (1975).

[6] OSIPOV, V.K., CHISTYAKOVA, V.A., YUDKEVICH, M.S., Voprosy Atomnoj Nauki i Tekhniki, Ser. Fizika i Tekhnika Yadernykh Reaktorov 7 (29) (1982) 86.

[7] BAZAZYANTS, N.O., VYRSKIJ, M.Yu., GERMOGENOVA, T.A., et al., APAMAKO-2F - a system for supplying neutron constants for calculations of radiative transfer in reactors and shielding [in Russian], USSR, Academy of Sciences, Institute of Applied Mathematics, Moscow (1976).

[8] BASHMACHNIKOV, A.I., NF-6 constant supply system, [in Russian], Preprint No. 49 (408), NIIAR, Dimitrovgrad (1979).

[9] ABAGYAN, L.P., YUDKEVICH, M.S., Neutron data library for thermal reactor calculation [in Russian], Voprosy Atomnoj Nauki i Tekhniki, Ser. Yadernye Konstanty 4 (43) (1981) 24-52.

[10] LIMAN, G.F., MAJOROV, L.V., The NEWRAS program for calculating the differential scattering cross-sections of slow neutrons [in Russian], Voprosy Atomnoj Nauki i Tekhniki, Ser. Fizika i Tekhnika Yadernykh Reaktorov 8 (21) (1982) 32.

[11] LIMAN, G.F., The COLCST and ELCOHR programs for calculating total and elastic coherent cross-section scattering in thermal neutrons [in Russian], ibid, 5 (27) (1982) 74.

[12] GOMIN, E.A., MAJOROV, L.V., The TERMAC system for calculating neutron group cross-sections in the thermalization region [in Russian] ibid., p. 70.

[13] TEBIN, V.V., YUDKEVICH, M.S., Neutron cross-section calculation from evaluated resonance parameters [in Russian], Voprosy Atomnoj Nauki i Tekhniki, Ser. Yadernye Konstanty 2 (1978) 29.

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A NEW VERSION OF THE UNIFIED CONSTANT SYSTEM PACKAGE

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ABSTRACT

A unified constant retrieval system called OKS has been developed for convenient access to the constant systems ARAMAKO-2F, ARAMAKO-G, DENSTY, TERMAC and others, in calculating radiation transport, value functions and various functionals. Since the system was first developed in 1980 both its language and its functional contents have been improved and added to. In this paper the input language and performance of the new version are described.

The unified constant system OKS has been developed to provide convenient access to various constant systems in calculating radiation transport, value functions and various functionals (see diagram). The functional contents of the OKS system comprise the well-known constant system DENSTY [1], ARAMAKO-2F [2], ARAMAKO-G [3], the 49-group constant calculation system [4, 5], ARAMAKO-80 [6] and TERMAC [7] and the format converters ARVES [8] and JAST.

Since its development in 1980 the OKS system has been used for solving radiation shielding problems. Intensive work is now under way to develop the ZASHCHITA ("shielding") package [9], in which OKS will be used to solve both shielding and reactor physics problems.

In the course of operating the OKS system additions have been made both to its language and to its functional contents. By comparison with the version described in Ref. [10], the new version of the system [11] incorporates the constant systems TERMAC, ARAMAKO-80 and the 49-group neutron constant calculation system and the following improvements: development of

the JOIN operator, supplementary parpameters for the FORM operator and increased service program content.

OKS language operators

The function of the OKS system is to sequence operators. The operators divide into executable and non-executable according to their functional purpose. An executable operator determines a certain action such as a call for a constant program or a format conversion. A non-executable operator is a description of the objects used in the work of the executable operator. The order in which the operators perform is determined by the order in which they are recorded. The range of action of an executable operator extends to the non-executable operators recorded immediately after it, up to the next executable operator.

The following operators have so far been included in the OKS system: ZONE, CONST, DATA, FORM, TAPE, JOIN, END. Let us now describe them in greater detail.

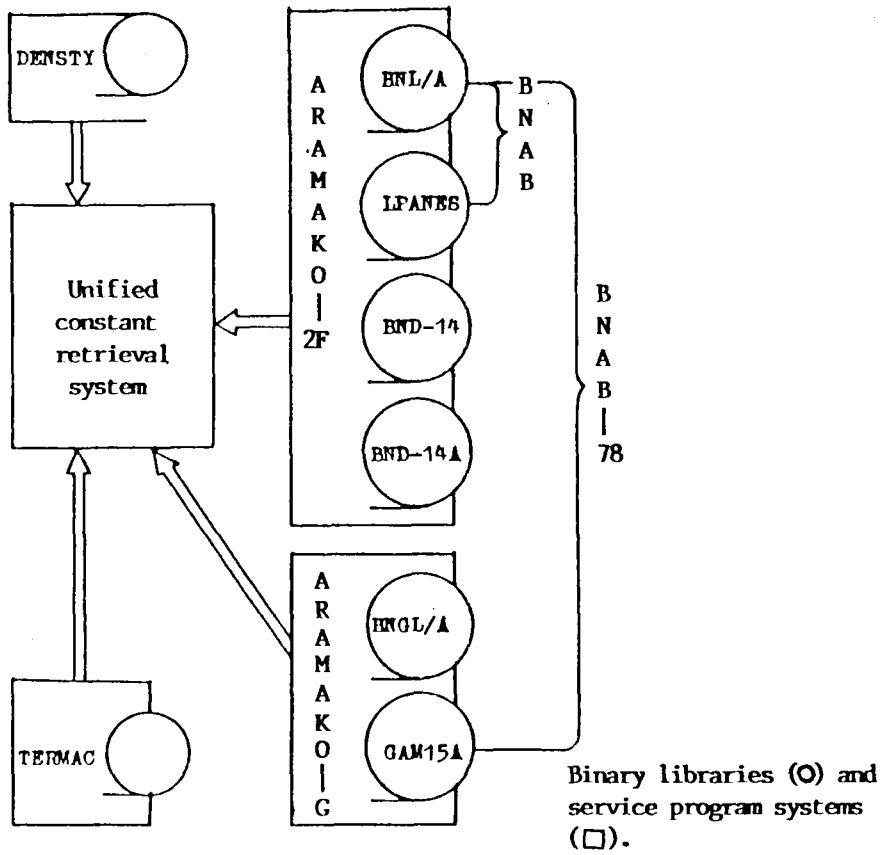
The ZONE operator (non-executable) describes one physical zone (substance), characterized by its physical homogeneous composition. In order to allow for situations in which isotopes within the zone are spatially distributed and have different temperatures, the temperature TI can be given for each isotope individually.

The ZONE operator takes the form:

ZONE: <zone number>, <T>, <name of isotope>, <nuclear concentation>, <TI>.

repeat k times

The zone number is a positive integer; T is the overall temperature of the zone (K). Next come the three parameters describing the isotope: TI is the temperature of the isotope. If TI is not stated, it is tacitly assured to be equal to T. The temperatures and nuclear concentrations are real numbers. The name of the isotope is an identifier. An identifier, in this system, is a



Binary libraries (O) and service program systems (□).

sequence (of letters, numbers and the symbols ".", "-" and "*"), starting with a letter. Identifiers must not exceed six characters in length.

Example 1:

ZONE: 7, 600., U-235, I.2IE-4,,ZR,0,0084. In this example two isotopes are described. The isotope temperatures are not stated and are taken to be equal to the temperature of the zone.

The CONST operator (executable) calculates the constants for one of the constant programs which make up the OKS system. The resulting constant file is given a name determined by the operator parameter. The CONST operator takes the form:

CONST: <file name>, <program name>, <mode>. The file name is the identifier by which the constant file obtained will be known. The program name is an identifier which unambiguously determines the constant system, its version, and also the program to be applied for calculating the required type of constants.

The following programs are now included in the OKS system:

NEUTR: calculation of neutron constants in 26- and 28-group approximation by means of the ARAMAKO-2F system [2], and in 49-group approximation using the 49-group constant system [5];

GAMMA: calculation of γ(G)-constants in 15-group approximation by means of the ARAMAKO-G [3] system;

N-G: calculation of neutron and G-constants (ARAMAKO-G);

NN-GG: calculation of neutron, N-G and G-constants (ARAMAKO-G);

CNN-GG: calculation of neturon, N-G and G-constants and their representation in the form of a single file in the FMAC5A (ARAMAKO-G) format;

DENSTY: calculation of 21-group neutron reactor constants by means of the DENSTY system [1];

RNEUT: calculation of neutron reactor constants by means of the ARAMAKO-80 system [6];

TERMAC: calculation of thermalization constants by means of the TERMAC system [7].

The "mode" parameter determines the choice of the program's mode of operation and is given by a list of sub-parameters, the length of which, as well as the meaning of each element of which, depends on the specific constant program concerned. Permissible parameter values are described in detail in the OKS system instructions.

Example 2:

CONST: A, NEUTR, 26,2,2,Ø; ZONE: 1,595., H,.452,,O,.226,,B-1Ø, 7.55E-9; ZONE: 2,595,.FE.,848. In this example the operator CONST is applied to two physical zones. It demands access to the NEUTR program. The neutron constant file thus calculated is given the name A.

The DATA operator (non-executable) is applied in cases where the executable operator parameter is a file of numbers or list of identifiers.

The DATA operator takes the form:

DATA: <file name>, <list>. The file name is an identifier. The list is a sequence of numbers or identifiers separated by commas.

Example 3:

CONST:G, GAMMA, 1, NGCOM; ZONE: 1,300., FE.,0847; ZONE: 2,300., H.,067, 0,.0335; DATA: NGCOM, 0,0,0,0,0,0,1,1,2,2,2,3,3,0,0.

Calculation of the γ-constants by means of the GAMMA program is called for. The third parameter, equal to unity, signifies that in the γ-constant file the angular dependence for the transition from one energy group to another will be given pointwise. The fourth parameter, NGCOM, is the name of the file whcih describes the convolution of the constants with respect to γ-quantum energy groups. The file consists of 15 whole numbers and is given by the DATA operator.

The FORM operator (executable) is designed to translate constants from one format to another. It takes the form:

FORM: <file name>, <format>, <file name>, <mode>; the first parameter is the file name, which is generated by the FORM operator; the second parameter is the format name; the third parameter is the name of the source file; the fourth parameter is the mode (this determines the mode of operation of the program carrying out the required format transformation). The mode is given by a list of subparameters. The length of this list and the sense of each of its elements depend on the specific transformation.

The following formats are included in the OKS system:

AMAC5A: conjugate constant format, obtained from the standard FMAC5A format as used in the shielding version of the ARAMAKO system;

ROZ-6: constant format for conjugate constants used in the ROZ-6 program;

AROZ-6: combined format, in which the constants consist of two consecutively recorded constant files, the first in the ROZ-6 format, the second in AROZ-6.

Example 4:

CONST: A, NEUTR, 26,2,2,Ø; ZONE: 1,595., H., 452,,0,. 226,, B-1Ø, 7.55E-9; ZONE: 2,595., FE,.848; FORM: B, ROZ-6, A,,,2,5.

File A, obtained through the NEUTR program, will be converted from format FMAC5A to format ROZ-6 and will be given the name B. A printout will be made of constants for group range 2-5.

The TAPE operator (non-executable) is designed to allocate the place in the external memory where a file with a given name is to be recorded. This file is generated by an expendable operator (to which the TAPE operator is applied). The same executable operator then records the file in the place allocated, the precise location of which in the external memory can be given either as the channel number, or as the mathematical number of the apparatus and the zone number. This is determined by the specific executable operator, the information for which is contained in the TAPE operator.

The TAPE operator takes the form:

TAPE: <file name>, <peripheral number>, <start>, <length>; <file name> - identifier; <peripheral number> - this or the channel number (in which case the third and fourth parameters may be omitted), or the mathematical number of the peripheral unit; <start> is the number of the initial zone; <length> is the number of zones.

Example 5:

CONST: A, NEUTR, 26,2,2,Ø; ZONE: 1,3ØØ,,FE,. Ø66,, 0-16.,Ø33; ZONE: 2,3ØØ., CR,. Ø4,,H,.ØØ1; FORM: B, CROZ-6, A, Ø,Ø,3,7; TAPE: B,5.

The B file in the CROZ-6 format will be recorded in channel 5, which corresponds to the magnetic tape with the mathematical number 45. The A file will be located on the OKS system backup. If this file is to be retained the TAPE operator must be written after the CONST operator with an indication of the location of file A in the external memory.

The JOIN operator (executable) is designed to combine two files represented in the same format into a single file in that format. In the

OKS system this is done for the FMAC5A format. The need for this operation stems from the fact that some constant systems place restrictions on the number of zones or isotopes which can simultaneously enter into a calculation. The JOIN operator allows such restrictions to be removed.

The operator takes the form: JOIN: <file name>, <format>, <file name>, <file name>, <mode>; the first parameter is the name of the file generated by the JOIN operator; the second is format FMAC5A; the third is the name of the first of the file to be combined; the fourth parameter is the name of the second such file; the fifth parameter is the mode of operation (this determines how the program combining the files operates). The mode consists of parameters whose values are not given here. The "mode" parameter may be omitted.

Both of the files to be combined may be calculated in a single exercise. It is also possible for one of the files to be obtained beforehand, in which case its storage location must be indicated by means of the TAPE operator.

Example 6:

CONST: B, NEUTR, 26,2,2,Ø; ZONE: 1,595., H,. 452,,0,.226,, B-1Ø, 7.55E-9; JOIN: C, FMAC5A, A, B; TAPE: A, 35,1,1ØØ; TAPE: C, 36,1,2ØØ.

The JOIN operator will combine files A and B in a single file C. It will read file A from magnetic tape 35, and file B from the OKS system backup.

The result will be recorded on magnetic tape 36.

The END operator is the end of the exercise. It takes the form: END.

Example 7:

The final form of an OKS system exercise is as follows:

CONST: A, NEUTR, 26,2,2,Ø; ZONE: 1,3ØØ., FE,.Ø66,,O-16,.Ø33; ZONE: 2, 3ØØ., CR,.Ø4,,H,.ØØ1; FORM: B, ROZ-6 A, Ø,Ø,1Ø),15; TAPE: B,5; END.

Access to the OKS system

The exercise to be performed by the system is recorded on punched cards using a standard alphanumeric device. The punch cards are stacked for reading

by the machine after entry of the command * EXECUTE. The OKS system is organized as a subprogram. Access to it from the user's program is achieved by means of the CALL (or CALL LOADGO) operator. For a single exercise the system may be used by means of the card * MAIN OKS1. The OKS system imposes no memory limitations on the program which calls up the system or on the constant retrieval programs which the OKS system addresses. This is made possible by special system devices incorporated in the OKS system.

REFERENCES

[1] MARIN, S.V., MARKOVSKIJ, D.V., SHATALOV, G.E., The DENSTY program for calculating the space-energy distribution of neutrons in one-dimensional geometry [in Russian], Preprint IAEh-2832, Moscow (1977).

[2] BAZAZYANTS, N.O., VYRSKIJ, M.Yu., GERMOGENOVA, T.A. et al., ARAMAKO-2F: a neutron constant supply system for calculations of radiative transfer in reactors and shielding [in Russian], USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1976).

[3] ABAGYAN, A.A., BARYBA, M.A., BASS, L.P. et al., ARAMAKO-G: a multigroup constant supply system for calculations of gammaradiation fields in reactors and shielding [in Russian], Preprint No. 122 USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1978).

[4] VYRSKIJ, M.Yu., DUBININ, A.A., KLINTSOV, A.A. et al., ARAMAKO-2F: a version of a system to supply constants for calculations of high-energy neutron transport [in Russian], Preprint No. 904, Institute of Physics and Power Engineering, Obninsk (1979).

[5] VYRSKIJ, M.Yu., DUBININ, A.A., ILYUSHKIN, A.I. et al., The 49-group constant system for calculating neutron transport in radiation shielding [in Russian], Third All-Union Scientific Conference on ionizing radiation shielding in nuclear installations (Abstracts), Tbilisi (1981).

[6] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for reactor and shielding calculation [in Russian], Ehnergoizdat, Moscow (1981).

[7] GOMIN, E.A., MAJOROV, L.V., The TERMAC program [in Russian], in Voprosy Atomnoj Nauki i Tekhniki, Ser. Fizkia i Tekhnika Yadernykh Reaktorov 5 (1982).

[8] VOLOSHCHENKO, A.M., KOSTIN, E.I., PANFILOVA, E.I., UTKIN, V.A., ROZ-6: a system of programs for solving the transport equation in over-dimensional geometries, Version 2: Instructions [in Russian], USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1980).

[9] BASS, L.P., GERMOGENOVA, T.A., KORYAGIN, D.A., et al., Software for reactor shielding physics problems [in Russian], Preprint No. 86 USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1981).

[10] GERMOGENOVA, T.A., KORYAGIN, D.A., DUKHOVITSKAYA Eh.S. et al., OKS: a program package for supplying constants [in Russian], in: Voprosy Atomnoj Nauki i Tekhniki, Ser. Fizkia i Tekhnika Yadernykh Reaktorov 4 (33) (1983).

[11] VOLOSHCHENKO, A.M., GERMOGENOVA, T.A., ISAENKO, T.G. et al., The unified constant supply system: OKS, Version 3.0 [in Russian], Preprint No. 20, USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1984).

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THE GROUP NEUTRON DATA LIBRARY (GNDL)

A.V. Voronkov, V.I. Zhuravlev, E.G. Natrusova

ABSTRACT

The paper describes the structure, organization and basic data representation formats of the GNDL, which was developed at the M.V. Keldysh Institute of Applied Mathematics of the USSR Academy of Sciences for the purpose of neutron data storage and retrieval. A simple method for linking up applications programs with the library is proposed.

In most reactor physics and penetrating-radiation shielding physics problems which can be solved by the group method there is a need for group constants, i.e. cross-sections for various neutron/nucleus interaction processes averaged over the energy range of the group. Owing to the extremely complex dependence of cross-sections on energy, and sometimes also because of a simple lack of data on the detailed behaviour of the cross-sections over the individual energy ranges, group microconstants for some isotopes are currently obtained by means of various not firmly established (or even arbitrary) algorithms and evaluations of both experimental and theoretically calculated material. In recent times this information has been obtained from various evaluated data libraries abroad. As a consequence, it is constantly being updated, so appropriate means are required for introducing changes, additions and corrections to the group microconstants. Since the number of isotopes used in reactor construction goes into the hundreds, and the number of groups used in calculation into the dozens, the group microconstants file must contain a sizeable body of numerical data which is very laborious and time-consuming to compile. Furthermore, this file is called for at the input stage of programs generating group macroconstants and must therefore be suitably organized both from the point of view of group microconstant control

and from that of the needs of the programs calculating the group macroconstants. At the ouput stage, the macroconstant calculation programs in turn generate a group macroconstant file which is comparable in volume to the group microconstant file and which is used by the reactor and shielding calculation programs, and for this reason the file must be suitably organized.

The USSR has now developed systems (such as ARAMAKO-2F [1], ARAMAKO-G [2], DENSTY [3], etc.) which generate group constants for use in calculation programs. Most of these systems obtain the group macroconstants from group microconstants, using for this purpose various methods (differing from library to library), such as the subgroup method, the separated resonances method, the self-shielding factors method, etc. The corresponding library programs are geared towards each system's specific group microconstant representation format, so it is difficult to combine them. However, experience shows that no one of the methods is better, in absolute terms, than any other over the entire energy range. Thus it is necessary to use different methods of obtaining macroconstants for different isotopes and energy intervals, and therfore a uniform group microconstant representation format is needed. Furthermore, the lack of unified inputs and outputs for these libraries makes it difficult to link the systems to calculation programs. The fact that, as a rule, such programs are linked to particular constant systems makes it difficult to compare both the quality of calculation methods and the quality of the group constants objectively.

In the present paper we briefly describe the Group Neutron Data Library (GNDL), which was developed at the M.V. Keldysh Institute of Applied Mathematics of the USSR Academy of Sciences for the purpose of storage and retrieval of nuclear data needed for calculations in reactor and radiation shielding physics problems. In planning the GNDL the following objectives were pursued:

- To establish a single format for the storage of various sets of neutron group constants. This would permit the standarization of

data handling procedures and the easy and convenient exchange of cross-section data between libraries; it would also facilitate changes and additions to the existing data;

- To offer some of the most widely used algorithms for converting microconstants into the group macroconstants needed for reactor and radiation shielding calculations;
- To simplify the process of linking up different calculation programs with library data.

Given these objectives, the GNDL uses two data representation formats: the textual group microconstant format GNDL/T and the binary group microconstant format GNDL/B. The textual format, based on the "one isotope - all groups" principle (i.e. all the data for one isotope are grouped together) is used for storing group microconstants and is designed for use in making changes and additions to data and in inter-library cross-section data exchanges. The binary format is geared to programs for obtaining macroconstants and other programs using group microconstants. It is based on the "one group - all isotopes" principle (i.e. the data on all isotopes for a single group are grouped together). By means of the special RTWB program, data from a textual format with a given number of groups can be converted to the binary format.

The GNDL software consists of:

- A set of programs for obtaining macroconstants (USCONS);
- A set of "access functions" programs;
- The library's set of service programs.

The function of the USCONS programs is to derive group macroconstants from microconstants recorded in the GNDL/B format. Up to the present time the following algorithms for macroconstant calculation have been included in USCONS: simple summation, the subgroup method, various versions of the separated resonances method and the self-shielding factors method.

Receiving its calculation task in a specially formulated language which describes the compositions of physical zones, temperatures and operating modes, the set of programs allows for different methods of macroconstant calculation in various energy ranges and for different physical zones. The data in the USCONS startup package are divided into three sections, called METOD ("method"), ZONA ("zone") and KONETS DANNYKH ("data end"). The package may contain only one KONETS DANNYKH section, but any number of METOD and ZONA sections, these being numbered in their order in the package.

The cards in the METOD section contain data decribing how constant calculation methods change according to groups. The USCONS source data package is taken to be broken down into the fields of application of the METOD sections according to the following relationship: the field of application of METOD section number N consists of all the ZONA sections in the package which lie between this section and METOD section number N + 1 (or the KONETS DANNYKH section, if N is the number of the final section of METOD). This relationship makes it possible to change the methods of constant calculation according to zones [4]. The cards in the ZONA section contain data describing the composition of a single physical zone. The name of the ZONA section is punched on the first card of the section, while the following cards receive the textual names of the isotopes entering into the composition of the zone along with their nuclear concentrations and temperaure [4].

The basic trend in linking constants applications programs nowadays is towards standardizing the output formats of the constant systems. However, this approach not only lacks effectiveness, but even to a certain extent acts as a brake on the development both of the constant systems themselves and on the calculation programs (experts avoid changing the output formats of a constant system because large numbers of alterations might arise in the calculation programs, while users avoid any remodelling of their input format so that they do not have to rewrite the program for linking up with the constant system). The main difficulty in linking up with the constant system

for the user is that of extracting the required number from the system's output format. It was primarily this problem which was intended to be solved by developing the GNDL system. This is achieved by introducing into the GNDL structure special program functions (access functions) which obtain a single element from the overall file of output data. As a result, the user need not know anything about the structure of the constant system output format; he can begin writing programs for filling the recording units of his input format. He adds his program to the constant system programs (which must allow for calling up an external function), and subsequently obtains his constants format through the combined operation of the programs. We believe that this method reduces the difficulties of linking the user's programs with the constant system by 80-90%.

The third set of programs (the service programs) are designed for users working with group microconstant libraries. The most important component of the set is the RTWB program, which, at the user's command, chooses data with a specific name from the GNDL/T format and records them on any carrier specified by the user in the GNDL/B format. In addition, the set of service programs includes programs for printing out the contents of the GNDL/B library. In general terms the GNDL is used as follows: let us suppose that a permanent archive in the GNDL/T format is filled, for example, by the group libraries ARAMAKO-2F [1], DENSTY [3] and BNAB-26 [5]. The user wishes to perform a series of calculations using constants from the ARAMAKO-2F library, supplemented by data on self-shielding factors from the BNAB-26 library, in order to compare the subgroup method of obtaining macroconstants with the self-shielding factors method. The user feeds the corresponding task to the RTWB program, which selects data labelled ARAMAKO-2F and BNAB-26 for the given isotopes, reprocesses them into the GNDL/B format and records them on the magnetic tape specified by the user, where a 26-group microconstant library is thus formed in which the resonance structure of the cross-sections is described by subgroups and self-shielding factors. Using the USCONS system

and specifying several of its operating modes, the user can obtain macroconstants in two ways. With the GNDL library organized in this way, the work carried out by a user engaged in reactor and shielding calculations can be made independent of the large-capacity constant archives, and the user can be assured of an effective supply of macroconstants for a wide series of calculations (i.e. without referring to the major constant archives he can conduct a whole series of calculations which does not call for any change in group division).

The basic data formats developed in the GNDL allow storage of group microconstants for the entire range of neutron energies which are of practical interest in reactor physics. The GNDL/T formats are versatile in the sense that almost any neutron interaction mechanism can be described precisely in them. They are also limiting in that only a limited number of different representations are permissible for data relating to any particular neutron interaction mechanism.

It should be noted that the GNDL/T format structure is a modification of that of the well-known ENDF/B-IV [6] evaluated data library. This modification has made it possible, without needing to change the quantity of data contained in the ENDF/B format records, to store in a single material (the basic unit of information in ENDF/B) the group microconstants corresponding to various group divisions.

We shall now described briefly the GNDL/T library formats, introducing definitions analogous to those from the GNDL/B library.

A material is defined as an isotope or mixture of isotopes. It may be a single nuclide; a natural element containing several isotopes; a molecule containing several elements; a standard mixture of elements (for example, a particular brand of steel). Each material in the GNDL/T library is given a unique identifying name consisting of no more than four letters or digits and starting with a letter.

The set of data for each material is subdivided into files, each of which contains a particular class of data and bears a two-digit identifying number MF. Each file is subdivided into sections, each of which is made up of data for a particular type of reaction and bears a three-digit identifying number MT. Note that the data in a material follow the ascending sequence of file numbers, while the data in each file follow the ascending sequence of section numbers.

The data in each section are subdivided into named subsections whose name contains not more than eight alphanumeric characters and starts with a letter. It is recorded in a special heading record called HEAD (see below) which always precedes the data set in the named subsection. The named subsection contains data for the type of reaction to which the section of which it is a subsection corresponds. It should be noted that although all data relating to a particular microconstant library held in the GNDL/T format archive are located in different sections, they are nevertheless located in identical named subsections. It is not absolutely necessary for all files, sections or named subsections to be present in each material.

The data for a specific material begin with the card SUBROUTINE (name of the material) and end with the two cards RETURN and END. All cards bearing data for this material begin with the letter C (the FORTRAN symbol for a comment line), i.e. formally the material is stored in the GNDL/T format as an empty SUBROUTINE with comments.

Each data set for a material is recorded by means of five format records:

HEAD - is the heading record, containing eight numbers and two textual constants;

LIST - is used for recording the series of real numbers B_1, B_2 ...;

TAB1 - is used for recording tabulated functions of a single variable y(x);

TAB2 - is used for recording tabulated functions of two variables y(x,z) (it determines how many values for z must be given and how to interpolate between their consecutive values);

CONTE - has four forms (NEND, SEND, FEND, TEND) which are used to signal the end of a named subsection, section, file or tape, respectively.

Standard computer operation with editor programs is achieved using the following data arrangement on a conventional 80-column punched card divided into ten fields:

Field	Columns	Description
1	1-1	C - FORTRAN symbol for a comment line
2	2-12	Data
3	13-23	Data
4	24-34	Data
5	35-45	Data
6	46-56	Data
7	57-67	Data
8	68-69	MF
9	70-72	MT
10	73-80	Serial number of card in material

Thus, by removing from the card the MAT field (the serial number of the material in the ENDF/B library) and moving the MF and MT fields accordingly, it is possible, without losing any of the information on the cards (the total length of data fields on punched cards in the ENDF/B and GNDL/T libraries is identical), to free columns 73-80 for consecutive numbering of the punched cards in the material. This permits data to be edited in the standard operating mode with practically any text editor program available as part of the computer software. All real numbers in the LIST, TAB1 and TAB2 records are punched onto cards in the E11.4 format, while all whole numbers from these records, apart from MF and MT, are punched onto the cards in the I11 format. The MF-number is punched in the I2 format, and the MT-number in the I3 format.

Data from the widely known group libraries ARAMAKO-2F, DENSTY, BND-49, BNAB-26 etc. are currently being converted to GNDL format by means of the

BFGNDL programs specially developed for this purpose. Data from other group microconstant libraries can easily be converted to GNDL by means of these programs.

REFERENCES

[1] BAZAZYANTS, N.O., VYRSKIJ, M.Yu., GERMOGENOVA, T.A. et al., ARAMAKO-2F: a neutron constant supply system for calculations of radiative transfer in reactors and shielding [in Russian], USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1976).

[2] ABAGYAN, A.A., BARYBA, M.A., BASS, L.P. et al., ARAMAKO-G: a multigroup constant supply system for calculations of gamma radiation fields in reactors and shielding [in Russian], Preprint No. 122, USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1978).

[3] MARIN, S.V., MARKOVSKIJ, D.V., SHATALOV, G.E., The DENSTY program for calculating the space-energy distribution of neutrons in one-dimensional geometry [in Russian], Preprint No. 2832, Institute of Atomic Energy, Moscow (1977).

[4] VORONKOV, A.V., ZHURAVLEV, V.I., NATRUSOVA, E.G., USCONS: a set of GNDL programs for group macroconstant calculation (instructions for users) [in Russian], USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1983).

[5] ABAGYAN, L.P., BAZAZYANTS, N.O., BONDARENKO, I.I., NIKOLAEV, M.N., Group constants for nuclear reactor calculations [in Russian], Atomizdat, Moscow (1964).

[6] GARBER, D., DUNFORD, C., PEARLSTEIN, S., Data formats and procedures for the nuclear data file, BNL-NCS-50496 (ENDF-102) (1975).

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THE ARMAN'YAK CODE

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ABSTRACT

The ARMAN'YAK (acronym from the Russian for "automated calculation of few-group neutron-nuclear constants") code is intended for compiling, on a computer's magnetic carrier, a library of files of nuclear concentrations, neutron spectra and few-group constants for further use as a simplified few-group system supplying constants for limited purposes. It may also be used in the preparation of constants for individual few-group calculations.

Description of the program

The ARMAN'YAK code is written in the FORTRAN-IV language and implemented on the BEhSM-6 computer at the Institute of Physics and Power Engineering (Obninsk). The capacity of the working memory is 32K; the working magnetic drum has from 80 to 150 sections, depending on the parameters of the problem; the magnetic carrier for the file library is a tape or disk with the ARAMAKO system. The operating system is "Dispak" ("Dubna") and the monitoring system "Dubna". The text volume of the programs is over 3000 punched cards. The full set of programs occupies 26 zones on a magnetic tape or disk in the octal number system.

Problem

For few-group fast-reactor calculations use is made of few-group macroconstants and block microconstants obtained by convolution of the corresponding multigroup constants. These are prepared by a constant supply system (e.g. ARAMAKO) for predetermined zone compositions, taking account of resonance self-shielding effects and the like. It is often necessary to calculate many versions for the same reactor differing only by slight changes

in zone composition. In such cases it is cumbersome to refer to the main multigroup constant supply system every time there is a change; it is better to recalculate few-group macroconstants from the small-group block microconstants already calculated for the particular reactor. The ARMAN'YAK programs are designed to meet this need, i.e. to compile, on a computer's magnetic carrier, the values necessary for few-group constant calculation (nuclear concentrations and multigroup integral zone spectra entered from punched cards) and the few-group macroscopic and block microscopic constants in each zone (calculated by convolution with the weight of the corresponding integral spectrum of the 26-group microconstants and corresponding macroconstants; the latter are in turn calculated on the basis of the BNAB-78 library [1] by means of the ARAMAKO set of programs [2]). The library compiled by the ARMAN'YAK programs can serve as the data base for a simplified constant supply system to be used in calculation tasks for a given project.

The few-group constant calculation program which forms part of the ARMAN'YAK code can also be used as a subprogram preparing constants for a set of programs designed for individual small-group calculations. In this case, the source data required for few-group constant calculation (nuclear concentrations and spectra with whose weight the few-group constants are convoluted) can be either entered from punched cards or read from an appropriate data library compiled in advance by means of a suitable ARMAN'YAK module.

Solution

When the ARMAN'YAK code operates in the library compilation mode, four mutually independent programs are used:

INLIB - is used for marking out the magnetic carrier and for compiling the library catalogues;

FORMCO - assembles files of nuclear concentrations for one or several physical zones of the reactor under consideration;

FORMF1 - assembles files of 26-group integral neutron spectra, fluxes and, possibly, currents, with whose weight the 26-group constants must then be convoluted into few-group constants (with the number of groups not exceeding 26);

CONSTM - calculated few-group macro- and microconstants for isotopes entering into the reactor composition, by means of a convolution of 26-group block microconstants. The latter are calculated using the ARAMAKO [2] system.

Prior to convolution, the 26-group elastic slowing-down cross-sections are corrected for the difference in shape between the within-group spectrum and the standard one used in calculating the tabulated values of the slowing-down cross-sections. The shape of the within-group spectrum is evaluated by means of a binodal piecewise-linear approximation of the multigroup histogram of the integral spectrum β_r the zone [3]. The convolution of the transport cross-sections and of the first angular momenta of the slowing-down cross-sections is carried out with the weight of the integral currents. If these are not directly stated they are evaluated by one of the following methods:

- The current spectrum is assumed to be identical with the flux spectrum;
- The current is taken to be proportional to the flux divided by the transport cross-section;
- The integral 26-group current spectra are calculated as an approximation of the material parameter of each of the zones under consideration.

When calculating few-group microconstants, the special GENER subprogram makes it possible, if so desired, to combine some of the last nuclides on the list of those forming part of the reactor into a "generalized" nuclide characterized by a single set of microconstants in each zone. For example, all the components of stainless steel can be combined into a single

generalized nuclide "steel". In the ARMAN'YAK mode of operation under consideration, the CONSTM program enters the compiled few-group constant files in the library. The user may choose whether the nomenclature of the few-group constants is to correspond to the requirements for calculations in the P_1 approximation or in the diffusion approximation.

The CONSTM program may also be inserted into the set of programs designed for individual few-group calculations. In this mode of operation the few-group constant files do not have to be entered in the library. The nuclear concentrations and integral spectra used to obtain them may either be entered on punched cards while accessing the CONSTM program or read from the library (if they were previously entered there).

Limiting the complexity of the problem

The number of files compiled in the library may not exceed 20; the number of zones for which data are represented in a file may not exceed 999; the number of zones for which few-group constants can be calculated in a single problem package may not exceed 100.

Typical calculation time

The preparation of 4-group constants in the format necessary for reactor calculations in three-dimensional hexagonal geometry (TRIGEX program) on the basis of 26-group constants generated by the ARAMAKO programs for 16 nuclides and 10 zones takes 45 s. The concentrations file in the file library (a recording in the file of the concentrations of 18 nuclides for 20 physical zones of the reactor) takes approximately 15 seconds to produce.

Special features of the program

Few-group constants are recorded by the CONSTM program in the library being assembled only if the nuclear concentrations and integral spectra necessary for the calculation are read by this program from the library being

assembled, (rather than directly from the punched cards, as is possible when the CONSTM program is being used in the operational preparation of few-group constants for individual calculation). This ensures that all information used in obtaining the few-group constants remains intact in the completed library, which may be of great importance in the subsequent analysis of calculation results.

Auxilary and accompanying programs

The programs and constant libraries of the ARAMAKO system are used in the operation of the ARMAN'YAK programs. Exchanges with the external memory (magnetic tape, drum, disk) are performed by the RDWRTD program, which gives direct access to the ARAMAKO system [2]. The input of source data is carried out by non-format input programs [4].

Present state of the program

The main program in the ARMAN'YAK system, CONSTM, is used by the Institute of Physics and Power Engineering for the operational preparation of few-group constants for neutron-physical reactor calculations in three-dimensional hexagonal geometry using the TRIGEX program [5]. The library compilation programs are used as a back-up to the archive of calculated versions when analysing the results of experiments conducted on the BN-350 reactor using the TRIGEX program (only the nuclear concentrations and integral spectra are retained). Work is in progress to include the TRIGEX program in the set of programs for reactor run calculation. This set of programs will work in conjunction with few-group constant libraries generated by means of the ARAMAN'YAK set of programs.

REFERENCES

[1] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for reactor and shielding calculation [in Russian], Ehnergoizdat, Moscow (1981).

[2] BAZAZYANTS, N.O., VYRSKIJ, M.Yu., GERMOGENOVA, T.A. et al., ARAMAKO-2F: a neutron constant supply system for calculation of radiative transfer in reactors and shielding [in Russian], USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1976).

[3] NIKOLAEV, M.N., RYAZANOV, B.G., SAVOS'KIN, M.M., TSIBULYA, A.M., Multigroup approximation in neutron transport theory [in Russian], Ehnergoatomizdat, Moscow (1983).

[4] IL'YASHENKO, A.S., LIMAN, G.F., Non-format input programs in FORTRAN [in Russian], Preprint No. 2293, Institute of Atomic Energy, Moscow (1973).

[5] SEREGIN, A.S., Annotation of TRIGEX programs for small-group neutron-physical reactor calculation in three-dimensional hexagonal geometry [in Russian], Voprosy Atomnoj Nauki i Tekhniki, Ser. Fizika i Tekhnika Yadernykh Reaktorov, 4 (33) (1983) 59.

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A LIBRARY OF NEUTRON DATA FOR CALCULATING GROUP CONSTANTS

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ABSTRACT

This paper describes the first version of a computerized library evaluated neutron data files (FOND) which includes data on the 67 most important nuclear reactor and radiation shielding materials. The data are represented in the ENDF/B format. The sources of data were the results of evaluations of data from differential neutron physics experiments conducted both in the USSR and abroad. The first version of the FOND library is not intended for use in reactor and shielding design calculations, but rather to serve as the basis for developing a corrected version which will guarantee adequate description of the results of a representative set of macroscopic experiments, and for generating multigroup constant systems in methodological research.

The computerized evaluated neutron data library described in the present paper is an integral part of the SOKRATOR system for supplying constants for nuclear reactor and radiation shielding calculations [1]. Together with the GRUKON applications program package [2] it forms the MIKRO subsystem for the periodic generation of sets of group constants for individual nuclides independently of the composition of the medium.

So far only an initial version of the computerized library of evaluated neutron data files (FOND) has been produced. The library includes whole sets of evaluated neutron data in the energy range 10^{-4} eV–20 MeV for the 67 most important nuclear reactor and radiation shielding materials, for the actinide isotopes formed in the process of nuclear fuel burnup and for ^{197}Ag, the cross-section for radiative capture on which is used as a standard for neutron cross-section measurements (the remaining nuclei whose cross-sections are used

as neutron standards are included among the reactor materials). It is also proposed that the FOND library should contain evaluated neutron data for those fission fragment nuclei which contribute most to reactor slagging and poisoning. Although it was decided to compile evaluated data files for the 27 most important types of fission fragment, this task has so far not been completed for most of these fragments. These data will therefore be incorporated into the FOND library at a later stage.

The data in the FOND library are represented in the format used by the American national evaluated nuclear data library, ENDF/B [3]. The library contains those evaluated neutron data which the compilers of the first version considered to be the most reliable. However, the reliability of the data in the first version of the FOND library was not such that they could be recommended for use in design calculations for nuclear power installations. For such purposes, it is necessary:

(1) To use group constants obtained from the FOND library as a basis for calculating the already measured characteristics of a representative set of critical assemblies and shielding compositions, and then, after comparing these calculation results with the experimental data, to evaluate the nature and magnitude of the errors in predictions of reactor and shielding characteristics calculated on the basis of FOND library data;

(2) To conduct a partial re-evaluation of the data for certain nuclides in the light of all existing experimental data and recent nuclear reaction theory concepts, taking into account also the results of analysing discrepancies between calculated and experimental data on critical assemblies and shielding compositions;

(3) To repeat the calculations mentioned in paragraph (1) for the improved version of the FOND library, and to ensure that it allows an accuracy of theoretical predictions no worse than that assured

by the BNAB-78 group constant system which is currently in use (for fast reactor and radiation shielding calculations) [4].

Until this work has been completed there is no reason to abandon the present systems for supplying constants for multigroup calculations. However, in the case of fast reactor calculations, changing from the BNAB-78 constant system to constants based on the first version of the FOND library will lead to less accurate results. From the point of view of the main users of neutron constants - nuclear power plant designers - the first version of the FOND library is useful only as a source of data needed to supplement existing group constant systems with data for new nuclides in respect of whose constants no great degree of accuracy is called for. A further directly practical application of the first version of the FOND library consists in using it as a basis for generating fine-group (hundreds or thousands of groups) constant systems for the purpose of developing corresponding constant supply systems and checking the accuracy of the multigroup approximations used (of groups 21, 26, 28). Note that, in principle, there is no difference between the status of the first verison of the FOND library as defined above and the status of the latest versions of national evaluated neutron data libraries in the USA (ENDF/B-V), the Federal Republic of Germany (KEDAK-3), the United Kingdom (UKNDL) and Japan (JENDL-2). In these countries (not to mention France, which does not have a national evaluated neutron data library of its own), design calculations are based on approved group constant systems, not on evaluated data libraries.

The establishment of the FOND library completes the development of the MIKRO subsystem - the final structural element of the SOKRATOR system. Other structural elements of the SOKRATOR system are the MAKRO subsystem, which operationally prepares all the constants needed for multigroup calculations of specific reactor or shielding variants, and the INDEhKS subsystem, the functions of which include automated analysis of discrepancies between calculation and experiment in data from macroscopic experiments and correction

List of isotopes contained in the FOND library

No	Isotope	Evaluated data
1	1-H-1	S(tot, el, gam), A, GF, AF
2	1-H-2	S(tot, el, 2n, gam), A, GF, AF
3	1-H-3	S(tot, el, non, 2n), A, E
4	2-He-3	S(tot, el, non, 2n, p, d), A
5	2-He-4	S(tot, el) A
6	3-Li-6	S(tot, el, in, in(i), 2nalf, alf, p,t), A, E, GF, AF
7	3-Li-7	S(tot, el, in, 2n, 2nalf, in(i), in(c), gam, d) A, E, GF, AF
8	4-Be-9	S(tot, el, 2n(i), gam, p,d,t,alf), A, E, GF, AF, EF
9	5-B-10	S(tot, el, in(i), gam, p, d, alf, t 2alf),A, GF, AF
10	5-B-11	S(tot, el, in, 2n, in(i), in(c), gam, p, t, alf), A, E, GF, AF, EF
11	6-C-12	S(tot), el, in, in(i), in(c), gam, p, d, alf), A, E, GF, AF
12	7-N-14	S(tot, el, in, 2n, in(i), gam, p,d,t, alf, 2alf), A, E, GF, AF
13	8-O-16	S(tot, el, in, in(i), gam, p, d, alf), A, GF, AF
14	9-F-19n	S(tot, el, non, in, 2n, n`alf, n`p, in(i), in(c), gam, p,d,t,alf),A,E,GF,AF,EF
15	11-Na-23	RP,S(tot, el,in,2n, in(i), in(c), gam, p, alf), A, E
16	12-Mg-nat	S(tot, el, non, in, 2n, n`alf,n`p, in(i), in(c), gam, p, alf),A,E,GF,AF,EF
17	13-Al-27	RP,S(tot, el, in, in(i), in(c), 2n, gam, p, alf), A, E
18	14-Si-nat	S(tot, el, in, 2n, n`p, in(i), in(c), gam, p, d, alf), A, E
19	17-Cl-nat	S(tot, el, in, 2n, n`alf, n`p, in(i), in(c), gam, p, alf), A,E,GF,AF,EF
20	19-K-nat	S(tot, el, in, 2n, n`alf, n`p, in(i), in(c), gam, p, alf) A, E, GF, AF, EF
21	20-Ca-nat	S(tot, el, in, 2n, n`alf, n`p, in(c), gam, p, alf), A,E,GF,AF,EF
22	22-Ti-nat	S(tot, el, non, in, 2n, in(i), in(c), gam, p, alf), A, E, GF, AF, EF
23	23-V-nat	S(tot, el, non, in, 2n, n`alf, n`p, in(i), in(c), gam, p, d, t,alf),A,E,GF,AF,EF
24	24-Cr-nat	RP,S(tot,el,in,2n,n`alf,n`p,in(i),in(c),gam,p,d,t,alf) A,E,GF,AF,EF
25	25-Mn-55	RP,S(tot, el,in, in(i),in(c), 2n, n`alf, n`p, gam, p, d, He3, alf), A,E
26	26-Fe-nal	RP,S(tot,el,non,in,2n,n`alf,n`p,in(i),in(c),gam,p,d,t, He3,alf) A,E,GF,AF,EF
27	27-Co-59	RP,S(tot,el,in,2n,in(i), in(c), gam, p, d, t, alf), A, E, GF, AF
28	28-Ni-nat	RP,S(tot,el, in,2n, n`p, in(i), in(c), gam, p, alf), A, E, GF, AF, EF
29	29-Cu-nat	RP,S(tot, el, non, in,2n,3n,n`p,n`alf, in(i),in(v),gam,p,d,He3,alf) A,E,GF,AF,EF
30	31-Ga-nat	S(tot,el, in, 2n, in(c), gam, p, alf), A, E, GF, AF, EF
31	39-Y-89	RP, S(tot, el, in, in(i), in(c), gam)A, E
32	40-Zr-nat	S(tot, el, in, 2n, 3n, in(i), in(c), gam, p), A, E, GF, AF, EF
33	41-Nb-93	RP, URP,S(tot, el, in, 2n, 3n, n`alf, in(i), in(c), gam, p, alf), A, E, GF, AF
34	42-Mo-nat	RP,S(tot,el, in, in(i), in(c),gam), A, E
35	48-Cd-nat	S(tot, el, non, in, 2n, in(i), in(c), abs, gam, p, alf), A, E
36	63-Eu-151	RP, URP, S(tot,el,non,in,2n,3n,n`alf,n`p, in(i),in(c),gam,p,d,t,He3,alf)A,E,GF,AF,EF
37	63-Eu-153	RP,URP,S(tot,el,non,in,2n,3n,n`p, in(i),in(c),gam,p,d,t,He3,alf)A,E,GF,AF, EF
38	64-Cd-nat	RP,S(tot,el, in, 2n,3n, in(c), gam), A, E
39	73-Ta-181	RP,URP,S(tot, el, in, 2n, 3n, in(i), in(c), gam, p), A, E, GF,AF, EF
40	74-W-182	RP,URP,S(tot,el,in,2n,3n, n`p, in(i), in(c), gam, p, alf), A, E, GF, AF, EF
41	74-W-183	RP, URP,S(tot, el, in, 2n, 3n, n`p, in(i), in(c), gam, p, alf),A,E,GF,AF,EF
42	74-W-184	RP,URP,S(tot,el,in,2n,3n,n`p,in(i),in(c), gam, p, alf), A,E,GF,AF,EF
43	74-W-186	RP,URP,S(tot,el,in,2n,3n, n`p, in(i), in(c), gam, p, alf), A,E,GF,AF,EF
44	75-Re-185	RP,URP,S(tot,el,in,2n,3n,in(i),in(c), gam)A, E
45	75-Re-187	RP,URP,S(tot,el,in,2n,3n, in(i), in(c), gam), A, E
46	75-Au-197	RP,S(tot,el,in,2n,3n,in(i), in(c), gam, p, alf) A, E
47	82-Pb-nat	S(tot,el,in,2n,3n,in(i), in(c), gam), A, E, GF, AF, EF
48	90-Th-232	NU,RP,URP,S(tot, el,in, 2n, 3n, f, in(i), in(c), gam), A, E
49	91-Pa-233	NU,RP,URP,S(tot,el, in, 2n,3n, f, in(i), in(c), gam), A, E
50	92-U-233	NU, RP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E
51	92-U-234	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E
52	92-U-235	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E
53	92-U-236	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E
54	92-U-238	NU, RP, URP, S(tot, el, in, 2n, 3n, 4n, f, in(i), in(c), gam) A, E
55	93-Np-237	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E

List of isotopes contained in the FOND library

No	Isotope	Evaluated data
56	93-Np-239	NU, S(tot,el, in, 2n, 3n, f, in(i), in(c), gam), A, E
57	94-Pu-238	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E
58	94-Pu-239	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E
59	94-Pu-240	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E
60	94-Pu-241	NU, RP, URP, S(tot, el, non, in, 2n, 3n, f, in(i), in(c), gam, A, E
61	94-Pu-242	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E
62	95-Am-241	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A, E, GF, AF, EF
63	95-Am-242M	NU, RP, URP, S(tot, el, in, 2n, 3n, f, 4n, in(i), in(c), gam), A,E,GF,AF,EF
64	95-Am-243	NU, RP, URP, S(tot, el, in, 2n, 3n, 4n, f, in(i), in(c), gam), A, E, GF, AF, EF
65	96-Cm-242	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam), A,E,GF,AF,EF
66	96-Cm-244	NU, RP, URP, S(tot, el, in, 2n, 3n, f, in(i), in(c), gam),A,E,GF,AF,EF
67	96-Cm-245	NU, RP, S(tot, el, in, 2n, 3n, f, 4n, in(c), gam), A,E, GF, AF, EF

of constants. The MAKRO subsystem functions applicable to the 26- or 28-group approximation are at present carried out by the ARAMAKO-2F system [5], while the functions of the INDEhKS system are carried out by the CORE set of programs [6], which includes a library of errors in the evaluated data (a covariance matrix), a library of calculation/ experiment discrepancies and their errors, and a library of factors for the sensitivity of macroexperiment results to constants. However, the completion of all the structural elements of the SOKRATOR system does not mean it has actually been put into operation; this stage will not be reached until systematic use of all three subsystems has made it possible to develop a version of the FOND library which can be recommended for practical use.

Choice of format for the FOND library

The initial version of the evaluated neutron data representation format used in the SOKRATOR system's computerized library was developed in 1972 [7] on the basis of a critical analysis of the only data representation format known at that time, the one used by the British UKNDL [8]. This format is known as the SOKRATOR format. In the mid-1970s a description of the data representation format used in the American ENDF/B library became available [9]. This format had been developed on the basis both of experience

with operating UKNDL and of experience gained in the United States with the formal structuring of large data files such that standardized program elements could be used in accessing a library. As a result it is both more convenient in practice (than the UKNDL and SOKRATOR formats), and versatile. These advantages were the reason why European countries quickly learnt how to process evaluated data in the ENDF/B format, too, while Japan, in compiling its own national evaluated neutron data library (JENDL), decided to use the ENDF/B format directly. This situation, and the fact that programs were being developed to translate data from the ENDF/B format into the British and West German library formats, led the IAEA Nuclear Data Section to decide to recommend a format for the international exchange of evaluated data. In view of the advantages and international status of the ENDF/B format it was decided to use it as of the very first version of the SOKRATOR system's evaluated data library. At the same time the library was given the special name FOND, since using the same name, SOKRATOR, to describe the format, the library proper and the entire system was a source of some confusion.

It should, however, be noted that the potential of the ENDF/B is utilized only insofar as the processing programs allow. The set of programs used in the USA for processing ENDF/B library data imposes many limitations on the format's potential. The most important limitations are those relating to the representation of data on the resonance structure of cross-sections. For example, data for one isotope must have one and the same boundary between the resolved and unresolved resonance regions and for s- and p-resonances. In practice, this means that the region of full resolution is taken by evaluators to be equal to the region for s-resonances, while the contribution of p- and d-resonances is subsumed under "non-resonance backing". This results in underestimates of the resonance self-shielding of those cross-sections, especially the capture cross-section, to which the contribution of p- and d-resonances is particularly great. In the unresolved resonance region, fluctuations in the mean cross-sections due to input states, or even to simply

statistical fluctuations in the widths and distances are described in the ENDF/B system by giving the energy dependence of the mean widths, usually for the p-wave. This leads to underestimates of resonance self-shielding. An ENDF/B format whose capabilities are limited by the existing versions of the American processing programs we shall call ENDF/B-V. The above-mentioned shortcomings of this format and others were noted at the IAEA consultants' meeting in late 1981 [10]. However, despite these shortcomings, when the first version of the FOND library was established it was decided to use the ENDF/B-V format without alteration.

Selecting evaluated neutron data

The time factor was of great importance in compiling the first version of the FOND library. It was decided to compile this version in 1982 so that practical library work could commence in 1983. For this reason, the data for the FOND library were selected only from among those data sets which were available in the ENDF/B format. The results of all Soviet evaluations carried out at the Institute of Physics and Power Engineering (Obninsk) or at the Institute of Heat and Mass Exchange of the Byelorussian Academy of Sciences (Minsk), as well as the results of evaluations conducted at the Dresden Technological Univesity, had already been represented in this format. The following data were drawn from the international evaluated neutron data exchange fund for analysis:

- From the ENDF/B-V library [11]: neutron standards data, data for secondary actinide nuclei not entering into the composition of unirradiated fuel, and also data on fission fragment nuclei which are not stable isotopes of reactor construction materials; these data were last reviewed over the period 1975-78;
- The ENDF/B-IV library [12], containing data for the majority of stable nuclei and actinide nuclei; evaluated in the early 1970s;
- The ENDL-78 library [13], developed at the Lawrence Livermore

Laboratory (USA), containing data for the majority of stable nuclides; evaluated 1970-75;

- The JENDL-1 library [14], the first version of the Japanese national evaluated neutron data library, containing data on the main reactor materials and the most important fission fragments.

Work with these computerized libraries was conducted on the BEhSM-6 computer, which was equipped with the appropriate software: a text editor program [15], the capabilities of which had been specially extended for work with textual libraries like ENDF/B [16], and the GRUKON applications program package [2] for obtaining group constants. In order to make the existing evaluated data compact, they were converted into 28-group form with a BNAB structure [4]. The following were used in comparing the results of different evaluations.

- Short descriptions (and sometimes graphs) contained in the accompanying documentation library;
- Group constants;
- Heading information contained in the evaluated data files, and, if necessary, the evaluated data themselves.

The following factors are taken into account in selecting data for the FOND library:

- Completeness of the experimental data evaluated and year of evaluation;
- Description of the resonance structure of the cross-sections (preference being given to data in which the resonance structure is described by resonance parameters, and, in the unresolved resonance region, by average parameters);
- Use of modern calculation methods for evaluating neutron cross-sections and spectra (the coupled-channel method for evaluating low-level excitation cross-sections at high energies,

consideration of pre-equilibrium processes in evaluating secondary neutron spectra, etc.);

- Completeness of the neutron reaction set represented.

Some of the evaluated data selected were replaced by more up-to-date, reliable or complete data (this could mean, for example, including resonance parameters from the most recent BNL compilation [17] or mean resonance parameters evaluated by averaging the resolved resonance parametes and fitting to the average cross-sections in the unresolved resonance region [18]; or it could mean replacing the calculated energy dependence of the cross-section for a particular important reaction by an experimental curve obtained in recent measurements). A written validation is prepared for each data file selected for the FOND library. At present such validations exist only as working material, but in the future it is intended to include most of them in the 451st (heading) section of each data set.

Contents of the FOND library

The list of evaluated neutron data which make up the FOND library is given in the table, which indicates both the nuclides and the actual data used in the evaluation. The following notation is used to describe the tabulated data: NU - characteristics of delayed and prompt neutrons; RP - resolved resonance parameters; URP - mean resonance parameters; S(x) - neutron cross-sections for the (nx) reaction; A(x) - angular distributions of secondary neutrons from the (nx) reaction; E(x) - the corresponding energy distributions; AE(x) - the corresonding energy-angular distributions; GF(x) - data on the large number of photons produced in the (nx) reaction; AF(x) - angular distributions of these photons; EF(x) - their energy distributions. For inelastic scattering, the indices i and c respectively indicate the discrete levels and the continuum of unresolved levels of the target nucleus.

Most of the evaluated isotope data analysed by us were obtained from the Nuclear Data Centre with the co-operation of V.N. Manokhin and A.I. Blokhin. The means for transferring data from the ES computer to the BEhSM-6 computer were developed by V.V. Evstifeev. V.V. Sinitsa made it possible to obtain group constants using the GRUKON applications program package, the calculations being performed by Zh.A. Korchagina. Some data were obtained directly from evaluators V.A. Kon'shin, N.O. Bazazyants, G.N. Manturov and L.P. Abagyan. The major task of editing the files was carried out by L.V. Petrova. To all of the above the authors express their gratitude.

REFERENCES

[1] NIKOLAEV, M.N., supplying nuclear data for fast reactor calculations [in Russian], Voprosy Atomnoj Nauki i Tekhniki, Ser. Yadernye Konstanty 8 (1) (1972) 3.

[2] SINITSA, V.V., Preprint No. 1188 [in Russian], Institute of Physics and Power Engineering Obninsk (1981).

[3] Data formats and procedures for the evaluated nuclear data file, BNL-NCS-50496 (ENDF-102), 2nd ed. (1979).

[4] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for reactor and shielding calculation [in Russian], Ehnergoizdat, Moscow (1981).

[5] BAZAZYANTS N.O., VYRSKIJ, M.Yu., GERMOGENOVA, T.A. et al., ARAMAKO-2F: A neutron constant supply system for calculations of radiative transfer in reactors and shielding [in Russian], Preprint, USSR Academy of Sciences Institute of Applied Mathematics, Moscow (1976).

[6] MANTUROV, G.N., Preprint No. 1034 [in Russian], Institute of Physics and Power Engineering, Obninsk (1980).

[7] KOLESOV, V.E., NIKOLAEV, M.N., See [1] Part 4, p.3.

[8] NORTON, D.S., UKAEA nuclear data library, AEEW -N 824 (1968).

[9] Data formats and procedures for the evaluated nuclear data file, BNL-NCS-50496 (ENDF-102) (1975).

[10] Proceedings of IAEA consultants' meeting on U and Pu resonance parameters, INDC (NDS)-129GJ, Vienna (1981).

[11] ENDF/B Summary documentation, BNL-17541 (ENDF-201), 3rd ed. (1979).

[12] Ibid., 2nd ed. (1975).

[13] HOWERTON, R.J., MACGREGOR, M.H., UCRL-50400, v. 15, Part D, Rev. 1 (1978).

[14] Japanese Evaluated Nuclear Library, ver. 1, JENDL-1 JEARI 1261, NEANDC (J), 59/1, (1979).

[15] MAZNYJ, G.L., Programming on the BEhSM-6 in the "Dubna" system [in Russian], Nauka, Moscow (1978).

[16] CHISTYAKOVA, V.A., YUDKEVICH, M.S., Preprint No. 3046 [in Russian], Institute of Atomic Energy, Moscow (1978).

[17] MUGHABGHAB, S.F., DIVADEEMAN, M., HOLDEN, N.E., Neutron cross-sections, Vol. 1, Neutron resonance paraemters and thermal cross-sections, Part A, Academic Press (1981).

[18] KONONOV, V.N., YURLOV, B.D., MANTUROV, G.N., et al., in: Neutron physics (Proc. Fourth All-Union Conference on Neutron Physics, Kiev, 1977), TsNIIatominform, Moscow, Part 2 (1978) 211.

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THE INDEhKS PROGRAM AND ARCHIVE SYSTEM

G.N. Manturov

ABSTRACT

This paper describes a set of programs for the comparative analysis of calculated and experimental data from integral and macroscopic experiments and for evaluating the accuracy of nuclear reactor parameter calculations by analysing the sensitivity of calculated reactor parameter values to the nuclear physics constants used in the calculations and to the uncertainties in those constants. The paper also describes applications of this system to reactor and shielding problems.

In 1972, S.M. Zaritskij, M.N. Nikolaev and M.Yu. Orlov (of the Institute of Physics and Power Engineering) drew up a work plan for developing computer programs and archives to which the name INDEhKS[*] (Russian acronym for "correction of neutron data on the basis of analysis of results of macroscopic experiments") was given. Their function is:

- To process and store evaluated results of macroscopic experiments along with the corresponding calculated data, in a form suitable for use in correcting constants;
- To calculate and store coefficients for the sensitivity of measured values and reactor parameters to nuclear constants;
- To carry out corrections on neutron constants in order to obtain the best agreement between calculations and experimental results, by varying the constants within the limits of the evaluated errors;

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[*] This system comprises a set of programs used on a fairly powerful computer (e.g. the BEhSM-6), linked to a single constant supply system, and interlinked through computer archives.

- To determine the accuracy of calculated predictions of neutron physics parameters for planned reactors before and after correction of constants;
- To estimate nuclear data requirements, taking into account the accuracy called for in the calculation of the different reactor parameters;
- To evaluate the data yield of different experiments in order to select the optimum experimental program.

The INDEhKS system had to include:

- Macroexperiment evaluation programs ("evaluation" here meaning determination of that proportion of the discrepancy between calculated and measured values which is due to inaccuracies in the constants used for the calculation; determination of covariance matrices for the uncertainties in experimental and calculated data; and determination of coefficients for the sensitivity of calculated values to constants);
- Archives containing the results of macroexperiment evaluation;
- A constant preparation system to reprocess evaluated nuclear data files into group constants;
- Programs to evaluate differential nuclear physics experiments so as to produce evaluated nuclear data and covariance matrices for nuclear constant uncertainties;
- Archives of covariance matrices for group constant uncertainties;
- Programs for statistical analysis of discrepancies between calculated and experimental results, using sensitivity coefficients and covariance matrices for constant uncertainties and also the results of calculations and measurements.

Such a system has been set up [1]. Its structure is shown in Fig. 1. The INDEhKS system is occupied by the CORE set of statistical analysis programs (see Fig. 2). The source data for CORE are supplied by the following

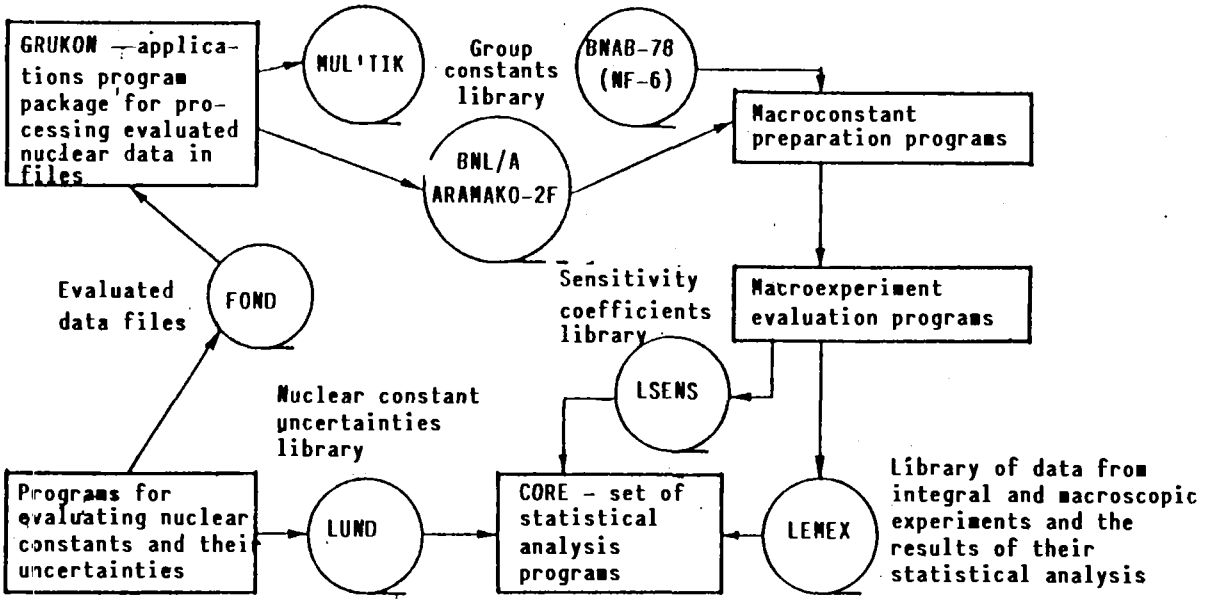

Fig. 1. The INDEHKS System

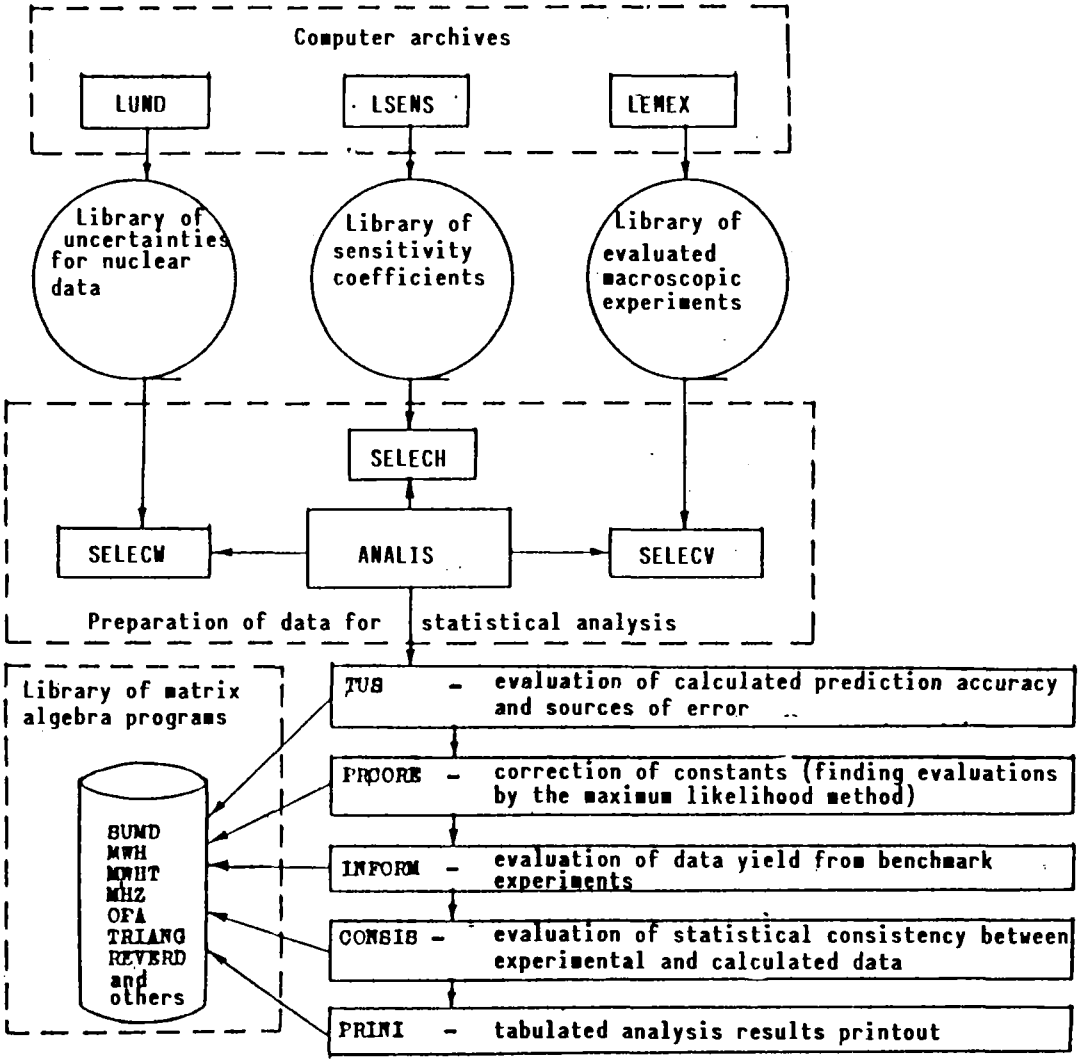

Fig. 2. CORE program structure

computer libraries: Library of Uncertainties for Nuclear Data (LUND), Library of Evaluated Macroscopic Experiments (LEMEX) and Library of Sensitivity Coefficients (LSENS). The algorithms contained in the CORE programs apply methods for the statistical processing of experimental data. A small specialized procedures library has been developed to carry out matrix algebra operations, including matrix summation (SUMD), multiplication (MWH, MWHT, MHZ), transposition (OPA), inversion (REVERD) and other operations on matrices. The second part of the INDEhKS system is made up of programs and archives which keep the computer libraries LUND, LEMEX and LSENS.

In the present version of the INDEhKS system the following programs are used for calculating radiaton fields together with their functionals and sensitivity coefficients and for evaluating macroexperiments:

- For multigroup reactor calculations: NULGEO for B_o-approximation calculations; KRAB1 for one-dimensional P_1- and S_N-approximation calculations; TVK-2D for two-dimensional diffusion calculations in RZ- and XY-geometries; reactor and shielding calculation programs using the Monte Carlo method in real three-dimensional geometry; TRIGEX for calculations in three-dimensional hexagonal geometry; and VPS for reactor calculations taking into account the real heterogeneity of fuel arrangements;
- For calculations of neutron and gamma fields in radiation shielding: ROZ-5, ROZ-6 and ROZ-11, and also the ZAKAT program for calculating sensitivity coefficients.

The range of calculation programs may be extended or changed to accommodate new demands and developments.

Constants for reactor and shielding calculations are supplied by the SOKRATOR ("system to supply constants for nuclear reactor and radiation shielding calculations") system [2]. Its main element is a library of evaluated neutron data files (FOND) recorded in textual form in the ENDF/B

format [3] on computer data carriers. The present version of the FOND library corresponds, for the most part, to those data which were used to obtain the BNAB-MIKRO constant system [4]. The processing of FOND library data (and, if necessary, those of other evaluated data libraries as well) into group constants for arbitrary division into groups is carried out by means of the GRUKON ("group constant calculation") applications program package [5]. By using the FOND-GRUKON channel it is possible to renew and supplement the contents of the second constants library, ARAMAKO ("automated calculation of macroscopic constants") [6, 7], which is in itself a specialized system for supplying constants for multigroup calculations of radiation fields in reactors and shielding. Using the present version of the ARAMAKO system it is possible in practice to carry out 26-, 28- or 49-group neutron calculations, and also calculations of γ-fields in a 15-group approximation. It is intended at a later date to connect this to the MUL'TIK multigroup constants library (approximately 300 groups). The BNAB-78 constant system [4] is being used as a standard constant base, with a more detailed breakdown of the high neutron energy region when necessary [6]. The processing of group library data into macroscopic constants required for radiation field calculations, and also the production of constants necessary for calculating the functionals of these fields, is performed by programs of the ARAMAKO system.

The LUND library contains covariance matrices for BNAB-MIKRO group constant uncertainties, from which the BNAB-78 constant system, used in practical calculations, differs by only a few ^{238}U cross-sections corrected on the basis of data from experiments on fast critical assemblies [4]. The evaluation of these covariance matrices is described, together with the corresponding numerical data, in Ref. [4]. Apart from the covariance matrix of the main constants library the LUND library can also store covariance matrices for the uncertainties of different constant versions.

The LSENS and LEMEX libraries are added to as follows. The LSENS library is added to by means of programs. The results of sensitivity

coefficient calculations obtained using the NULGEO, TVK-2D or ZAKAT programs are entered by means of special interface modules. The LEMEX library can only be added to manually. It receives:

- The symbolic names of experiments and of functionals measured therein;
- Experimental results, including all corrections necessary for applying these results to a miscalculated experimental model (type A correction), and also the covariance matrix for the uncertainties in the experiments taking into account the errors in the type A corrections;
- Calculation results, including all corrections necessary for applying them to a miscalculated experimental model (type B correction), and also the uncertainties matrix for the calculation results, taking into account the errors in the type B corrections.

Considerable experience has so far been gathered in using the INDEhKS system to analyse the sensitivity of reactor and shielding characteristics to constants. Thus, in Ref. [9] the sources of error in calculating the criticality coefficient, breeding ratio and core breeding ratio of a large plutonium fast breeder reactor are analysed, and ways of increasing the accuracy of calculated predictions of fast reactor characteristics are indicated. Reference [10] contains evaluations of the accuracy of calculated predictions of fast reactor characteristics obtained using the BNAB-78 group constant system. These came to $\pm$ 1.4% for the criticality coefficient and $\pm$ 0.035 for the breeding ratio. Reference [4] describes both the heuristic correction of BNAB-MIKRO as a result of which the BNAB-78 constant system was produced and an algorithmic correction which confirmed the results of the authors' research. Reference [11] contains an evaluation of the accuracy of fast reactor shielding calculations.

As is evident from this description, the existing version of the INDEhKS system is geared towards processing and analysing the results of

reactor and shielding benchmark experiments, and also towards evaluating the accuracy of calculated predictions of the characteristics of planned fast reactors and shielding. An advanced program system may also, of course, be used in other fields where the problem arises of correcting a large number of parameters in accordance with the results of indirect experiments.

REFERENCES

[1] MANTUROV, G.N., Software for problems of analysing the sensitivity of reactor characteristics to nuclear constants [in Russian], Preprint No. 1034, Institute of Physics and Power Engineering, Obninsk (1980).

[2] NIKOLAEV, M.N., Supplying nuclear data for fast reactor calculations [in Russian], Yadernye konstanty 8, Part 1 (1972) 3.

[3] Data formats and procedures for the evaluated nuclear data file, BNL-NCS-50496 (ENDF-102, 2nd ed. (1979).

[4] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for reactor and shielding calculations [in Russian], Ehnergoizdat, Moscow (1981).

[5] SINITSA, V.V., The GRUKON package. Part 1. The conversion program [in Russian], Preprint No. 1188, Institute of Physics and Power Engineering, Obninsk (1981).

[6] BAZAZYANTS, N.O., VYRSKIJ, M.Yu., GERMOGENOVA, T.A. et al., ARAMAKO-2F: a neutron data supply system for radiative transfer calculations in reactors and shielding [in Russian], Preprint, Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1976).

[7] ABAGYAN, A.A., BARYBA, M.A., BASS, L.P. et al., ARAMAKO-G: a multigroup constant supply system for calculations of gamma-ray fields in reactors and shielding [in Russian], Preprint No. 122, Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1978).

[8] GERMOGENOVA, T.A., KORYAGIN, D.A., LUKHOVITSKAYA, Eh.S. et al., The unified constant supply system OKS [in Russian], Preprint No. 140 Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1979).

[9] ALEKSEEV, P.N., MANTUROV, G.N., NIKOLAEV, M.N., An evalaution of the uncertainties in the calculation of criticality coefficients and breeding ratios for fast power reactors due to inaccuracies in neutron data [in Russian], At. Ehnerg. 49 4 (1980) 221.

[10] MANTUROV, G.N., NIKOLAEV, M.N., An evaluation of the accuracy of calculated predictions of fast breeder reactor characteristics using the BNAB-78 constant system [in Russian], "Nejtsonneya fizika" (Neutron physics) (Proc. Fifth All-Union Conference on Neutron Physics, Kiev, 15-19 September 1980), Part 3, TsNIIatominform, Moscow, p. 316.

[11] MANTUROV, G.N., SAVITSKIJ, V.I., ILYUSHKIN, A.I., Evaluation of the constant component of the uncertainty in calculating fast reactor shielding [in Russian], ibid., p. 323.

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ON THE PRESENT STATUS OF THE ARAMAKO SYSTEM

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ABSTRACT

This paper reviews the present status of the ARAMAKO multigroup constant calculation system for solving neutron and gamma quantum transport equations and for calculations of linear and bilinear functionals of their fields.

ARAMAKO is a system for supplying constants for neutron and gamma field calculations for fast reactors and radiation shielding in a multigroup approximation. At present the system consists of a data base and the corresponding service routines, program packages for multigroup constant preparation and the KRAB-1 program package for one-dimensional reactor calculations.

The data base contains the following files:

BNL/A - A 26-group basic library of neutron/matter interaction cross-sections with subgroup representation of cross-section resonance structure in binary format. It contains data on nuclides from Refs [1-3] and on a number of other nuclides now being used experimentally;

DOPPLER - A 26-group binary format library containing Doppler increases in cross-section resonance self-shielding factors [1-3];

LPANES - A 26-group binary format library containing elastic scattering anisotropy parameters [3, 4];

LHYDR-26 - A 26-group binary format library containing data on the interaction of neutrons with hydrogen [1];

LHYDR-28 - As LHYDR-26, but with supplementary data on the first

and zeroth groups of the energy division used in the BNAB-78 library [3];

BND-14 - A two-group binary format library containing neutron/matter interaction data for the first and zeroth energy division groups used in the BNAB-78 library [3];

BNGL/A - A group constant binary format basic library containing abundances and 15-group spectra for gamma quanta produced in neutron reactions [3];

SAI - The detailed behaviour of the mass coefficients of gamma attenuation in gamma interactions, in binary format [5];

BGL/A - The detailed behaviour of gamma quanta/matter interaction cross-sections, in binary format. This library was obtained by computer processing of the SAI file;

GAM15G - A 15-group library of gamma quanta/matter interaction data;

TEMBR - A 26-group library of group constants, in textual format [6];

OLN - A working library containing BNL/A data or the TEMBR file. Note that all the calculation programs in the ARAMAKO package use data from this library only, and that the library itself is generated by special software. When the TEMBR file is being used, DOPPLER files also are generated by special programs. The data presentation formats are described in Refs [6-9].

The ARAMAKO program packages may be divided arbitrarily into component parts.

I. The ARAMAKO-OKS program package consists of:

(1) Programs to supply 28- or 26-group constants for use in calculating neutron transport in reactors and radiation shielding

(consisting of extensive homogeneous zones), using spherical harmonic methods, Yvon's method, the discrete ordinate method and others. In these programs the anisotropy of elastic scattering is represented by the first six terms (fifteen in the case of hydrogen) in a Legendre polynomial serial expansion. Both the total macroscopic cross-section and the elastic scattering cross-section are averaged taking into account the fine structure of the flux anisotropy up to the sixth angular moment, it being assumed that $\Sigma^{g}_{t\ell} \approx \Sigma_{tmin}$ when $\ell \geq 6$ (as can be observed in practice);

(2) Programs to supply constants for calculating sources of secondary gamma radiation, based on calculating the neutron fields in 28- and 26-group approximations;

(3) Programs for averaging group constants, based on the detailed behaviour of gamma quanta/matter interaction cross-sections;

(4) Programs to supply multipgroup constants for gamma quanta transport equations, based on the GAM15G library;

(5) Programs combining programs (1), (2) and (4).

The program package detailed above is included in the unified constant system (OKS) applications program package [10] and is used mainly in shielding physics research. However, with the ROZ-VI program [11] a one-dimensional zero-power reactor can be calculated, i.e. this constant supply program package does not take the Dopper effect into account.

II. The ARMAKO-R program package is basically designed to perform simple calculations of fast power reactors and includes:

1. Programs preparing group constants for calculating neutron fields in the P_1 diffusion approximation as well as higher approximations. The scattering indicatrix, for programs solving transport equations by the discrete ordinates method or the Monte Carlo method, is taken into account by

two terms in a Legendre polynomial serial expansion or by a transport approximation.

These programs prepare constants mainly for calculating integral neutron physics characteristics of reactors, such as the criticality coefficient k_{eff}, the breeding ratio and its components, the burnup rate, the efficiency of control and safety system elements, the sodium effect and the Doppler reactivity effect. Differential characteristics can also be obtained with these programs, for example the reaction rate and heat production distributions. The zones of the reactors calculated must be homogeneous and
sufficiently extensive for the group approximation to be applicable. When fast reactors with heterogeneous cores are calculated, the use of group constants obtained by this program package can lead to errors whose magnitude must be evaluated by comparison with the results of calculations using non-group methods.

In these programs, resonance structure is taken into account on the basis of the concept of a dilution cross-section and of subgroup representation of neutron/matter interaction cross-sections. This reduces the time taken by the BEhSM-6 computer to produce the constants for a typical multizone reactor variant to approximately one minute. The Doppler effect is allowed for by interpolating tables of Doppler coefficients for self-shielding factor increases between temperature base points and by extrapolating exponentially for temperatures over 2100 K. Changes in the cross-section self-shielding coefficients resulting from changes in the dilution cross-section due to the Doppler effect are neglected. The error associated with these approximations in calculating the basic reactor characteristics is small compared with the other methodical errors in a 26-group approximation.

The resonance self-shielding of ^{233}U, ^{235}U and ^{232}Th cross-sections at energies below 46.5 eV is allowed for by approxiation to infinite mass.

2. Programs for correcting the elastic slowing-down cross-section and the fission neutron spectrum. These procedures are necessary to reduce the methodical error in the criticality coefficient k_{eff} from 3 to 1%. In these programs, an integrated spectrum is calculated for each homogeneous reactor zone in a 26-group approximation with uncorrected cross-sections and fission neutron spectrum $\chi(\bar{\nu} = 2.4)$. The spectrum for zones where $\nu\Sigma_f \neq 0$ in a material parameter approximation is asymptotic, but it is an equilibrium spectrum for zones where $\nu\Sigma_f = 0$. Further, the spectra are approximated by a broken line, and corrections are made to the elastic slowing-down cross-section on the basis of the within-group spectra evaluated in this way. Multigroup spectra are also used to determine the value of $\bar{\nu}$, which is used to obtain a more precise fission neutron spectrum.

3. Programs preparing constants for calculating sources of secondary gamma radiation, based on calculating neutron fields in a 26-group approximation and 15-group macroscopic constants entering into the integro-differential equation for gamma quanta transport in the approximation of isotropy of the scattering indicatrix.

4. Programs preparing constants for calculating energy release fields in the reactor taking energy transport by gamma quanta into account.

The algorithms used for preparing constants in the ARAMAKO-OKS and ARAMAKO-R packages are described in some detail in Refs [3, 8, 12].

III. The ARAMAKO-K program package is designed to prepare 26-group constants used in applications programs for numerical analysis of experiments on fast critical assemblies. It differs from the ARAMAKO-R package in:

- The programs to prepare microscopic constants for calculating local reactivity coefficients for small samples. These programs contain algorithms for averaging the sample cross-sections taking into account spectrum perturbation of the spectra of the surrounding medium.
- The programs for calculating the homogenized macro- and

microscopic constants for heterogeneous media. These programs calculate cells of heterogeneous lattices in plane and cylindrical geometry using the first collision probability method in a subgroup transport approximation. An option for calculating cluster-type cells consisting of N-angle right prisms with cylindrical inclusions is available;

- The programs to prepare constants in which resonance self-shielding of cross-sections is allowed for by averaging over all possible combinations of subgroups of the resonant nuclides; this significantly increases the processor time required, even when preparing constants for homogeneous media.

IV. The KRAB-1 program package for one-dimensional calculation of reactors, is a constituent part of the ARAMAKO system and a tool for methodically evaluating various algorithms for preparing multigroup and few-group constants.

The structure of the ARAMAKO system described above is such that it can be run on the BEhSM-6 computer. Work is now being done on transferring the system to the ES computer. For example, programs from the ARAMAKO-R package for preparing constants for homogeneous media and for correcting elastic slowing-down cross-sections and fission neutron spectra are being applied industrially. Transfer to the ES is being carried out taking the capabilities of these computers into account, but still preserving the formats and sequences of input and output information so as to minimize the alterations required to access the system from the applications programs.

REFERENCES

[1] ABAGYAN, L.P., BAZAZYANTS, N.O., BONDARENKO, I.I., NIKOLAEV, M.N., Group constants for nuclear reactor calculations [in Russian], Atomizdat, Moscow (1964).

[2] KHOKHLOV, V.F., SAVOS'KIN, M.M., NIKOLAEV, M.N., ARAMAKO set of programs for calculating group macroscopic and block microscopic cross-sections on the basis of a 26-group system of constants broken down into subgroups [in Russian], Yadernye Konstanty 8 3 (1972) 3-132.

[3] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for reactor and shielding calculations [in Russian], Ehnergoizdat, Moscow (1981).

[4] BAZAZYANTS, N.O., ZABRODSKAYA, A.S., NIKOLAEV, M.N., "Gruppovye parametry anizotropii rasseyaniya nejtronov", Yadernye Konstanty 8 2 (1972) 3-96; [Translation: Group parameters for the anisotropy of neutron scattering, Nuclear Constants 8 2 (1974) 1-101, INDC(CCP)-39/U].

[5] STORM, Eh., ISRAEL', Kh., Gamma-ray interaction cross-sections [in Russian], Atomizdat, Moscow (1973).

[6] OSIPOV, V.K., CHISTYAKOVA, V.A., YUDKEVICH, M.S., TEMBR: a format for textual recording of multigroup constant libraries for reactor and shielding calculation [in Russian], Voprosy Atomnoj Nauki i Tekhniki, Ser. Fizika i Tekhnika Yadernykh Reaktorov 5 27 (1982) 62.

[7] BAZAZYANTS, N.O., VYRSKIJ, M.Yu., GERMOGENOVA, T.A., et al., ARAMAKO-2F: A system to supply neutron constants for radiation transport calculations for reactors and shielding [in Russian], Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1976).

[8] ABAGYAN, L.P., BARYBA, M.A., BASS, L.P., et al, ARAMAKO-G: A system to supply multigroup constants for calculating gamma-ray fields in reactors and shielding [in Russian], Preprint 122, Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1978).

[9] VYRSKIJ, M.Yu., DUBININ, A.A., KLINTSOV, A.A., et al., ARAMAKO-2F: A version of a system for supplying constants for high-energy neutron transport calculations [in Russian], Preprint No. 904, Institute of Physics and Power Engineering, Obninsk (1979).

[10] GERMOGENOVA, T.A., KORYAGIN, D.A., LUKHOVITSKAYA, Eh.S., et al., The OKS unified constant supply system, Preprint No. 140, Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1979).

[11] VOLOSHCHENKO, A.V., KOSTIN, E.I., PANFILOVA, E.I., UTKIN, V.A., ROZ-6: A system of programs for solving transport equations in one-dimensional geometries [in Russian], Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1980).

[12] NIKOLAEV, M.N., RYAZANOV, B.G., SAVOS'KIN, M.M., TSIBULYA, A.M., Multigroup approximation in neutron transport theory [in Russian], Ehnergoatomizdat, Moscow (1983).

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A METHOD AND A PROGRAM FOR ATUOMATIC PREPARATION OF FEW-GROUP CONSTANTS FOR REACTOR CALCULATIONS IN THREE-DIMENSIONAL HEXAGONAL GEOMETRY

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ABSTRACT

A method and a program are proposed for the automated preparation of few-group constants using 26-group calculation in three-dimensional hexagonal geometry. The distinctive feature of the method is the precise orientation of the multigroup calculation towards preparing few-group constants exclusively. Along with a natural simplification of the initial problem (large space lattice, reduced accuracy in termination of iterative process), this orientation has allowed approximations to be introduced through which the few-group constants can be calculated in times that are acceptable in practice while maintaining adequate accuracy of the results obtained. For example, the BEhSM-6 computer takes 9 minutes to prepare 4-group macroconstants for the SNR-300 prototype reactor (FRG). The proposed method is carried out by the SERP83 program which is written in FORTRAN.

Calculations in three-dimensional hexagonal geometry based on few-group diffusion approximation have become widespread in the practice of designing fast reactors and supplying calculations for their operation. Hence there is a need for maximum automation of the preparation of few-group constants, since this is at present usually done on the basis of a few multigroup calculations in one- or two-dimensional (R-Z) geometry and is highly dependent on the experience and physical intuition of the researcher. This circumstance makes multivariant calculation research and the comparison of results obtained by different authors extremely difficult. Moreover, this type of procedure is difficult to automate, both because of the complexities involved in

formalizing the construction of simplified models and because of the difficulty of making the inverse transition to hexagonal geometry.

The method we propose for automatic preparation of few-group constants is based on the use of three-dimensional 26-group calculations in hexagonal geometry. The distinctive feature of the method is the precise orientation of the multigroup calculation towards preparing few-group constants exclusively. Experience with (R-Z) geometry calculations shows that the accuracy required for the group fluxes used in the convolution of group constants is significantly less than that normally required of the fluxes used in calculating k_{eff} and heat production fields. Effective advantage may be taken of this fact in building up an algorithm of a 26-group calculation, and indeed this is the main subject of the present paper. We shall not touch on questions to do with methods of convoluting constants, and will use the method most widely used in practice, i.e. that of averaging (even the diffusion coefficient) over the mean integral flux for a given area. Our aim - which is to set up an engineering programme which will completely automate few-group constant preparation for reactor calculations in three-dimensional hexagonal geometry - can be achieved by solving the multigroup diffusion problem in the same calculation model as the few-group problem.

Multigroup calculation method

The fundamental difficulty in solving the problems mentioned above lies in obtaining the solution to a multigroup diffusion problem in three-dimensional hexagonal geometry:

$$-div D^{(g)}(\vec{r})\Phi^{(g)}(\vec{r}) + \Sigma^{(g)}_{y\beta}(\vec{r})\Phi^{(g)}(\vec{r}) = \sum_{\ell=1}^{g-1} \Sigma^{\ell\to g}(\vec{r})\Phi^{(\ell)}(\vec{r}) + \chi^{(g)}(\vec{r})Q(\vec{r}) , \qquad (1)$$

where the neutron source undergoing fission is

$$Q(\vec{r}) = \frac{1}{K_{эф}} \sum_{\ell=1}^{N} \nu\Sigma_f^{(\ell)}(\vec{r})\Phi^{(\ell)}(\vec{r}); \qquad (2)$$

and g is the group number (g = 1, 2, ..., N). The remaining symbols are conventional [1].

Even when requirements regarding the accuracy of iteration are comparatively low and the space lattice is coarse (one point on a hexagonal prism), three-dimensional 26-group calculations in hexagonal geometry in traditional form [calculation of k_{eff} and $\Phi^{(g)}(\vec{r})$] are very time-consuming. There is also a technical difficulty in carrying out such calculations due to the limited amount of working and external memory available to the computer in practice. The end result is that existing programs for three-dimensional multigroup calculations in hexagonal geometry, such as JAR [2], cannot be used effectively to prepare few-group constants in serial calculation research. There is thus a practical need for the original problem (1), (2) to be simplified, and the goal we have set ourselves - to use the solution obtained solely in order to convolute group constants - enables us to do so. Let us now set out the main simplifications.

The source iteration method [1] is the one normally used to solve the hypothetically critical problem (1), (2) with its appropriate boundary conditions. We know that the zonally integral fluxes used in preparing few-group constants converge more quickly than the detailed spatial distribution of the group fluxes. For this reason, the number of external iterations required to obtain the integral spectra can be significantly lower than in solving problem (1), (2) in the traditional manner to within the accuracy normally achieved in practice. The number of external iterations can be reduced even further by improving the choice of initial fission source distribution $Q_o(\vec{r})$, usually set equal to a constant. In the method we propose, the number of external iterations is equal to unity and the distribtion $Q_o(\vec{r})$ required for the calculation is taken from the one-group (N = 1) solution to problem (1), (2).

Experience with these calculations shows that in energy spectrum formation, and consequently also in averaging the constant in a specific

array, a determining influence is exerted by no more than two layers of the surrounding arrays. Hence it is clear that for our given problem the structure of the local fission source is the most important, and it is sufficiently well described by a one-group calculation. Data are set out below which support this conclusion. In practice, however, calculation models may obviously be encountered (not often, we hope) where the above approximation will prove inadequate. We have guarded against this situation by providing a possibility of fission source recalculation followed by the multigroup calculation, i.e. an external iteration option. There is yet another way of increasing accuracy: by better defining the initial distribtuion $Q_o(\vec{r})$, for example through using a 26-group solution to problem (1), (2) while retaining the non-iterative (without external iterations) version of the multigroup calculation.

We noted above that the averaging of constants in practical calculations is done using not the spatial distribution $\Phi^{(g)}(\vec{r})$, but rather the integral fluxes $\bar{\Phi}_i^{(g)}$ averaged over some areas V_i. These areas (homogeneous as a rule) are chosen such that the spectrum within them varies only slightly and the few-group constants can consequently be considered independent of the space co-ordinate. Thus, in terms of our ultimate goal, there is no need to keep the 26-group fluxes for all the grid points of the calculation lattice. However, in solving problem (1) the spatial distributions $\Phi^{(g)}(\vec{r})$ must be kept, as they are used in calculating the slowing-down source for subjacent groups. In order to avoid this, the following approximation is adopted to calculate the slowing-down neutron source:

$$\sum_{\ell=1}^{g-1}\Sigma^{\ell\to g}(\vec{r})\Phi^{(\ell)}(\vec{r})\approx\Sigma^{g-1\to g}(\vec{r})\Phi^{(g-1)}(\vec{r})+\frac{\sum_{\ell=1}^{g-2}\Phi^{(\ell)}(\vec{r})}{\sum_{\ell=1}^{g-2}\bar{\Phi}_i^{(\ell)}}\sum_{\ell=1}^{g-2}\Sigma^{\ell\to g}(\vec{r})\bar{\Phi}_i^{(\ell)}\Bigg|_{\vec{r}\in V_i}. \qquad (3)$$

Approximation (3) is satisfied for the first three groups, and in the absence of hydrogen for all groups below the eleventh. This follows from the assumption that within areas V_i the spatial distribution of the fluxes $\Phi^{(g)}(\vec{r})$ is identical in all groups, i.e. the energy spectrum does not change. This is not so in reality. However, as we have already said, we choose areas V_i in just such a way that the spectrum varies only slightly, and we can therefore expect approximation (3) to be satisfied with sufficient accuracy. The practical absence of external iterations and approximation (3) are the main features of the method we propose.

Problem 1 is converted into finite difference form for a space lattice with grid points at the centres of gravity of hexagonal prisms. The height of the calculation area is divided into flat layers. The resultant system of linear algebraic equations is solved by iteration. To speed up the iterations and reduce calculation time, the following methods are used:

1. Over-relaxation [1]. The acceleration parameter ω is calculated at the 8th iteration for the first energy group and at the 5th for the remaining groups.

2. To set an initial flux distribution for groups below the first, we use the formula

$$\varphi_0^{(g)}(\vec{r}) = \frac{\sum_{\ell=1}^{g-1} \Sigma^{\ell\to g}(\vec{r})\varphi^{(\ell)}(\vec{r}) + \chi^{(g)}(\vec{r})Q(\vec{r})}{B_g^2(\vec{r})D^{(g)}(\vec{r}) + \Sigma_{yg}^{(g)}(\vec{r})}, \tag{4}$$

where $B_g^2(\vec{r})$ is determined from the calculation of the previous group on the assumption that the spatial functions of neutron fluxes in neighbouring groups are similar:

$$B_g^2(r) = \frac{\sum_{\ell=1}^{g-2} \Sigma^{\ell\to g}(\vec{r})\varphi^{(\ell)}(\vec{r}) + \chi^{(g-1)}(\vec{r})Q(\vec{r})}{\varphi^{(g-1)}(\vec{r})D^{(g-1)}(\vec{r})} - \frac{\Sigma_{yg}^{(g-1)}(\vec{r})}{D^{(g-1)}(\vec{r})}. \tag{5}$$

The effectiveness of approximation (5) is borne out by the data in Table 1, which shows the number of iterations involved in calculating a test

model of the West German SNR-300 reactor [2] with an accuracy for the local fluxes of $\varepsilon < 10^{-2}$, where

$$\varepsilon = \max \left\{ \left| \frac{\varphi_j^{(g)}(\vec{r}) - \varphi_{j-1}^{(g)}(\vec{r})}{\varphi_{j-1}^{(g)}(\vec{r})} \right| \right\} \qquad \text{j being the number of iterations.} \qquad (6)$$

It can be seen from Table 1 that the approximation (4), (5) has an advantage over $\Phi_0^{(g)}(\vec{r}) = 1$ for all groups. The advantage is particularly large in the 9th group and below. Overall, the number of iterations is reduced almost by half. In the 6th and 14th groups, approximation (4) with $B_g^2 = 0$ proves more effective owing to the influence of powerful oxygen resonances in the former and sodium resonances in the latter. As a result of this influence, the spatial functions of the fluxes for the 5th and 6th groups, and for the 13th and 14th groups, differ sharply from each other, so that calculating $B_g^2(\vec{r})$ using the flux function from the preceding group in accordance with formula (5) becomes invalid. For this reason, $\Phi_0^{(g)}(\vec{r})$ for the 6th and 14th groups should be calculated with $B_g^2 = 0$ when calculating reactors with oxide fuel and sodium coolant.

3. In an iterative calculation of the spatial distribution of group fluxes, it is desirable to vary the accuracy of the iteration as a function of the relative magnitude of the flux and of its contribution to the reactor characteristic being calculated. This can be done by introducing a variable criterion for exit from the iterative procedure dependent on the problem conditions, group number and contribution of the given calculation grid point to the unknown functional. For our problem we adopted the criterion

$$\varepsilon = \max \left\{ \left| \frac{\varphi_j^{(g)}(\vec{r}) - \varphi_{j-1}^{(g)}(\vec{r})}{\varphi(\vec{r})} \right| \right\} < \varepsilon_0 , \qquad (7)$$

where $\Phi(\vec{r})$ is the total flux obtained from a one-group solution to problem (1), (2).

Table 1

Number of iterations to calculate SNR-300 reactor

Group	I	2	3	4
I	I6	I6	I6	8
2	23	I5	I3	2
3	22	I3	I4	3
4	2I	I5	I3	6
5	I9	II	I3	5
6	20	I7	I3	II
7	I9	I3	I2	8
8	I8	I2	I0	9
9	I8	9	I0	7
I0	I7	9	9	4
II	I6	4	8	4
I2	I4	6	7	4
I3	9	4	4	3
I4	I5	I2	8	I0
I5	I7	8	I0	5
I6	I7	5	I0	3
I7	I7	6	9	2
I8	I8	5	I0	2
I9	I8	7	9	2
20	I9	6	9	2
2I	I9	8	I0	2
22	20	9	9	2
23	2I	7	9	2
24	2I	7	8	2
25	22	8	8	2
26	I8	6	6	2
Total iterations	474	238	257	II2

Note: In column 1, $\Phi_0^{(g)}(\vec{r})=1$ is taken as the initial approximation; in column 2, the initial distribution is calculated according to formula (4) with the parameter $B_g^2(\vec{r})$ as defined by formula (5); in column 3, the calculation of $\Phi_0^{(g)}(\vec{r})$ is carried out in accordance with formula (4) with $B_g^2=0$; column 4 gives the number of iterations involved in calculating the SNR-300 reactor using the ε criterion with $\varepsilon_0 = 10^{-2}$, the initial distribution being calculated in accordance with formulae (4) and (5).

Note that there is a limitation within the program according to which less than two iterations are not carried out. Comparison of the four-group macroconstants calculated using criteria (6) and (7) shows that the difference does not exceed 1%. The total number of iterations, as can be seen from Table 1, is reduced to less than half.

4. The convergence of the iterative process of different points in the calculation lattice is not identical. Sub-regions exist where the solution process stops significantly faster than for the reactor as a whole. For example, the spatial distribution of fluxes in the core as a rule converges faster than in the blanket. The property of non-identical convergence can be exploited to save calculating time. This can be done by identifying sufficiently large sub-regions in which a solution can be obtained with fewer iterations, and arranging for these sub-regions to be by-passed when the extra iterations are carried out. The sub-regions must be large enough for the time saved in by-passing them to be greater than the time lost in arranging the by-pass (identification, checking of conditions and so forth). The choice of these sub-regions is determined both by the conditions of the problem and by the actual algorithm used for its numerical solution. In the SERP83 program, calculation layers were chosen to act as such sub-regions, and the iterations are carried out in accordance with the following scheme.

The calculation is performed layer by layer from top to bottom or vice versa. The "exit from iteration" condition is checked at each calculation layer. Whenever the criterion is fulfilled for a given layer, that layer is excluded from the iteration process. Once the criterion has been satisfied in this way for each layer, one further iteration is carried out on all the layers. If, after this, the criterion proves not to have been fulfilled for the reactor as a whole, the iterations are continued on the usual lines, with every layer being recalculated. However, experience with calculations of the SNR-300, BN-350 and BN-600 reactors has shown that a single final, full iteration (for all layers) is quite sufficient. Data characterizing the iteration process for the SNR-300 prototype reactor from this point of view are set out in Table 2. 1 indicates that the calculation is carried out for that layer, 0 indicates that the layer is left out of the iteration process. The data are for the 5th group. The iterations are carried out using Seidel's method with an accuracy of $\varepsilon_0 = 10^{-2}$ in accordance with criterion (6).

Table 2

The iteration process for the 5th group for the SNR-300 prototype reactor

Iteration number	Layer number																			
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
3	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
4	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	1	0
5	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

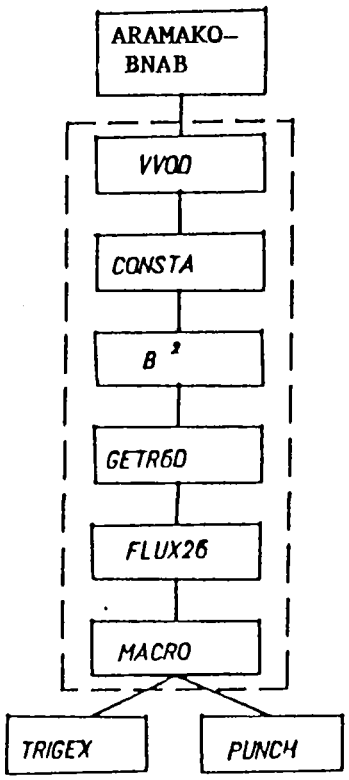
It can be seen that this approach allows real savings in terms of computing time.

The method proposed is carried out by the SERP83 program, which includes calculation of 26-group fluxes in three-dimensional hexagonal geometry and preparation of few-group constants on this basis.

The SERP83 program (See blocked diagram on page 76).

ARAMAKO-BNAB: a source library of 26-group cross-sections supplied by processing programs for calculating block micro- and macroconstants.

VVOD: input of initial data, separated into two basic groups. The first group, which contains the cartogram and service information for allocating the external memory, selecting computing and printing modes and so forth, corresponds wholly to the initial data format of the TRIGEX program [3]. The second group of initial data gives the mode of operation for the ARAMAKO system [4] and contains the concentrations and temperatures of the physical areas in the system to be calculated. In addition, data are entered on the boundaries of the broad groups. In contrast to the TRIGEX program, in



Block diagram of SERP83 program

which a layer-by-layer formulation of the calculating cartogram is adopted, the SERP83 program has an additional, much less time-consuming package option for describing reactor geometry and composition.

CONSTA: a module selecting and converting the 26-group constants calculated by the ARAMAKO system into the SERP83 internal format.

B^2: flux calculations in a B^2 approximation for all the physical areas in the system being examined. In areas containing fissile isotopes, the value of B^2 is determined from the criticality condition, while in non-fission areas $B^2 = 0$.

On the basis of the spectra thus obtained, corrections to the slowing-down cross-section [5] (BJTJ-ARAMAKO sub-routine) and fission spectra $\chi_i(g)$ (XIN-ARAMAKO sub-routine) are calculated. These spectra are used to obtain the one-group constants required by the GETR6D module.

GETR6D: one-group calculation of the hypothetically critical problem (1), (2) in three-dimensional hexagonal geometry to obtain the initial distribution of sources $Q_o(\vec{r})$. The module is a simplified version of the TRIGEX program's basic iteration block.

FLUX-26: for 26-group calculation of problem (1) in three-dimensional hexagonal geometry with a known source $Q_0(\vec{r})$. Output is in the form of spectra integral over the separate areas.

MACRO: calculation of macroscopic few-group constants (D, Σ_{rem}, $\nu\Sigma_f$, $\Sigma_f + 0.35\Sigma_c$, $\Sigma^{i\to j}$) and of the corrections to the slowing-down cross-section and recalculation of fission spectra using the integral spectra obtained. Results are printed out or punched on cards (in the input format for the TRIGEX program) or can also be transferred directly into the TRIGEX program via the COMMON block. This is more efficient, as not only the constants required for the calculation, but also the initial few-group fluxes can be transferred in this case, thus cutting down the number of iterations required in the TRIGEX program and so reducing overall computing time.

The program is written in FORTRAN and run on the BEhSM-6 computer. The program volume is 2200 operators. The computing time for the SNR-300 reactor (397 assemblies, 20 horizontal layers) is approximately 9 min, that for the BN-350 (721 assemblies, 24 horizontal layers) approximately 20 min.

Calculation results. Tables 3 and 4 set out the results of the calculations of the few-group constants $D^{(g)}$ and $\Sigma^{(g)}_{rem}$ carried out for the SNR-300 prototype reactor. The data in column 1 represent 26-group fluxes calculated by Seidel's iterative method to an accuracy of $\varepsilon_0 = 10^{-2}$ in accordance with criterion (6), the initial distribution $Q_0(\vec{r})$ being obtained from a one-group calculation. Column 2 shows analogous results for the case where the initial distribution of the source is given by the formula

$$Q_0(\vec{r}) = \nu\Sigma_f^i\Big|_{\vec{r}\in V_i}, \tag{8}$$

where $\nu\Sigma_f^i$ are one-group constants calculated in a B^2 approximation. The difference between the first and second sets of results characteristics the sensitivity of the few-group constants to the shape of the source used in

Table 3

Diffusion coefficients for various versions of the SNR-300 prototype reactor calculation

	I	2	3	4
	Low enrichment zone			
I	2,636	2,635	2,616	2,629
2	I,556	I,55I	I,566	I,555
3	0,8I48	0,8I52	0,8I64	0,8I47
4	0,9672	0,9669	0,962I	0,9672
	High enrichment zone			
I	2,632	2,633	2,613	2,626
2	I,566	I,573	I,574	I,565
3	0,8028	0,8026	0,8044	0,8029
4	0,9500	0,9497	0,9455	0,9497
	Lateral blanket			
I	2,099	2,I00	2,066	2,095
2	I,I66	I,I82	I,I86	I,I65
3	0,7068	0,7063	0,7I20	0,7069
4	0,8II9	0,8II9	0,8II5	0,8II9
	Core control rod			
I	4,388	4,388	4,363	4,373
2	2,808	2,805	2,833	2,807
3	I,2II	I,2II	I,227	I,2I2
4	I,696	I,695	I,694	I,695

Table 4

Removal cross-section for various versions of the SNR-300 prototype calculation

	I	2	3	4
	Low enrichment zone			
I	0,03583	0,03585	0,03053	0,03580
2	$0,0^{2}5509$	$0,0^{2}5580$	$0,0^{2}5593$	$0,0^{2}55I8$
3	0,0I707	0,0I7I2	0,0I904	0,0I7I0
4	0,02687	0,02694	0,02826	0,02828
	High enrichment zone			
I	0,03626	0,03621	0,03I30	0,03632
2	$0,0^{2}6I65$	$0,0^{2}6084$	$0,0^{2}6290$	$0,0^{2}6I67$
3	0,0I882	0,0I878	0,02095	0,0I882
4	0,03356	0,03367	0,03496	0,03358
	Lateral blanket			
I	0,04492	0,04448	0,03754	0,04498
2	$0,0^{2}6305$	$0,0^{2}5962$	$0,0^{2}597I$	$0,0^{2}63II$
3	0,0I572	0,0I563	0,0I770	0,0I574
4	0,0I388	0,0I388	0,0I434	0,0I388
	Core control rod			
I	0,0I855	0,0I854	0,0I579	0,0I862
2	$0,0^{2}I800$	$0,0^{2}I82I$	$0,0^{2}I76I$	$0,0^{2}I805$
3	$0,0^{2}6366$	$0,0^{2}6403$	$0,0^{2}8249$	$0,0^{2}6380$
4	$0,0^{3}8936$	$0,0^{3}90I4$	$0,0^{3}9282$	$0,0^{3}8960$

Note: In columns 1–3 the criterion for completing the iteration process is determined by formula (6), in column 4 by formula (7). In columns 1, 3 and 4 the initial source distribution $Q_0(\vec{r})$ is derived from a one-group calculation, and in column 2 from formula (8). Corrections b_j are made to the slowing-down cross-section in columns 1, 2 and 4, while in column 3 $b_j = 1$.

the multigroup calculation. Clearly, this sensitivity is not great. Although approximation (8) is an extremely crude estimate of $Q_0(\vec{r})$ compared with the one-group calculation, the differences in the diffusion coefficient do not exceed 1%. For the removal cross-section the differences do not exceed 1.5%, with the exception of the 2nd group for the lateral blanket, where the difference is 5.5%. Such a small dependence of the few-group constants on the shape of the source $Q_0(\vec{r})$ is indirect evidence that estimating this distribution with a one-group calculation is adequate for the given problem.

Column 3 of Tables 3 and 4 shows results obtained without corrections to the slowing-down cross-section, i.e. without the correction factor $b_i = 1$. We see that the differences in the diffusion coefficient are within 1%, apart from the 1st group for the lateral blanket, where the difference is 1.5%. The differences are significantly greater for the removal cross-sections. Thus, in the last group the difference is as high as 15%, in the 2nd it is 5%, in the 3rd, 13% (30% for a control rod) and in the 4th group around 5%. Hence it is clear that introducing the coefficient b_i has a profound effect on few group constant calculation. Column 4 contains results analogous to those in column 1 again with an accuracy of iteration for the 26-group calculation of $\varepsilon_0 = 10^{-2}$, but with the "exit from iteration" criterion as defined by formula (7). When this is done, the differences in the few-group constants do not exceed 1%, which indicates that this criterion is valid for the problem in question. Note that in switching from condition (6) to condition (7) the number of iterations is reduced by more than half (see Table 2).

REFERENCES

[1] SHISHKOV, L.K., Methods of solving the diffusion equations of a two-dimensional nuclear reactor [in Russian], Atomizdat, Moscow (1976).

[2] ZIZIN, M.N., SHISHKOV, L.K., YAROSLAVTSEVA, L.N., Test neutron physics calculations of nuclear reactors [in Russian], Atomizdat, Moscow (1980).

[3] SEREGIN, A.S., Notes on the TRIGEX program for few-group neutron physics calculation of a reactor in three-dimensional hexagonal geometry [in Russian], Voprosy Atomnoj Nauki i Tekhniki, Ser. Fizika i Tekhnika Yadernykh Reaktorov 4 33 (1983) 59-60.

[4] BAZAZYANTS, N.O., VYRSKIJ, N.Yu., GERMOGENOVA, T.A., et al., ARAMAKO-2F - a system for preparing neutron constants for calculations of radiation transport in reactors and shielding [in Russian], Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1976).

[5] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for reactor and shielding calculation [in Russian], Ehnergoizdat, Moscow (1981).

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A PROGRAM FOR CALCULATING GROUP CONSTANTS ON THE BASIS OF LIBRARIES OF EVALUATED NEUTRON DATA

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ABSTRACT

The GRUKON program is designed for processing libraries of evaluated neutron data into group and fine-group (having some 300 groups) microscopic constants. In structure it is a package of applications programs with three basic components: a monitor, a command language and a library of functional modules. The first operative version of the package was restricted to obtaining mid-group non-block cross-sections from evaluated neutron data libraries in the ENDF/B format. This was then used to process other libraries. In the next two versions, cross-section table conversion modules and self-shielding factor calculation modules, respectively, were added to the functions already in the package. Currently, a fourth version of the GRUKON applications program package, for calculation of sub-group parameters, is under preparation.

The GRUKON (group constant calculation) program is part of the system for supplying constants for nuclear reactor and radiation shielding calculations (SOKRATOR) [1]. The GRUKON program, along with the FOND library of evaluated neutron data files [2], forms the MIKRO sub-system, which is designed to generate periodically, for a given set of nuclides, multigroup and fine-group constants (having, respectively, several tens and several hundreds of groups), independently of the composition of the medium. As an example, we may cite the well-known BNAB system [3] and also the MUL'TIK system of 250 groups (in the slowing-down region), which is currently being developed for checking multigroup approximations [4].

In structure, GRUKON is a package of applications programs [5] whose basic components are:

- A set of functional modules which carry out various structural conversions on neutron cross-section data;
- Systems software to sequence processing by the functional modules (according to task) and to provide information links between modules;
- A command system by means of which the user runs the data structure conversion program.

Data exchange between the functional modules is by standard information units (standard representations) which are stored in the package's working library, or standard representations library (BSP). The GRUKON package of applications programs can thus be described as a program package with standard function loading. A description of the package hardware and capabilities and of its operating instructions is contained in Refs [6-9].

Structure of the function loading

All conversions carried out by GRUKON can be divided into four groups:

- Data input from punched cards or from evaluated data libraries, converted into standard form and entered in the BSP;
- Algorithmic conversions, which switch from one method of representing cross-section data to another;
- Editing conversions, which change only the locations of data within the BSP without altering the internal structure of the standard representations;
- Output of data from the BSP, i.e. to an alphanumeric printer in the form of lists or annotated tables, or converted into group constant library format and entered in the device indicated.

The second group of conversions being the more important, we shall examine it in greater detail. The conversions in this group are chosen in such a way as to facilitate the transition from the representation of cross-section data used in the evaluated data libraries to the representation

of data as constants. As we know, the evaluated data libraries represent cross-section resonance structure by means of resolved resonance parameters (R), tables of cross-section energy dependences (S) and mean resonance parameters (U), whereas cross-section group functionals (F) and sub-group parameters (P) are characteristic of group constant libraries. The problem is thus how to make the transition from the R, S, U set to F or P representation. In the GRUKON package this transition is accomplished by the following modules:

- Calculation of the detailed cross-section behaviour from the resolved resonance parameters (R/T-S);
- Calculation of the cross-sections for a given temperature (S/T-S);
- Calculation of the energy dependence of the expected values of the cross-section functionals on the basis of the energy dependence of the mean resonance parameters (U/D-F);
- Addition of various cross-section components given by the detailed behaviour and reduction to a general set of fundamental energies (S/C-S);
- Computation of group functionals on the basis of the detailed cross-section behaviour (S/G-F);
- Computation of group functionals on the basis of the energy dependence of the expected values of the cross-section functionals (F/G-F);
- Convolution of the cross-section functionals given for the various components of the cross-sections (F/C-F);
- Obtaining of sub-group parameters on the basis of the dependence of the cross-section group functionals on the cross-section environment, dilution and temperature parameters (F/-P).

The conversion system is shown in Fig. 1. The special feature of this system is that it does not involve the limitations usually applied by processing programs to evaluated data libraries, namely (1) that the total

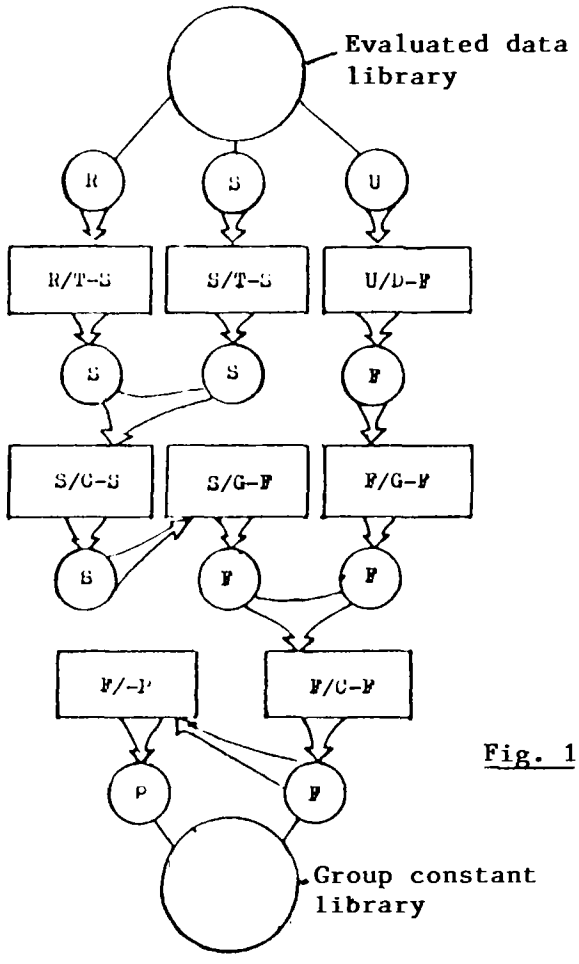

Fig. 1. System for converting evaluated neutron cross-section data into group constants

cross-section must be given for a set of fundamental energies representing a combination of all sets for national cross-sections; and (2) that the resolved and unresolved resonance regions must not overlap, even if the resonances are related to different systems [10]. This feature increases the system's ability to represent cross-section resonance structure in evaluated data libraries.

At present, the capabilities of the GRUKON applications program package's loaded functions are greater than required to solve the basic problem. It has been found that these are closely related problems which can be solved to some extent using the existing functional modules, such as analysis of microscopic experiment data, evaluation of neutron cross-sections and generation of evaluated data libraries. However, it was considered useful to expand the set of modules so as to cover these areas more fully. For example, a group of modules for converting cross-section tables has appeared

which is designed to automate the generation of detailed cross-section behaviour files, and the capabilities of the S/G-F, U/D-F and F/C-F modules were increased so that experimentally measurable transmission and self-indication functions could be calculated as well as the block cross-sections used in group constant libraries.

Currently, the total number of functional modules (including the input/output and editing modules) is 28 [9].

Conversion control and data exchange organization

There are two levels of data conversion control in the GRUKON package. The first level of control uses what is termed a conversion program, fed in from punched cards at the beginning of the calculation by the monitor program of the package (Fig. 2). The conversion program uses stationary language (see below) to establish the sequence in which the functional modules are called up and to determine the location of data in the BSP.

The second control level - control of module operating mode - uses "conversion parameters". The parameters are entered from punched cards by the INPUT module and stored in the BSP along with the basic cross-section data, from which they differ only in name (both the basic data and the parameters have the same formal structure of standard representations. As the set of parameters is specified for each module, their conventional names coincide with the names of the corresponding conversions. For example, in the case of the module for calculating detailed behaviour from resonance parameters (R/T-S), the conversion parameters are named R/T-S and contain the number of the resonance formula, the numbers of temperatures for which the cross-sections must be computed, the energy interval boundaries, the accuracy of interpolation between fundamental energies, and temperature values. All data entered into the BSP (irrespective of whether they are external input or the results of calculations) are logged by the monitor program in the BSP catalogue, in which are entered: the data name, the number of the device in

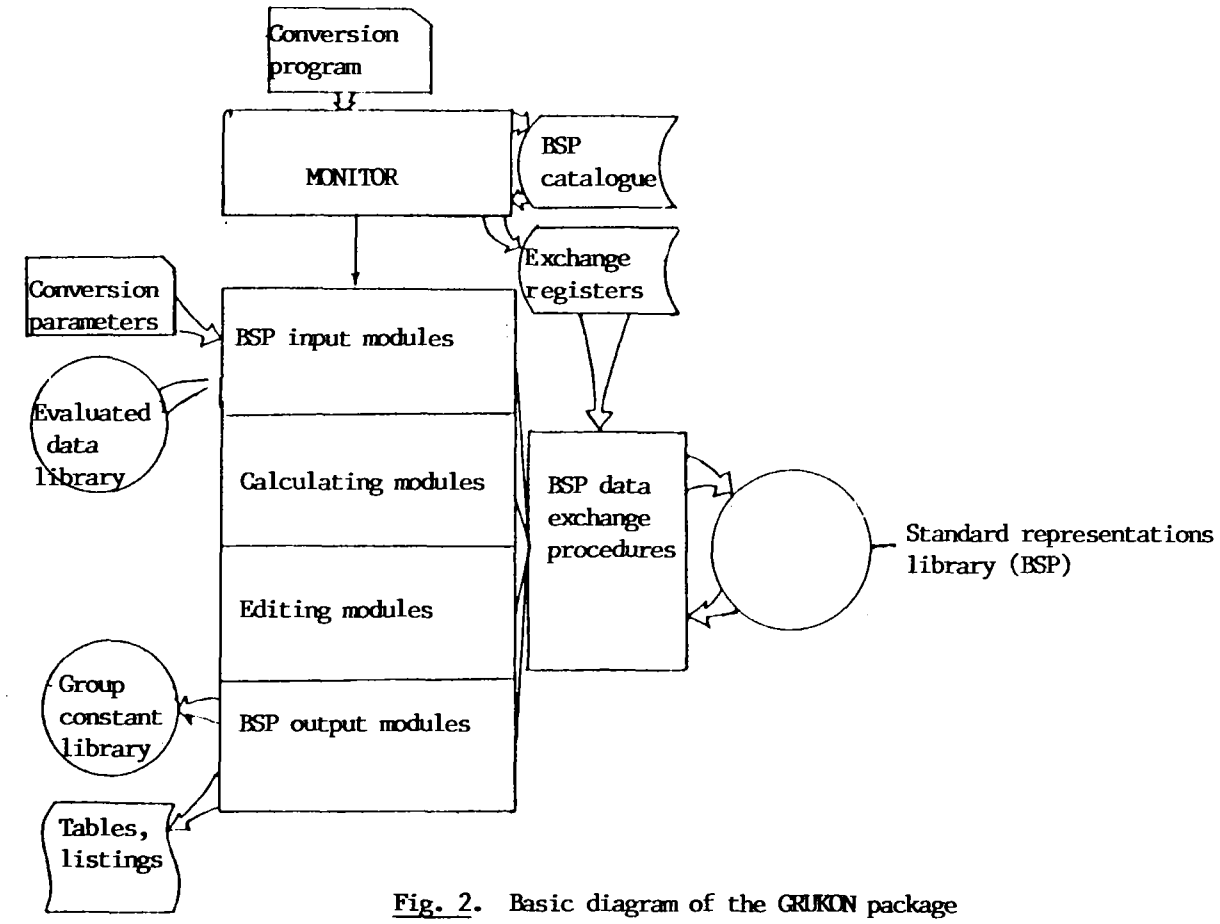

Fig. 2. Basic diagram of the GRUKON package

which they are stored, the initial address of the data, and their length (in words). Before calling up the next module, the monitor program analyses the next command in the conversion program, determines the address of the source data to be used in the conversion and builds up exchange registers from them. In this way the system exchange procedures used in the telefunctional modules for reading and writing data from the BSP are adjusted to a particular operating mode. Information on the location of data is thus excluded from the telefunctional modules, which much simplifies programming them. At the same time, correct use of the systems procedures for data exchange with the BSP provides a data link between modules and protects the BSP. Information is exchanged between the modules and the BSP along three channels: the first carries source data, the second carries the parameters, and calculation results are recorded through the third. Information is fed through each of the channels page by page by way of the corresponding buffer arrays (sheets).

The devices to which the data channels are attached may be either the same or different; in the latter case, the page/channel correspondence is not observed and pages are exchanged taking the access frequency into account.

Command system

Four groups of commands are used in the conversion program:

- For data conversion (including input, output, editing and algorithmic conversions);
- For catalogue generation (enter in catalogue, alter data names and print out catalogue contents on alphanumeric printer);
- For designating the working field of the BSP library;
- For control (repeat command groups, end conversion).

The commands in the first group have the most general structure, so we shall confine our remarks to them. The conversion command has a three-address structure: I, J, K, <k-data name>, <k-data address in BSP>; where I, J and K are the addresses in the BSP catalogue of the source data, the parameters and the conversion results, respectively (data address in the catalogue means the number of the catalogue line on which they are recorded). Apart from data addresses, a comand may also indicate the name assumed by a conversion result and the address at which the data should be entered in the BSP (if the address is omitted, the results are entered in the BSP working field starting at the first free word). Address in the BSP means the device number, the number of the first word, and the number of words occupied by the data. Note that a need to indicate the BSP address does not often arise so the command structure is usually fairly simple. The remaining commands are a subset of the conversion commands; for example, the command to end conversion consists of one name, written ,,,END. There is a detailed description of the command system used in the GRUKON package in Ref. [6]. The return to "code programming" in the input language of the GRUKON package might appear to be a backwards step, unless it is taken into account that the appearance of

higher-level languages was related to the requirements of automated programming, which do not arise in this case.

Operating experience and prospects for program development

Since the first operative version of the GRUKON package was put on the BEhSM-6 computer, it has been used for the preliminary processing of data available to the author from foreign data libraries (the American libraries ENDL-78 [11] and ENDF/B-IV [12], some files of ENDF/B-V [13], and also the Japanese library JENDL-J [14] into 28-group non-block cross-sections averaged with standard spectrum weighting in the BNAB group division [3]. Cross-section evaluation calculations were carried out and detailed behaviour files were generated from the FOND evaluated data library.

Mid-group values for cross-sections were obtained for basic reactor materials using the 250-group MUL'TIK division, and work began on calculating the sub-group parameters. Currently, the algorithms for obtaining sub-group parameters are being run in, and work has begun on transferring the program to the ES-1060 computer. It is proposed in the immediate future to include in the package modules for processing data on neutron angular and energy distributions, functioning in an autonomous mode for the time being.

REFERENCES

[1] NIKOLAEV, M.N., "Obespechenie raschetov bystrykh reaktorov yadernymi dannymi", Yadernye Konstanty 8 1 (1972) 3. [Providing nuclear data for fast reactor calculations, Nuclear Constants, 8 1 (1974) 1; INDC(CCP)-38/U].

[2] KOSHCHEEV, V.N., NIKOLAEV, M.N., A library of neutron data for calculating group constants [see present publication, fifth Abstract].

[3] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for calculating reactors and shielding [in Russian], Ehnergoizdat, Moscow (1981).

[4] DOLGOV, E.V., SAVOS'KIN, M.M., TSIBULYA, A.M., On the development of a fine-group constant system [see present publication, final Abstract].

[5] BASS, L.P., GERMOGENOVA, T.A., ZHURAVLEV, V.I., et al., Preprint No. 44, Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1979).

[6] SINITSA, V.V., Preprint No. 1188, Institute of Physics and Power Engineering, Obninsk (1981).

[7] SINITSA, V.V., Preprint No. 1189, Institute of Physics and Power Engineering, Obninsk (1981).

[8] SINITSA, V.V., Preprint No. 1332, Institute of Physics and Power Engineering, Obninsk (1982).

[9] SINITSA, V.V., Preprint No. 1429, Institute of Physics and Power Engineering, Obninsk (1983).

[10] MacFARLANE, R.E., BOICOURT, R.M., NJOY: A neutron and photon cross-section processing system. Trans. ANL, 22 (1975) 720.

[11] HOWERTON, R.J., MacGREGOR, M.H., The LLL evaluated nuclear data library (ENDL), UCRL-50400, California, Livermore, 15 (1978) Part D, Rev.1.

[12] ENDF/B Summary documentation, BNL-17541 (ENDF-201), 2nd Ed. Upton, New York (1975).

[13] Ibid. 3rd Ed. Upton, New York (1979).

[14] Japanese evaluated nuclear data library, Ver.1, JENDL-1, JEARI-1261, NEANDC (J) 59/1. Tokai-mura, Ibaraki-ken (1979).

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EVALUATION OF THE METHODICAL ERROR IN 26-GROUP APPROXIMATION

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ABSTRACT

The accuracy of calculation of linear and bilinear functionals using a 26-group approximation is evaluated by comparing fine-group (288 groups) calculations with group (26 group) calculations. It is demonstrated that multigroup calculations of fast reactors call for the calculation of slowing-down cross-sections on the basis of an approximative evaluation of the within-group spectrum. At present levels of accuracy of nuclear data the methodical error of a 26-group approximation is acceptable. In order further to increase the accuracy of calculated predictions of the main physical characteristics of fast reactors to the level required, it will be necessary to make a transition to a fine-group system of constants. Multigroup calculations cannot provide accuracies of the central reactivity coefficients better than tenths of a per cent (up to 1%) of the reactivity coefficient of the basic fuel isotope.

In order to determine the methodical error in a 26-group approximation [1], a comparison must be made with calculations performed in a more detailed energy division with the same source information. The standard used for this purpose in the present work was a 288-group system of constants which was worked out on an M-222 computer and corresponds in its energy structure to the BNAB 28-group constant system [2]. Division of the group library (28 groups) into a fine-group (288-group) library was carried out as follows: the -1th group (14.0-14.5 MeV) was made into a single fine group; the 0th group (10.5-14.0 MeV) was divided into three fine groups; the 1st group (6.5-10.5 MeV) into five fine groups, and groups 2-8 inclusive (lower boundaries 4.0, 2.5, 1.4, 0.8, 0.4, 0.2 and 0.1 MeV) into nine fine

groups. The remaining groups were divided into 12 fine groups each. All the fine groups within the same broad group have the same width on the lethargy scale. A sub-group approximation is used to describe the unresolved resonance structures of the cross-sections within the fine groups. The M-222's limited memory places a restriction on the total number of sub-groups in all the fine groups of a given broad group, which must not exceed a certain number (nine or 12). This is achieved by combining fine groups with similar mean cross-sections into a broader fine group. The number of sub-groups in each fine group must not exceed four.

The fine-group averaged cross-sections for ^{238}U are shown in Fig. 1; the numbers denote the number of sub-groups in a given fine group. The fine-group averaged capture cross-sections are set off from the total cross-sections by hatching. As the diagram shows, the first seven strong resonances of ^{238}U are well described in the fine-group energy approximation we have adopted, bearing in mind that the resonance structure not resolved by the fine groups is taken into account in the sub-group approximation. In

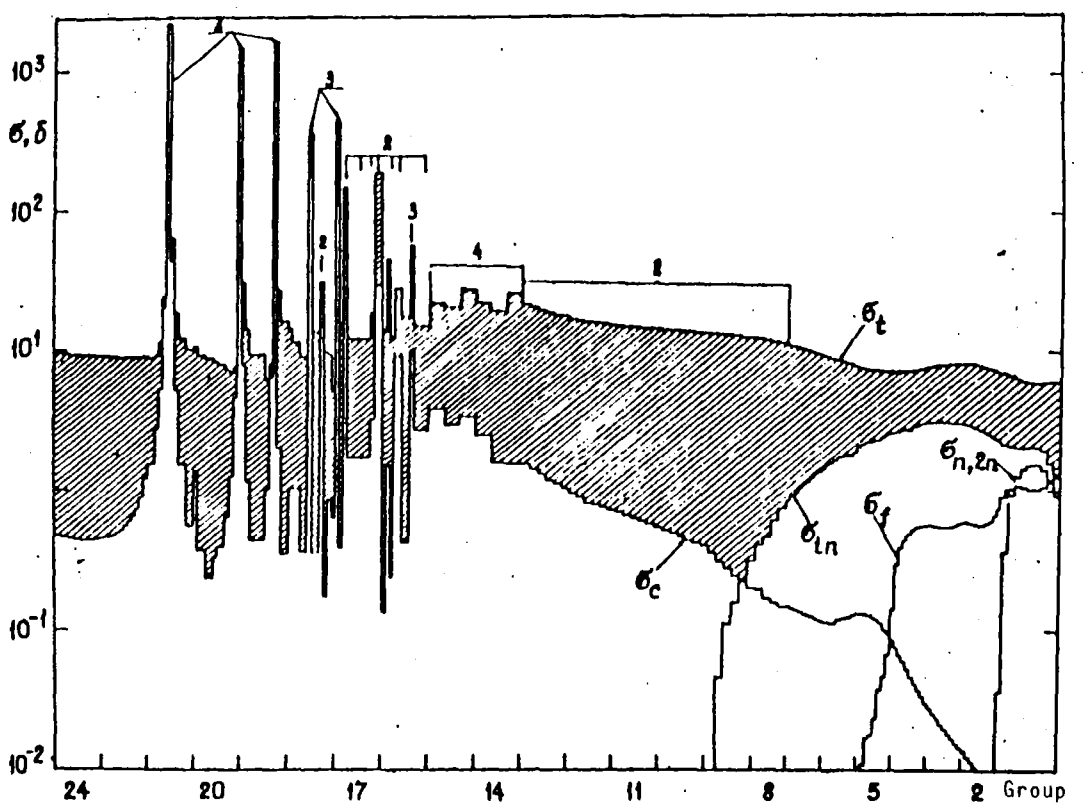

Fig. 1. Fine-group averaged cross-sections for ^{238}U

building up a fine-group system of constants, special attention must be paid to those isotopes which most affect the calculation characteristics of fast reactors. Fine-group constants for the isotopes ^{10}B, ^{12}C, ^{16}O, sodium, aluminium, iron, nickel, ^{235}U, ^{238}U, ^{239}Pu and ^{240}Pu were prepared on the basis of UKNDL and Soviet files. Information for isotopes not listed above was taken from the ARAMAKO constant library [3].

Calculation method

A set of programs was written for work with the fine-group constant library which is capable of:

- Preparing fine-group block macro- and microconstants;
- Calculating fine-group fluxes and importances in a B_0 approximation;
- Convoluting fine-group constants into 26-group constants, weighted with both standard spectra and calculated fluxes;
- Carrying out 26-group calculations of fluxes and importances for convoluted constants;
- Calculating linear flux functionals (reaction rates) and bilinear flux and importance functionals (sample reactivities) in group and fine-group divisions;
- Calculating correction factors to constants reflecting the effect of the difference in shape between within-group and standard spectra on the results of averaging 26-group constants;
- Introducing corrections into the basic physical characteristics (integral fluxes, k_{eff}, central reactivity coefficients) calculated in a 26-group approximation to account for the shape of the within-group spectrum.

This set of programs was used to evaluate the accuracy of the 26-group approximation. The results of the 26-group and 288-group calculations were compared in a diffusion B_0 approximation for media studied on the BSF and

KBR critical assemblies and also for media making up the core of a fast reactor prototype.

For each medium a basic version of the calculation in a fine-group approximation - version A - and three 26-group calculations were performed:

- Version B: calculation using constants averaged and weighted with the fine-group fluxes obtained in version A;
- Version C: calculation using constants averaged and weighted with the standard spectrum and with slowing-down cross-sections as in version A;
- Version D: calculation using constants averaged over the standard spectrum and with slowing-down cross-sections obtained either for the standard spectrum or evaluated by one of the approximation methods [4] as follows:

  MG - An approximative fine-group method which does not take into account the energy dependence of the cross-sections within the limits of the group. The probability of sub-group scattering leaving a neutron within the same BNAB group was treated as varying linearly from zero at the lower energy boundary of the group to twice the mid-group value at the upper. Inelastically scattered neutrons are distributed uniformly over the remaining parts of the group;

  GG - Calculation of the shape of the within-group spectrum using the Greuling-Goertzel continuous slowing-down model. The cross-sections are treated as constant within the group limits;

  PA - Parabolic evaluation of the spectrum shape. The parabola parameters are determined from the conditions for neutron flux conservation in a given group and in two neighbouring groups (the fluxes being determined in a preliminary calculation);

DU - Two-node evaluation of the spectrum shape, consisting in approximating a histogram of the previously calculated scattering density by a partly continuous broken line with two nodes in each group. The values at the nodes are determined from the conservation condition for the mid-group scattering density Q and the equality of the derivative dQ/dU (in the interval between points lying wholly within a single group) with the mean value of the derivatives of adjacent parts of the broken line. The node positions are optimized to give the smoothest possible approximation;

LI - Evaluation of spectrum shape by linear interpolation of group fluxes.

Calculation of linear functionals of the flux

The results of calculating linear functionals of the flux are shown in Tables 1 and 2. All the values obtained for versions A and B agree (this was a method of testing that the program was functioning correctly). Comparison of the data obtained in versions A and B shows that, even when accurate slowing-down cross-sections are retained, using standard rather than real spectra in averaging the capture and fission cross-sections leads to errors in the criticality coefficient k_{eff} (0.8% in the BFS-38 assembly) and the core breeding ratio (0.5% for the fast reactor prototype).

Using the standard spectrum in calculating slowing-down cross-sections (version D, correction factor $b_j = 1$) leads to errors in k_{eff} (3.5% for the BFS-31 assembly). These figures can be explained from Tables 3 and 4, which show the effect of the difference between standard and real spectra on the capture and fission cross-sections to be greatest at low energies and to result in lower group fluxes for the standard 26-group calculation because of the overestimation of the absorption cross-sections when averaged over the standard spectrum. This is to be expected, since the within-group spectra for

Table 1

Comparison of the functionals calculated according to different slowing-down models

Functional	I	$\delta I = (I_\alpha / I_{mul'tik} - 1)100\%$					
	Version		Version D methods				
	A, B	C	MG	GG	PA	DU	LI	$b_1 = 1$
	BFS-33 assembly							
k_{eff}	0,9612	+0,3	-0,1	+0,6	+0,9	+0,2	+0,4	+2,8
$\bar{\nu}$	2,5115	+0,1	+0,1	+0,1	+0,1	+0,1	0	+0,2
Σ_f	0,00249	+0,5	+2,4	+0,9	0	+0,6	-0,6	+3,2
Σ_o	0,00402	+0,1	-2,7	0	-1,3	+0,4	-0,3	-1,1
f^8/f^5	0,0209	+2,0	+3,2	+4,8	+4,1	+2,2	-1,3	+6,0
f^9/f^5	0,9105	+0,4	-0,7	+0,5	+0,9	+0,5	+0,8	+1,4
f^{10}/f^5	0,1878	+0,1	-2,6	+1,4	+2,4	0	-1,8	+5,1
σ^8/f^5	0,1402	-0,2	+0,7	-0,1	-0,7	0	-0,1	-3,7
σ^8/f^9	0,1540	-0,6	+1,4	-0,6	-1,6	-0,8	-0,9	-5,1
α^5	0,2846	0	+1,4	-0,1	-0,7	+0,2	0	-0,2
α^9	0,2917	+0,2	+3,4	+0,3	-1,8	+0,6	-0,5	+1,4
	Baker's core model							
k_{eff}	1,000	+0,4	+0,2	+1,0	+1,5	+0,7	+0,5	+3,3
$\bar{\nu}$	2,807	0,0	0,0	0,0	0,0	0,0	0,0	+0,1
Σ_f	0,00166	+0,8	+2,1	+1,5	+1,8	+1,0	+0,7	+4,6
Σ_o	0,00261	+0,3	+0,2	-0,1	-0,7	0,0	0,0	-0,8
f^8/f^5	0,0195	+2,3	+2,7	+5,3	+4,5	+2,8	+0,4	+8,8
f^9/f^5	0,871	+0,8	+0,2	+1,1	+1,6	+1,3	+1,1	+2,5
f^{10}/f^5	0,167	+0,5	-0,8	+1,6	+0,6	+0,3	-2,4	+5,2
σ^8/f^5	0,136	+0,2	+0,3	0,0	-0,2	+0,5	0,0	-3,1
σ^8/f^9	0,156	-0,7	+0,1	-1,1	-1,0	-0,7	-1,2	-5,4
α^5	0,297	+0,4	+0,4	+0,3	+0,8	+0,7	+0,7	+0,9
α^9	0,352	-0,8	+1,2	-1,4	-2,1	-1,5	-1,7	-0,6
CBR($\delta = 0$)	1,039	-0,4	-0,2	-0,8	-1,3	-0,3	-0,8	-5,3
CBR($k_{eff}=1$)	1,039	+0,6	+0,3	+1,8	+2,5	+1,5	+0,3	+3,2

CBR = core breaking ratio

these energy regions in fast reactors are harder than the standard spectrum. In Table 4, significant errors stand out in the ^{238}U fission cross-sections and in the fourth group, which gives rise to almost half of all ^{238}U fissions in the reactor. This effect considerably exceeds the increase in the inelastic scattering cross-section for this group and is not compensated by it. Moreover, averaging the inelastic scattering cross-sections over the standard spectrum can lead to an underestimate of the inelastic transition cross-sections accompanied by large energy losses, i.e. to an understatement of the fission neutron removal cross-section below the ^{238}U fission threshold. Although this does not always occur (in particular, this does not

Table 2

Comparison of functionals calculated in different approximations

Functional	BFS-30				BFS-31				BFS-35			BFS-38			
	I	δI, %			I	δI, %			I	δI, %		I		δI, %	
	Version		Version D		Version		Version D		Version		Version D	Version		Version D	
	A,B	C	GG	$b_j=1$	A,B	C	GG	$b_j=1$	A,B	C	$b_j=1$	A,B	C	DD	$b_j=1$
k_{eff}	1,000	0,2	0,2	0,7	0,9808	0,5	1,0	3,5	0,9651	0,6	0,7	0,9459	0,8	0,9	1,1
ν	2,500	0,1	0,1	0,2	2,8634	0,0	0,0	0,1	2,5504	0,1	0,1	2,849	0,0	0,0	0,0
Σ_f	0,00393	0,5	0,7	2,4	0,00226	0,8	1,4	4,3	0,00356	0,6	1,4	0,00283	0,9	1,5	1,8
Σ_a	0,00706	0,4	0,2	1,3	0,00434	0,1	0,0	-0,9	0,00585	-0,2	0,6	0,00570	-0,2	0,2	0,2
f^0/f^5	0,0447	2,0	4,6	6,2	0,0200	2,2	4,8	5,9	0,0224	2,6	4,3	0,0209	2,6	4,1	3,8
f^9/f^5	1,082	0,0	0,2	-0,2	0,899	0,5	0,7	1,4	1,088	0,3	0,3	1,075	0,3	0,5	0,3
f^{10}/f^5	0,335	0,0	1,9	4,3	0,180	0,2	-1,5	5,2	0,254	1,4	5,3	0,242	1,6	4,6	5,2
σ_θ/f^5	0,124	0,1	0,1	-0,8	0,1395	0,0	0,0	-3,7	0,121	-0,4	0,4	0,123	-0,1	0,2	-0,3
σ_g/f^9	0,115	0,0	0,0	-0,6	0,1552	-0,6	-0,6	-5,0	0,111	-0,4	0,1	0,114	-0,5	-0,2	-0,7
α^5	0,224	0,0	-0,3	-0,3	0,2882	0,0	-0,2	-0,2	0,226	-0,7	-1,0	0,231	-0,7	-1,0	-1,1
α^9	0,150	0,8	0,3	6,7	0,3043	0,0	-0,3	1,8	0,132	-0,3	3,6	0,139	-0,2	-0,3	4,0

Table 3

Comparison of group fluxes calculated according to different slowing-down models (Baker core)

Group number	φ	$\delta\varphi = (\varphi_\alpha / \varphi_{mul'tik}^{-1})100\%$						
	Version	Version D methods						
	A,B	C	MG	GG	PA	DU	LI	$\delta_j = I$
1	0,36	0,0	+1	+1	+1	+1	+1	+10
2	1,83	+0,1	0	0	0	0	0	+5
3	4,75	-0,5	+1	+1	+1	+1	+1	+2
4	9,98	+0,1	+6	+1	+3	0	+2	+7
5	11,54	+0,3	-5	0	+1	-10	-20	+8
6	21,94	-0,5	-7	0	-5	+10	+8	+12
7	27,91	+0,3	-6	-1	+2	-2	+8	+2
8	32,08	-0,2	-2	-1	+2	-3	-6	-4
9	29,72	-0,1	0	-1	-1	-2	+1	-6
10	23,92	-0,1	+2	0	+2	+5	+5	-8
11	19,43	-0,1	+2	+1	+3	0	+3	-9
12	10,06	-0,6	+2	0	-3	+1	+16	-7
13	4,02	-0,0	-10	-13	-10	-1	+2	-10
14	6,90	-3,6	-1	-6	-25	-15	-7	-12
15	3,19	-1,8	+2	-1	+6	-1	-3	+4
16	1,20	0,89	0,94	0,89	1,02	0,90	0,91	1,15
17	0,26	0,85	1,00	0,91	1,11	1,07	1,04	1,69
18	$0,0^{2}30$	0,76	1,70	1,05	1,36	1,28	1,43	3,34
19	$0,0^{2}21$	0,80	2,70	1,70	3,1	3,8	2,1	13,8
20	$0,0^{3}12$	0,94	2,5	1,82	3,7	4,8	7,1	35
21	$0,0^{5}34$	0,66	2,6	1,36	10,2	11,0	25,7	203
	209,10	-0,1	-1,9	-0,5	-0,3	-0,3	-0,2	-1,3

Note: Below the 15th group the ratio/$\gamma\alpha/\gamma$ mul'tik is given.

happen for the core of the prototype), the total inaccuracy effect caused by averaging over the standard spectrum leads to an overestimate of σ_f^8 by 2-3%.

Let us now examine how the choice of one or another slowing-down model affects the shape of the spectrum. We can see from Table 3 that where the cross-sections vary smoothly models MG and GG provide acceptable accuracy of calculating the spectrum in the energy region where there are no sources of fission or inelastic scattering (or where they are insignificant, i.e. below the ninth group). At higher energies the errors in the flux calculation increase significantly. The accuracy of reconstructing spectra by means of interpolation models is appreciably poorer. Where resonance features appear in the spectra (13th group), none of the approximative slowing-down models was capable of describing these to accuracies better than 10%. Table 5 shows the

Table 4

Errors in group constants due to standard averaging method (Baker core)

Group number	$\delta\Sigma_c$	$\delta\Sigma_f$	$\delta\Sigma_{in}$	$\delta\sigma_f^8$	$\delta\sigma_c^8$	$\delta\sigma_f^9$	$\delta\sigma_c^9$	$\delta\sigma_f^5$	$\delta\sigma_c^5$	$\delta\sigma_c^{Na}$	$\delta\sigma_c^{Fe}$
I	-0,3	+0,2	0	+0,2	-0,3	+0,I	-0,3	+0,2	-0,2	+0,I	-0,2
2	-0,3	0	-0,I	+0,I	-0,6	0	-0,6	0	-0,6	+0,2	-0,4
3	+I,2	0	+0,8	+0,2	-3,3	-0,2	-3,3	-0,5	-6,I	-0,6	-I,2
4	-3,I	+I,3	+0,6	+2,0	-3,3	0	-2,6	0	-3,9	-0,8	+0,2
5	-2,3	+2,5	+3,3	+I0,6	-2,0	+0,8	-4,I	+0,5	-2,9	-2,5	-8,3
6	+0,3	+0,2	+2,4	+I0,0	+0,6	+0,2	-2,3	-0,2	-I,I	-2,0	+0,3
7	-0,7	+0,2	+I,3	+4,0	-0,7	+0,2	-I,I	-0,3	-I,2	-I,2	-0,6
8	0	0	0	-	0	0	0	0	0	0	0
9	+0,8	0	-2,3	-	+0,8	0	+0,4	+0,2	+0,4	+0,4	+0,4
I0	+0,3	+0,I	+I,I	-	+0,4	+0,I	+I,0	+0,3	+0,6	+0,7	+2,5
II	+0,6	+0,2	-	-	+0,4	+0,2	+I,I	+0,5	+0,5	+0,7	+3,6
I2	+0,9	+0,7	-	-	+0,7	+0,7	+3,0	+I,5	+I,3	+I,5	-7,I
I3	+I,3	+0,3	-	-	+0,7	+0,3	+0,2	+0,I	0	+I0,0	-I,4
I4	+6,2	+3,3	-	-	+3,8	+3,3	+4,0	+0,6	+I,7	-5,9	+I8,0
I5	-I,8	+9,I	-	-	-0,3	+9,I	-4,6	+4,6	+4,7	-0,6	+3,9
I6	+7,3	+I2,	-	-	0,0	+I2	+I7	+6,5	+3,2	+I,9	+5,3
I7	+7,0	-5,5	-	-	+9,3	-5,5	+5,I	+0,2	+5,2	+3,7	+5,9
I8	+4,8	+I7	-	-	-3,4	+I7	+9,8	+24	+8,5	+7,4	+8,9
I9	-25	+24	-	-	-I9	+24	-32	+7,6	+I,6	+6,3	+9,6
20	-33	+85	-	-	+66	+05	+07	-I9	-3,3	+9,2	+9,6
2I	+70	-I8	-	-	+I45	-I8	-27	-49	-I5	+I4	+I4

Table 5

Comparison of corrections to slowing-down cross-sections obtained using different methods

Group number	Mul'tik	MG	GG	PA	DU	LI
I	3,44	2,38	2,38	2,38	2,38	2,38
2	I,67	I,60	I,60	I,60	I,60	I,60
3	I,28	I,I8	I,I8	I,I8	I,I8	I,I8
4	I,34	I,29	I,I4	I,I9	I,30	I,42
5	I,24	I,34	I,2I	I,I8	I,45	I,77
6	I,24	I,34	I,2I	I,30	I,I0	I,I6
7	I,06	I,I6	I,07	I,04	I,08	0,97
8	0,99	I,03	0,99	0,96	I,02	I,05
9	0,96	0,98	0;96	0,96	0,98	0,95
I0	0,92	0,92	0,9I	0,89	0,87	0,89
II	0,88	0,88	0,86	0,83	0,87	0,83
I2	0,87	0,86	0,85	0,86	0,8I	I,03
I3	0,82	0,94	0,94	0,89	0,92	0,8I
I4	0,70	0,76	0,74	0,98	0,85	0,76
I5	0,67	0,69	0,67	0,74	0,7I	0,73
I6	0,5I	0,6I	0,58	0,63	0,69	0,69
I7	0,38	0,62	0,49	0,54	0,55	0,64
I8	0,23	0,36	0,32	0,46	0,60	0,66
I9	0,37	0,4I	0,37	0,43	0,46	0,60
20	0,I0	0,I5	0,II	0,4I	0,38	0,60
2I	0,09	0,I4	0,II	0,I2	0,74	0,77

values of the correction factors b_j for these same versions calculated using various slowing-down models. In all versions, these corrections were calculated for the standard spectrum (fission neutron spectrum) in the first three groups.

From the data we have examined, it is clear that the GG method is to be preferred in the region below the inelastic scattering threshold. In the 1-4 MeV region, where the largest proportion of ^{238}U fission takes place, none of the methods provides acceptable accuracy in describing the shape of the within-group spectrum: the values of the correction factor b_j differ substantially from those obtained in the fine-group calculation, which also explains the considerable errors in the group fluxes for these energy regions.

To illustrate this, Fig. 2 shows the fine-group fluxes and collision densities calculated for the composition of a fast reactor core. The good energy resolution of the fundamental resonances for ^{23}Na, ^{56}Fe and ^{16}O are evident in the diagram.

Calculation of bilinear flux and importance functionals

Taking as an example the calculation of central reactivity coefficients using a fine-group constant system, let us evaluate the accuracy of the calculation of bilinear flux and importance functionals in a 26-group approximation. In so doing, we shall evaluate those differences between bilinearly averaged constants and constants averaged with respect to flux which are due to the smooth energy dependence of the importance function. These differences reflect the indirect effect of a change in the concentration of the i-th isotope on the macroconstants for the medium; such a change brings about some alteration in the shape of the within-group spectrum, and consequently also in the constants averaged over that spectrum. As to the differences between bilinearly averaged and flux-averaged constants due to the correlation between the resonance structures of the importance function and the isotope collision density, they are examined in Refs [4, 5].

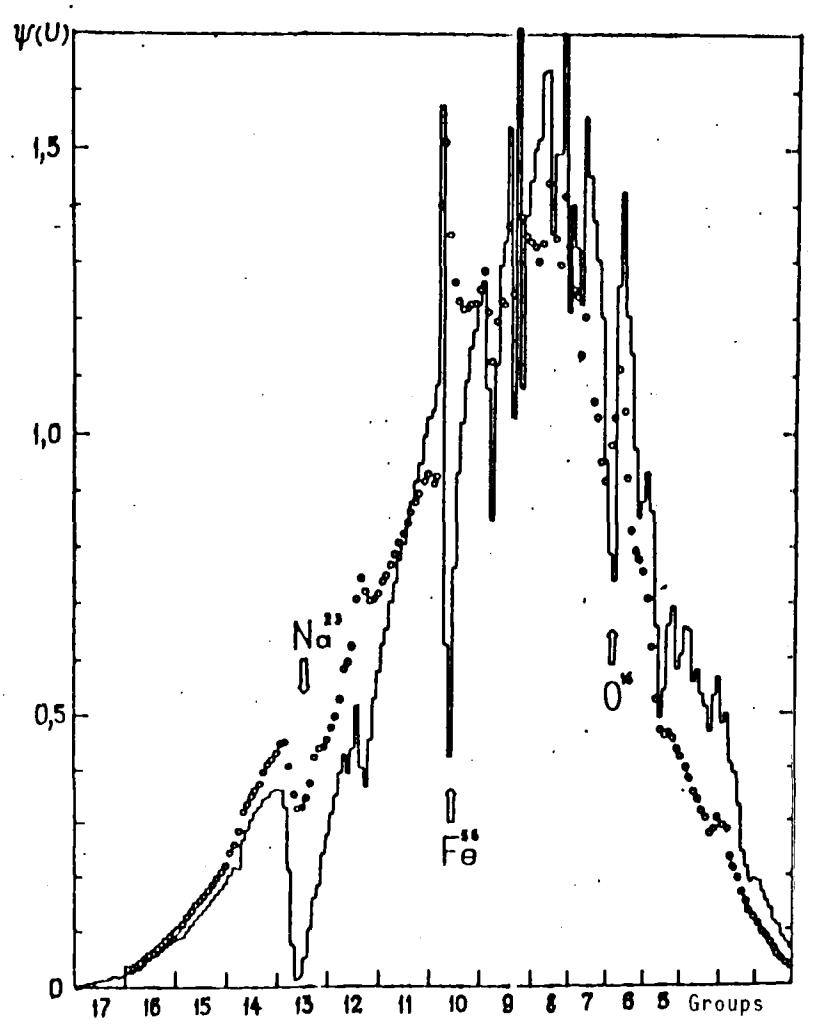

Fig. 2. Calculated flux (⌐¬) and collision (o) densities in Baker prototype core

Of course, the fine-group calculations partially take resonance effects into account insofar as the 288-group approximation allows the cross-section resonance structure to be resolved. Apart from the 288-group calculation of the reactivity coefficient (version A), three types of 26-group calculation were carried out, as described above (versions B, C and D).

Table 6 shows the results of a fine-group calculation of the ratio between the reactivity coefficients of the substances indicated and that of ^{235}U. Table 7 gives the errors in the respective group calculation versions, in per cent. These data show that the corrections, as a rule, amount to tenths of a per cent of the ^{235}U reactivity coefficient. Therefore the usual group calculations of small reactivity coefficients contain significant errors. We can see from the data in Table 7 that if the slowing-down cross-sections are not recalculated in the group calculations, the error in the reactivity coefficients of the scattering materials will in

Table 6

Reactivity ratios β_α calculated in a fine-group approximation $\left[\beta_\alpha^A = (KP_\alpha/KP_{235_U})100\%\right]$ (Version A)

Assembly	^{9}Pu	^{10}B	^{40}Pu	^{8}U	Nickel	Iron	Chro-mium	Alumi-nium	Sodium	^{12}O
BFS-26	132	-293	-16,9	-29,1	-0,59	-0,04	-0,17	0,56	1,43	2,16
BFS-27	150	-234	21,8	-14,6	-0,22	0,64	0,49	1,19	2,18	2,77
BFS-28	153	-81	36,4	-5,3	-1,37	-0,66	-0,73	-0,62	0,16	0,18
BFS-30	157	-88	39,8	-4,7	-1,34	-0,66	-0,63	-0,34	0,31	0,71
BFS-31	125	-67	13,0	-6,4	-1,30	-0,94	-1,04	-1,09	-0,10	-0,99
BFS-33	121	-82	11,6	-7,2	-0,91	-0,74	-0,80	-0,73	-0,46	-0,13
BFS-36	144	-42	26,2	-5,5	-1,92	-1,34	-1,50	-1,37	-1,68	-2,23
BFS-38	138	-34	24,2	-5,0	-1,97	-1,31	-1,68	-1,68	-2,07	-2,91
KBR-3	116	-176	-41,6	-31,1	-0,70	-0,42	-0,56	-0,23	-0,85	-0,04
KBR-7	132	-235	-66,3	-46,2	-0,69	-0,50	-0,64	-0,02	-0,10	0,24
Baker	111	-95	33,6	-7,3	-1,00	-0,73	-0,94	—	-0,53	-0,49

many cases be reduced. Of course, this sort of error compensation is no reason to recommend not increasing the accuracy of slowing-down cross-sections when carrying out multigroup calculations.

Table 8 shows the distribution of the contributions of the slowing-down cross-sections for graphite to the group reactivity coefficients for various calculation versions, taking the BFS-33 assembly as an example. The group (version B) and fine-group importance spectra for this assembly are shown in Fig. 3. In groups 1-9, where the importance of lethargic neutrons drops, the contributions to the reactivity coefficient from graphite are negative, whereas at lower energies (not considering regions of resolved resonances) they are positive. Figure 3 shows that, in the energy region where the sole source of neutrons in a given group is elastic slowing down from an adjacent group, the importance calculated in a group approximation agrees with the importance of neutrons slowing down elastically within it.

As a result, it appears that for groups 10-13 the group importance $\bar{\phi}_g^+$ is less than the averaged fine group $\langle\phi\rangle_g^+$. At higher energies, when the neutron source is distributed more uniformly over the group, $\bar{\phi}^+ \approx \langle\phi\rangle_g^+$, and in high-energy groups $\bar{\phi}_g^+$ is close to the neutron importance near the lower-energy boundary of the group, i.e. also in the region in which the source neutrons are concentrated. The distribution of the importance

Table 7

Differences in reactivity coefficients calculated in group and in fine-group approximations $\left[(\beta_\alpha^B - \beta_\alpha^A)/\beta_\alpha^A\right]$

Assembly	^{9}Pu	^{10}B	^{40}Pu	^{8}U	Nickel	Iron	Chro-mium	Alumi-nium	Sodium	^{12}C
					Version B					
BFS-26	-0,4	-1,1	-1,6	0,4	21	116	60	2	-29	-3
BFS-27	-0,6	-1,8	-0,2	0,9	157	-25	-36	-2	-5	-5
BFS-28	0,0	0,3	-0,2	2,1	23	10	15	-10	-243	-170
BFS-30	-0,2	-0,8	-0,3	1,4	22	0	19	-14	-61	-35
BFS-31	-0,2	-1,7	0,8	-2,8	2	1	1	-5	900	7
BFS-33	-0,3	-1,8	3,4	-2,6	17	9	5	2	-200	69
BFS-35	0,2	2,0	0,2	-0,2	-8	-7	-8	1	-6	-7
BFS-38	0,3	3,7	0,1	0,5	-7	-1	-6	-21	-2	3
KBR-3	-0,3	1,0	-0,5	2,2	-6	3	-5	8	-64	21
KBR-7	-0,4	2,7	-1,3	4,6	-1	10	0	450	30	16
Baker	-0,4	-3,3	11,9	-3,5	3	1	-2		8	15
					Version C					
BFS-26	0,3	-4,1	-15,0	-2,1	20	193	56	-1	-32	-4
BFS-27	-0,1	-4,1	5,0	-1,7	168	-31	-35	-3	-6	-6
BFS-28	-0,2	-0,5	-0,2	1,0	27	11	16	-7	-247	-176
BFS-30	-0,3	-1,8	-0,2	0,2	26	2	21	-8	-65	-38
BFS-31	0,4	-1,6	+1,6	-2,3	3	4	0	-2	900	6
BFS-33	0,0	-3,5	2,8	-4,5	21	12	6	5	-200	83
BFS-35	0,5	1,5	1,9	-0,1	-7	-6	-8	3	-5	-7
BFS-38	0,6	3,1	2,0	0,5	-6	1	-5	3	2	-1
KBR-3	1,3	-3,1	-4,5	-6,2	-7	5	-6	10	-62	-60
KBR-7	2,4	1,2	-1,0	-3,0	-1	12	-2	470	34	12
Baker	0,8	-3,3	-23,2	-2,4	5	6	-2	-	7	12
					Version D					
BFS-26	3,6	-4,0	21,0	-1,6	8	+42	-16	12	-10	-8
BFS-27	1,5	-4,0	9,7	-7,7	73	4	4	5	-4	-8
BFS-28	-0,2	-4,6	7,9	0,5	-1	-8	-5	-16	150	74
BFS-30	0,0	4,4	6,9	-0,8	0	-12	-6	-47	22	13
BFS-31	2,0	10,9	1,0	5,0	14	3	-2	-3	-263	-16
BFS-33	1,5	5,4	2,1	0,9	0	6	4	6	-36	-30
BFS-35	0,3	0,9	7,3	0,1	-13	-8	-8	2	-12	-17
BFS-38	0,3	1,7	6,8	1,2	-7	20	-5	3	-2	-7
KBR-3	6,0	0,3	40,5	1,2	2	3	-7	-4	-27	-194
KBR-7	5,2	-5,5	36,6	-8,8	0	1	-8	63	72	-41
Baker	3,6	8,8	-47,0	5,4	-3	7	0	-	-12	-15

spectrum and the energy behaviour of the flux and cross-sections enables us to explain all discrepancies between the group contributions to the graphite reactivity coefficient (column B of Table 8) and the multigroup contributions (column A).

Table 9 shows the contributions from the principal neutron processes to the reactivity coefficients of various materials in the BFS-33 assembly. It is seen that the main difference between the multigroup calculation

Table 8

Group contributions of the slowing-down cross-section for graphite to the reactivity coefficient for various calculation versions (BFS-33)

Group number	Version			
	A	B	C	D
I	-0,018	-0,022	-0,022	-0,010
2	-0,036	-0,042	-0,042	-0,030
3	-0,127	-0,259	-0,250	-0,170
4	-0,709	-0,663	-0,671	-0,668
5	-0,148	-0,109	-0,215	-0,175
6	-0,387	-0,246	-0,242	-0,408
7	-0,548	-0,574	-0,590	-0,494
8	-0,701	-0,727	-0,731	-0,614
9	-0,459	-0,453	-0,452	-0,311
10	0,521	0,510	0,506	0,513
11	0,869	0,728	0,715	0,811
12	0,605	0,582	0,555	0,615
13	0,443	0,357	0,336	0,423
14	0,120	0,121	0,168	0,226
15	0,014	0,016	0,007	0,012
16	-0,005	-0,004	-0,005	-0,010
17	-0,001	0,002	0,003	0,014
18	0,000	0,000	0,000	-0,007
19	0,000	0,000	0,000	-0,001
Total	-0,460	-0,663	-0,941	-0,981

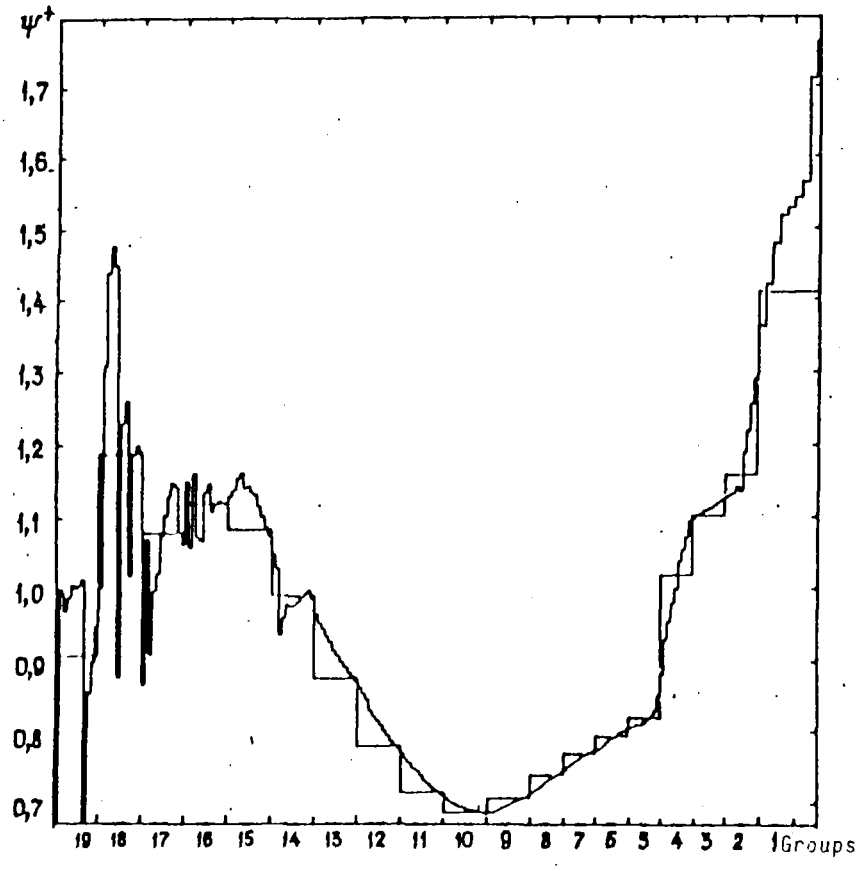

Fig. 3. Group and fine-group importance spectra in BFS-33 assembly

Table 9

Contributions to reactivity coefficients from various processes for four calculation versions (BFS-33 assembly)

Isotope	Method	Contribution to reactivity coefficient from				
		$\nu\sigma_f$	σ_a	σ_{in}	σ_{mod}	Total reactivity coefficient
^{235}U	A	725,6	-303,5	-7,17	0,08	415,0
	B	725,6	-300,9	-7,00	0,02	417,7
	C	724,5	-300,0	-7,07	0;02	417,5
	D	737,0	-319,4	-7,58	0,13	410,2
^{239}Pu	A	785,4	-280,3	-5,41	0,08	499,8
	B	785,4	-278,4	-5,62	0,02	501,4
	C	787,6	-279,1	-5,72	0,01	502,8
	D	809,0	-301,6	-6,26	0,13	501,3
^{238}U	A	16,4	-38,5	-7,85	0,06	-29,9
	B	16,4	-38,1	-7,56	0,00	-29,3
	C	16,7	-38,1	-7,66	-0,01	-29,0
	D	17,6	-39,2	-8,29	0,12	-29,8
Iron	A	-	-1,25	-2,03	0,22	-3,06
	B	-	-1,26	-1,92	-0,17	-3,35
	C	-	-1,31	-1,96	-0,18	-3,46
	D	-	-1,38	-2,13	0,30	-3,21
Sodium	A	-	-0,75	-1,51	4,19	1,93
	B	-	-0,72	-1,43	0,18	-1,97
	C	-	-0,76	-1,41	0,10	-2,07
	D	-	-0,80	-1,56	4,40	2,14
Carbon	A	-	-0,02	-0,08	-0,46	-0,56
	B	-	-0,02	-0,07	-0,86	-0,95
	C	-	-0,02	-0,07	-0,94	-1,03
	D	-	-0,03	-0,08	-0,28	-0,39

(version A) and the group calculation with "accurate" constants (version B) is caused by the difference in evaluating the contribution of elastic slowing down. In fine-group calculations, this contribution (through the energy dependence of the importance function within the group) takes into account also the effect of variation in the slowing-down properties of the medium on the mid-group constants. This effect is particularly apparent in the case of sodium.

It has been demonstrated that, in carrying out multigroup calculations of critical assemblies and fast power reactors, it is necessary to calculate the slowing-down cross-sections on the basis of an approximative evaluation of the shape of the within-group spectrum. Calculating the slowing-down cross-sections by the recommended approximation methods brings down the

methodical error in the multigroup calculation of k_{eff} from 3% to no more than 1% and that in the core conversion ratio to 2%. About half of this error is due to inaccuracy in evaluating the slowing-down cross-sections, and the other half to the effect of the indeterminacy of the within-group spectrum on the fission and capture cross-sections. At current levels of nuclear data accuracy, the methodical errors in 26-group approximations are acceptable. In order further to increase the accuracy of calculated predictions to the level required, it will be necessary to make a transition to a fine-group constant system.

Numerical comparison of the results of multigroup and fine-group calculations has shown that, in calculating the reactivity factors of scattering samples, it is important to take into account the perturbations they cause in the shape of the neutron spectrum. Multigroup calculations cannot provide accuracies of calculating reactivity coefficients better than a few tenths of a per cent (up to 1%) of the reactivity coefficient of the basic fuel isotope.

REFERENCES

[1] ABAGYAN, L.P., BAZAZYANTS, N.O., BONDARENKO, I.I., NIKOLAEV, M.N., Group constants for calculating nuclear reactors [in Russian], Atomizdat, Moscow (1964).

[2] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for calculating reactors and shielding [in Russian], Ehnergoizdat, Moscow (1981).

[3] KHOKLOV, V.F., SAVOS'KIN, M.M., NIKOLAEV, M.N., ARAMAKO set of programs for calculating group macroscopic and block microscopic cross-sections on the basis of a 26-group system of constants broken down into sub-groups [in Russian], Yadernye Konstanty 8 3 (1972) 3.

[4] NIKOLAEV, M.N., RYAZANOV, B.G., SAVOS'KIN, M.M., TSIBULYA, A.M., Multigroup approximation in neutron transport theory [in Russian], Ehnergoatomizdat, Moscow (1983).

[5] [Missing in original paper.]

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ON THE DEVELOPMENT OF A FINE-GROUP CONSTANT SYSTEM

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ABSTRACT

Errors in the multigroup approximation are the main methodical errors in the calculation of flux and importance spectra and functionals. To achieve the required accuracy in calculating the main characteristics of fast reactors a transition must be made from 26-group to fine-group approximation. A description is given of a fine-group system of constants along with a status report on its development.

The 26-group system of constants adopted for fast reactor calculation describes the energy dependence of the neutron flux and cross-sections in sufficient detail to meet the needs of serial calculations. However, a more detailed description of cross-section energy dependence is required for calculations of critical assemblies, when it is planned to use the results of measurements on these assemblies to correct constants, and also for final calculations of projected reactors and for test calculations to check 26-group approximations.

Errors in the multigroup calculation are the main methodical errors (as opposed to errors due to inaccuracies in the constants used) in calculations of neutron importance and flux functionals and spectra. These errors are caused by inaccuracy in describing the shape of the within-group spectrum adopted in averaging the group constants; for example, the standard 26-group constants are averaged in the first three groups with a weighting for the ^{235}U fission spectrum under the action of thermal neutrons, and in the remaining groups with a Fermi spectrum weighting. The neutron spectrum in the medium differs from the indicated standard spectrum. These differences affect

primarily the value of the group cross-section for elastic slowing-down of neutrons. Methods have now been developed of introducing corrections to the slowing-down cross-section for the shape of the within-group spectrum [1, 2]; however, none of these is to be preferred, since they all do not eliminate, but merely reduce (by a factor of about three) the error in the calculation results due to the impossibility of computing the slowing-down cross-section accurately.

Our inaccurate knowledge of the shape of the within-group spectrum is reflected in the results of averaging reaction cross-sections, primarily for those reactions whose cross-sections are strongly energy-dependent: ^{238}U fission, inelastic scattering at lower levels and radiative capture (particularly in wide and intermediate resonance regions).

Evaluations of the errors in critical assembly characteristics are shown in the table, from which we can see that the indeterminacies in the linear functionals due to errors in the group approximation are comparable to, or even in excess of, the experimental errors. As to the bilinear functionals (central reactivity coefficients), in their case the indeterminacies due to the group approach are even greater owing to the influence of the within-group structure of the importance and other effects.

Hence, it is necessary, in order to reduce the methodical error in calculating the values measured in critical assemblies to a level below that of the experimental error, and also to achieve the required accuracy in

Evaluation of errosion results of individual experiments, in %

Functional	Mean square deviation of results [3]	Error	
		Evaluated by experimenters [4]	26-group approximation [2, 5]
K_{eff}	0,7	0,3	0,8
$\sigma_f(^{238}U)/\sigma_f(^{235}U)$	5,3	3,0	4,0
$\sigma_f(^{239}Pu)/\sigma_f(^{235}U)$	3,3	2,0	2,5
$\sigma_f(^{240}Pu)/\sigma_f(^{235}U)$	10,0	5,0	5,0
$\sigma_0(^{238}U)/\sigma_f(^{235}U)$	2,3	2,0	2,0

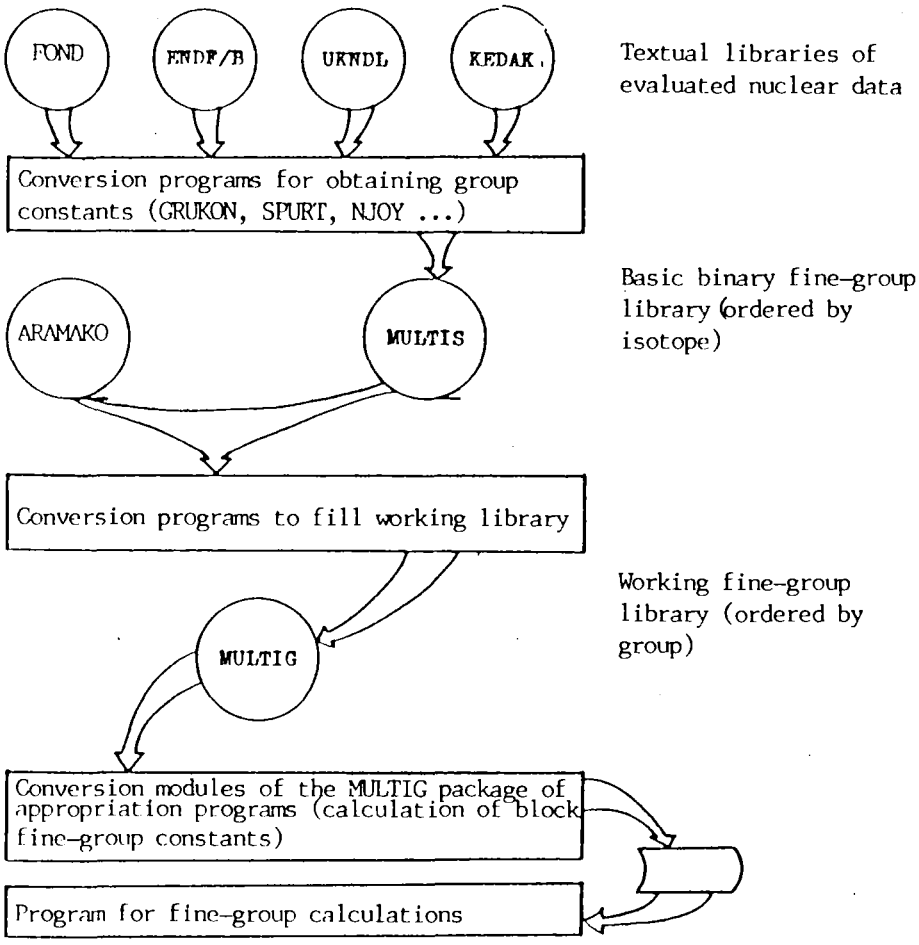

Diagram of system for providing constants for fine-group neutron calculations.

calculating the fundamental characteristics of fast reactors, to make a transition from 26-group approximation to multigroup approximation with a significantly larger number of energy groups. The main requirements which a system to provide constants for fine-group calculations must meet are as follows:

- The division into groups must correspond with the divisions in BNAB [6];
- The system must be capable of carrying out calculations using information from a fine-group library for a proportion of the isotopes and from a 28-group constant library for the rest [7];
- It must be capable of being programmed to fill the microconstant input library of the MULTIG system on the basis of evaluated data files.

The energy divisions for the fine-group constant system were chosen as follows. The energy region 10.5–20.0 MeV was divided into nine fine groups of equal width on the lethargy scale; the regions 2.5–4, 4.0–6.5 and 6.5–10.5 MeV were each divided into six equal fine groups; the regions 0.8–1.4 and 1.4–2.5 MeV were each divided into eight fine groups; the region 0.1–0.8 MeV was divided into twenty-seven fine groups, and the region 1 eV–0.1 MeV was divided into 180 fine groups of equal lethargy. The energy range below 1.0 eV is the thermalization region, for which no division into groups has been defined. In order to satisfy the second requirement, it was decided to include information from the 28-group library directly in the fine-group constant library so as to ensure uniform processing of the data.

Programs [8] are currently available which are designed to obtain group constants directly from files of evaluated nuclear data (for example, GRUKON [8], SPURT [9] and NJOY [10]). These are used in filling the MULTIS base fine-group library which is arranged in order of isotope. However, a more convenient library structure for carrying out calculations is to have the data arranged in order of energy variable (group). The MULTIG working library is of this kind, and features information from the ARAMAKO libraries along with fine-group data. The general outlines of the system for supplying the constants for fine-group neutron calculations are shown in the Figure. The structural unit for each fine-group library is the section, containing neutron data of a certain type. For the MULTIS library, a structure was chosen with four sections whose data are required for calculating neutron fields. The number of sections in the library can be increased if necessary.

In the first section, the following values are shown for each nuclide: ν, σ_f, σ_c, σ_{el} and σ_{in}, where ν is the total number of neutrons emitted per fission event, σ_f is the mid-group fission cross-section, σ_c is the mid-group cross-section for neutron absorption without fission (capture), σ_{el}, is the mid-group elastic scattering cross-section, and σ_{in} is the mid-group total cross-section for inelastic

scattering and the (n,2n), (n,3n) and (n,4n) reactions. The values of ν and σ_f are given for fissile isotopes only, and σ_{in} is shown only in groups where inelastic scattering occurs. All values are given for a temperature of 300 K and are computed by the GRUKON applications program package [on the basis] of evaluated nuclear data files in the ENDF/B library format.

The second section gives resonance structure data and temperature corrections. The resonance structure of the cross-sections is described using the sub-groups from Ref. [11]: the section gives fractions for the sub-groups A_j and resonance structure coefficients RK_x^j which are ratios of the cross-section of the j-th sub-group of a given process $x(x = f,c,el,in)^x$, calculated for a given temperature, to the mid-group cross-section at a temperature of 300 K. The sub-group fractions are considered to be independent of temperature; they are subject to the condition $\sum_j A_j = 1$. If $\sigma_x(T)$ is the mid-group cross-section for a process x at a temperature T, then $\sigma_x(T) = \sigma_x(T_o) \sum_j A_j RK_x^j(T)$. The GRUKON package is also called upon to prepare sub-group fractions A_j and coefficients RK_x^j (work on developing these blocks in the form required for filling the MULTIS library is not yet complete).

Section 3 is designed to describe the spectra of secondary neutrons in inelastic scattering. The spectrum of such neutrons consists of a superposition of spectra described by various formalisms, namely inelastic scattering with excitation of a particular level of the target nucleus, evaporation of one neutron and successive evaporation of several. The library gives parameters characterizing these formalisms (excitation energies of discrete levels, reaction thresholds, number of neutrons evaporated, temperatures describing evaporation spectra for each neutron, fine-group matrix of inelastic transition probabilities) and the probabilities for each formalism in a given fine group.

Section 4 describes the elastic scattering anisotropy. It contains the mid-group scattering indicatrices in the form of a Legendre polynomial serial expansion. The software for this section has not yet been prepared. Remember that in this case each section contains information in order of nuclide. In the MULTIG working library the data hierarchy is different: in each energy group, information is given on the various types of reaction for all the nuclides. Each data type is described by its section. At present, it is intended that the library should have seven sections (this figure may be increased).

1. Mid-group constants section. Along with the data from section 1 of the MULTIS library this section gives the fine-group total cross-section σ_t, determined from the balance; the mean cosine of the elastic scattering angle μ_{el}; the mean cosine of the inelastic scattering angle μ_{in}; the abundance of secondary neutrons $r = (\sigma_{in} + 2\sigma_{n,2n} + 3\sigma_{n,3n} + 4\sigma_{n,4n})/(\sigma_{in} + \sigma_{n,2n} + \sigma_{n,3n} + \sigma_{n,4n})$; and KR, signifying the presence of resonance structure in the cross-sections of a given fine group.

2. Resonance structure section. Gives sub-group fractions A_j and resonance structure coefficients RK_x^j (for processes x = t,f,c,el,in).

3. Inelastic transitions section. For each nuclide, this section shows matrices of the probability of transitions from higher groups into a given fine group. For light isotopes, analogous matrices of the first angular moments of inter-group transitions are shown.

4. Elastic transitions section. Matrices of transition probabilities for elastic scattering and matrices of first angular moments are shown for all isotopes. We can see from the description of sections 3 and 4 that, in its finished state, the library contains data for supplying calculations in the diffusion and the P_1 approximation. A constant for calculations taking into account the anisotropy of elastic scattering of a higher order must be calculated using programs coming under the constant preparation function

block. In this process, information from the following sections is used.

5. Scattering anisotropy section. This gives harmonics (angular moments) of the mid-group scattering indicatrix in the form of a Legendre polynomial serial expansion.

6. Wide-group constants section. This is designed to supply ARAMAKO system calculations with constants. The information from this section is given only in those fine groups which fall at the beginning of the energy interval described by the wide group. In calculations, in the working memory they are converted by programs into formats which correspond to the description of the fine-group constants (sections 1-5); thus, a single algorithm prepares fine- and wide-group constants. The data for this section are taken from the files of the ARAMAKO constant supply system.

7. Doppler increases section. This is designed to take into account the temperature dependence of the wide-group cross-sections. The ideology of the calculation and the format for the data are the same as for the BNAB-78 constant system. The information is drawn from the ARAMAKO system's files of Doppler increases and is given only for the same fine groups as the data from section 6.

So far, sections 6 and 7 of the MULTIG library have been filled, and development of the software to fill sections 1-5 and to calculate block constants is in progress.

REFERENCES

[1] NIKOLAEV, M.N., RYAZANOV, B.G., SAVOS'KIN, M.M., TSIBULYA, A.M., Multigroup approximation in neutron transport theory [in Russian], Ehnergoizdat, Moscow (1983).

[2] DOLGOV, E.V., TSIBULYA, A.M., Evaluation of the methodical error in 26-group approximation [see present publication, previous abstract].

[3] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N., TSIBULYA, A.M., Group constants for calculating reactors and shielding [in Russian], Ehnergoizdat, Moscow (1981).

[4] KAZANSKIJ, Yu.A., DULIN, V.A., ZINOV'EV, V.P., et al., Methods for studying reactor characteristics on BFS critical assemblies [in Russian], Atomizdat, Moscow (1977).

[5] PIVOVAROV, V.A., Errors in approximating collision constancy in fine-group constants [in Russian], Voprosy Atomnoj Nauki i Tekhniki, Ser. Yadernye Konstanty 1 45 (1982) 14-23.

[6] ABAGYAN, L.P., BAZAZYANTS, N.O., BONDARENKO, I.I., NIKOLAEV, M.N., Group constants for calculating nuclear reactors [in Russian], Atomizdat, Moscow (1964).

[7] BAZAZYANTS, N.O., VYRSKIY, M.Yu., GERMOGENOVA, T.A., et al., ARAMAKO-2F - A system for supplying neutron constants for calculations of radiation transport in reactors and shielding [in Russian], Institute of Applied Mathematics, USSR Academy of Sciences, Moscow (1976);
VYRSKIJ, M.Yu., DUBININ, A.A., KLINTSOV, A.A., et al., ARAMAKO-2F - A version of a system for supplying constants for high-energy neutron transport calculations [in Russian], Preprint No. 904, Institute of Physics and Power Engineering, Obninsk (1978).

[8] SINITSA, V.V., The GRUKON package. Part 1. The conversions program [in Russian], Preprint No. 1188, Institute of Physics and Power Engineering, Obninsk (1981);
SINITSA, V.V., The GRUKON package. Part 2. Control parameters [in Russian], Preprint No. 1189, Institute of Physics and Power Engineering, Obninsk (1981).

[9] KOLESOV, V.E., KRIVTSOV, A.S., An algorithm and a program for preparing group constants for reactor calculations on the basis of the SOKRATOR system neutron data library [in Russian], in: Nejtronnaya fizika (Neutron physics) (Proc. 3rd All-Union Conference on Neutron Physics, Kiev, 9-13 June 1975), Part 1, TsNIIatominform, Moscow (1976) 140.

[10] MacFARLANE, R.E., BOICOURT, R.N., NJOY: A neutron and photon cross-section processing system, Trans. Am. Nucl. Soc. 22 (1975) 720.

[11] NIKOLAEV, M.N., Comments on the probability table method, Nucl. Sci. Eng. 61 (1976) 286.

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