Priorities in the development of nuclear constants support system for reactor and shielding calculations

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Available online 23 August 2016

Abstract
First priority tasks to be resolved in the development of new generation of nuclear data support systems for calculation of fast reactors on the basis of the unified ABBN-2020 multi-group system of neutron data retrieved from the ROSFOND files of evaluated neutron data are discussed. Along with the development of advanced system for provision of nuclear data support for neutronics calculations significant attention must be paid to the development and elaboration of methodologies and calculation codes for evaluation and ranging of calculation uncertainties in the calculations of nuclear facilities in order to be able to focus the efforts on the most important directions.

Development of the integral unified nuclear data support system and its implementation in the calculation codes will ensure not only the unification of the procedure for nuclear data preparation, which will allow enhancing reliability of their verification, but, as well, will enhance accuracy and reliability of calculation prediction of all the most important characteristics of the reactors under design, will ensure their licensing compliance, competitiveness and independence from foreign products.

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Keywords: Neutron data; ROSFOND; ABBN multi-group nuclear constants; Nuclear data support system; Calculations of fast reactors and radiation shielding.

Introduction
Neutron and gamma-radiation transport equation within the energy range important in the calculations of fast reactors and neutron shielding does not contain any more or less significant approximations. The accuracy of its solution is practically completely determined by the accuracy of knowledge about the characteristics of interaction of radiation with matter and only to a certain degree on the correctness of the calculation methodologies applied [1,2].

Provision of reliable data on the characteristics of interactions for calculation codes refers to the competence of the industry metrological service. As pertains to the international practices, the so-called “request lists” are formed reflecting the needs in nuclear data [3] for the most important outstanding tasks.

Bringing the methodologies for application of these characteristics in the calculations of radiation fields in compliance with existing level of knowledge about these characteristics must be regarded as one of the most important tasks in the development of new generation of codes.

Let us list the first priority tasks in this direction as applied to the main problems and methodologies of calculation of radiation fields.

Monte-Carlo method
Monte-Carlo method is from the point of view of methodology the most advanced among the contemporary methods used in calculations of neutron and gamma-fields [4,5]. The method allows describing energy dependences of characteristics of interaction with accuracy with which these characteristics “are known” [6]. Two problems still remain to be unsolved, at least as applied to indigenous calculation codes:
1. Codes implementing Monte-Carlo method mandatorily accompany the results of calculations with indication of statistical uncertainties predetermined by the finite number of simulated trajectories. For the current level of development of computers statistical uncertainties of calculation of main reactor characteristics are brought without any significant issues to the level which is insignificantly small as compared with uncertainties predetermined by the inaccuracy of knowledge about neutron and photon data (the so-called “nuclear data component of uncertainty”) and by the inaccuracy of knowledge about nuclear concentrations (the so-called “technological component of uncertainty”).

Provision for calculation codes of covariance data allowing estimating in objective (scientifically justifiable) way the uncertainties of calculation of reactivity effects and other functionals determining the conditions of safe operation refers to the number of first priority tasks. Real possibility to solve the problem is ensured by the available results of already implemented efforts (pilot versions of neutron covariance data [7] and methodologies for application of the data in question, for instance, SKALA code [8], in nuclear and radiation safety calculations are available).

2. Codes capable to calculate responses of local neutron flux sensors to fast changes of reactor criticality in emergency operation modes must be available for prevention of large-scale accidents.

Correct calculation of local functionals by Monte-Carlo method requires solution of non-homogenous adjoint equation which makes it necessary to abandon the detailed description of energy dependences of cross-sections and to pass on to the use of multi-group approximation.

Solution of this problem would allow more correctly and accurately calculating the ratio of effects of reactivity and ratios of cross-sections and involving experiments producing values measured using small samples on critical assemblies and reactor in the analysis of this sort.

In order to solve the above formulated problems codes implementing Monte-Carlo method must be supported not only with detailed energy dependences of cross-sections but, as well, with multi-group constants obtained on their basis. A special processing and preparation of group constants procedure is required for correct solution of the adjoint transport equation.

Combination of detailed and multi-group description of neutron data allows escaping unreasonably high expenditures of processor time in the calculations of reactors with high enough fuel burnup when the number of nuclides included in the composition of the core increases by two orders of magnitude. This is especially important in the implementation of dynamic calculations. Practical possibility of solution of the problem is ensured by the available results of preliminary studies because the systems for provision of calculations performed using Monte-Carlo simulation codes with combined detailed, group and/or multi-group neutron data are already available. Still further advancement in this direction is, however, necessary. For instance, the suggested approach implementing the combination of “group” isotopes into a single “macronuclide” with its own “macro-constants” will result in the significant reduction of computation time and in the reduction of statistical uncertainty (part of “subgroup” nuclides, description of interactions of neutrons with which is permissible to be described by blocked neutron group constants, can be included in the “macronuclide” as well).

3. In order to implement dynamic calculations computer codes must be supplied with data on the probabilities for neutron to be entered in a certain group of delayed neutrons and with effective half-life values for precursors of these groups.

Group method

Group method of solution of transport equation is widely applied in Russia and abroad both for calculation of reactor cores and for calculation of radiation shielding [2]. In the calculations of radiation shielding the time expended for solving specific problem is proportional to the number of energy groups for which nuclear data are prepared. The support program CONSYST for preparation of nuclear constants [9,10] (previously used the ARAMAKO program [11]) is capable to generate few-group constants by implementing evaluation of neutron spectra in B²-approximation applicable for fissile media where fission neutrons emitted in the material under examination serve as the main source of neutrons. In such cases B²-approximation proves to be correct enough in order to allow unify the initial multi-group constants into few-group ones on the basis of spectra calculated using this approximation (this is specifically what is done in the preparation of data for reactor calculations).

1. A priori evaluation of spectra is not possible in non-fissile materials used in different types of radiation shielding. Therefore, the number of groups which is used in the radiation shielding calculation codes is usually one order of magnitude larger [12] than it is applied in the reactor calculations. This results in increasing of expenditures of processor time and in the impossibility of implementation of multiple-variant optimization calculations within a reasonable time period. Elimination of the above drawback requires solution of the following problem: iterative refinement of problem-oriented few-group constants for calculations of radiation shielding. Sources of neutron moderation into the wider group from higher energy groups and differences between neutron inflows and leakages from adjacent media are evaluated during each iteration step. On the basis of this information the data preparation code calculates for each wide group its own value of the B² parameter ensuring maintenance balances,
evaluates the intra-group spectrum and prepares few-group constants for the subsequent iteration steps.

2. Another problem of classical multi-group method is the impossibility to calculate angular dependence of neutron cross-sections associated with the resonance self-shielding and boundary resonance effects. In radiation shielding, the purpose of which is to achieve the largest possible gradients of neutron flux, this represents a fairly significant problem. Solution of this problem is possible by the switching to the use of subgroup approximation and in order to implement such approach the system of data preparation must prepare problem-oriented subgroup macroconstants for each individual calculation task.

3. Improvement of data preparation programs is necessary in order to improve accuracy of calculations. The method for taking into account the resonance self-shielding effects implemented in the CONSYST code was developed already during the 1960s and is oriented toward the use of diffusion approximation [13]. Resonance self-shielding of angular distribution parameters is not taken into account in it; evaluation of resonance structure of neutron flux density does not take into account the flow component possessing different structure; the so-called “adjusted transport approximation” is used in the calculation of transport cross-sections. More advanced methodology for preparation of group constants was developed long ago and is to be implemented in the program for preparation of constants for the new generation of calculation codes. Possibility of refusal from the approximation of narrow resonances not applicable for group description of resonance self-shielding at low energies must be anticipated in this program as well. The above formulated problem can be solved by calculating neutron spectrum in low-energy region and by numerically solving moderation equation using the data on the detailed energy behavior of cross-sections for resonance isotopes.

4. Multi-group methods of solution of homogenous and non-homogenous adjoint transport equations are applied for solving a number of applied problems (for calculating sensitivity factors, for evaluating reactivity effects, etc.). It is known that conjugation and group averaging operations are not commutative and group constants weight-averaged using calculated importance functions must be used in the solution of the adjoint equation instead of using the weights of neutron flux density. Their spectra and, especially, their resonance structures are significantly different. However, these differences are neglected in the usual practice of calculations because of absence the programs for preparation of this type of constants. The above shortcoming can be eliminated in the new program for preparation of constants using the available methodologies at least during preparation of constants for calculation of importance functions relative to the asymptotic power. Also, additional methodological development efforts are needed for preparation of constants for solving problems of generalized perturbation theory.

5. Program of constant preparation must prepare the data on the energy yield and emission of gamma-quanta in neutron induced reactions and constants for calculations of gamma-fields. At the same time the user must be given the possibility to refuse from the description of transfer of energy by gamma-quanta. In this case the energy carried away by them must be accounted as the energy released locally at the spots of their formation which must be accounted for in the energy release constants prepared for this case. Such possibility is anticipated in the advanced CONSYST code.

**Diffusion approximation**

Few-group diffusion approximation is widely applied both in the reactor design codes and in the codes used for supporting operation of working reactors. Uncertainties of calculation results associated with this approximation are counterbalanced by introducing corrections evaluated for one or several base options of the reactor design under examination by comparing these results with results of precise calculations obtained, as a rule, using the Monte-Carlo method.

1. It is quite natural to formulate the problem of introduction of “corrections” not in the calculated results but, instead, in the nuclear constants used in the calculations in order to be able to obtain as the result of calculations correct values of not only the integral functionals but of the neutron fields as well. Here the corrections introduced in the obtained “problem-oriented” few-group constants must take into account not only the uncertainties of diffusion approximation, but also the uncertainties introduced by the accounting of heterogenous effects in the preparation of constants. The latter requires unifying the program used for preparation of nuclear constants with the code for calculation of cell of heterogenous grid directed towards obtaining problem-oriented sets of constants.

2. Another important task is to implement the methodology of evaluation of components of uncertainties of calculation results associated with the constants and the technology taking into account the factor that in the initial, post-startup conditions the reactor was strictly critical. Taking this factor, resulting in the significant reduction of evaluated calculation uncertainty, into consideration is especially important in the calculation of the evolution of reactivity with burnup and other effects associated with variation of nuclide composition (breeding ratio, etc.). The problem of accounting the component of uncertainties of calculated results associated with nuclear constants using diffusion codes is already solved both methodologically and from the viewpoint of development of software tools. The only issue is that, when such approach is used, it is necessary for taking into account criticality in initial conditions to revise co-
variance matrices of uncertainties of nuclear constants which will require additional software and methodological development efforts.

Calculations of isotopic kinetics, fuel burnup, accumulation of fission products, transmutation of minor actinides

Information about cross-sections of separate reactions is required for analysis of nuclear fuel cycles including transmutation of radioactive wastes, analysis of approaches to be used for breeding radionuclides and other potential applications of nuclear reactions. Data on the generation of minor actinides, fission products and other nuclides produced in neutron induced reactions, necessary and sufficient for achieving the above purpose, are available in the group form convenient for applications. However, certain additional processing of these data is still required for their practical use, for instance, determining probabilities of threshold reactions in the total numbers of absorption, inelastic scattering and other reactions obtained in the calculation. Data on the cross-sections of yields and incineration of products of neutron induced reactions must be appropriately conjugated with data on radioactive decays which are also required for calculation of nuclide kinetics. The importance of the task of improving methodologies for application of results of measurements of irradiated fuel nuclide compositions and uncertainties of these measurements, in order to reduce the uncertainty of prediction of spent fuel isotopic composition and its characteristics, deserves a special notice. Importance of this task is associated with high level of average burnup of spent nuclear fuel in the cores of advanced fast reactors.

Transport and interactions of gamma-quanta with matter

Nuclear data for gamma-quanta are required both for calculating radiation and hydrogen safety in storage facilities and containers for spent nuclear fuel rods, and for correct calculation of energy release during neutronics calculations of reactor cores. The latter task is especially important in the case of calculation analysis of heavy liquid metal cooled fast reactor cores, because the gamma-radiation generated by neutrons releases significant part of its energy directly in the coolant, thus may significantly reduce the thermal load on the fuel pin cladding.

1. Possibility to perform calculations of sources of gamma-radiation from radioactive decay taking into account the contribution of all not too long-lived daughter radionuclides must be incorporated in the program for preparation of nuclear constants of new generation.
2. Gamma-radiation transport data applied at the present moment (both in 15 and in 127 group energy representation) were obtained on the basis of EPDL library used all around the world and must be supplemented in the same approximation with data allowing taking into account the bremsstrahlung radiation induced by Compton and photoelectrons.

Evaluation of accuracy of calculations

One of the important tasks addressed during the phase of design of fast reactor is to obtain evaluation (conservative) of the balance of reactivity within the system and to determine the margins required for compensation of excess of the reactivity taking into consideration the established nuclear safety regulations and rules. All sources and components of uncertainties in the calculations of neutronics characteristics must be determined in this case including the following:

(1) Methodological component which is the systematic uncertainty (a bias) associated with approximations used in the applied calculation codes under the solution of radiation transport equation, and with inaccuracies in the development of the model of the reactor core.
(2) Nuclear data component associated with existing uncertainties of neutron data (energy dependences of cross-sections, their resonance structure, angular dependences, etc.). According to their nature the uncertainties associated with nuclear constants have the random character and, quite often, they counterbalance each other because of their very (enormously) large number and variety.
(3) Unknown systematic uncertainty (a bias) associated with imperfection (as of today) of experimental methods (as, for instance, finiteness of energy resolution of experimental facilities) and of theoretical approaches. This type of uncertainty can be evaluated by calculating of numerous benchmark (test) models of experiments and then by their statistical processing.

The nuclear data support system of new generation, under the development (CONSYST/ABBN-2020), now is based on the ROSFOND national library of files of evaluated neutron data [14,15] which should follows to world newest evaluations of neutron data, uses modern methodologies, and must be provided with tools for substantiating accuracy and reliability of calculation prediction of characteristics of the designed reactor core [16,17], radiation shielding, safety parameters of both the reactor facility as self and of its fuel cycle along with supporting the calculations with required nuclear constants.

Development of appropriate verification databases of well evaluated (benchmark type) experimental data, as ICSBEP [18] or IRPhEP [19], development of respective methodologies and creation of system of computation codes for evaluation and ranking of calculation uncertainties ([20,21]) – all the above constitute the means for resolving the most important task in the field of provision of nuclear data support, i.e. evaluation of contributions from different sources of uncertainties [22] and analysis of permissible uncertainties in the calculations in order to focus efforts on the most vital directions.

Conclusion

In conclusion let us formulate in a concise form the first priority tasks which, as we realize, must be addressed and
resolved in the development of new generation of nuclear data support system for calculation of fast reactors:

- Development of advanced version of the ROSFOND library of files of evaluated neutron data on the basis of new evaluations and the newest experiments and calculation data including evaluation of covariances of uncertainties of cross-sections;
- Development of advanced version of the ROSFOND library of files of the ABBN-2020 universal system of multi-group nuclear neutronics constants including subgroups and detailed dependences of cross-sections (including, in particular, temperature dependences) and libraries of covariance matrices of uncertainties of multi-group data;
- Development of library of nuclear constants for calculations of isotopic kinetics and activation of materials, library of nuclear constants for gaseous fission products, solid fractions and slags;
- Development of advanced CONSYST-2020 software complex for supporting different neutronics codes and applications (including nuclear fuel cycle) with nuclear constants in different formats prepared using the ABBN-2020 universal system of multi-group constants and their detailed descriptions including the development within the framework of CONSYST code of the processing module for reformatting the ROSFOND files into the multi-group format of ABBN constants;
- Development of interface modules within the framework of CONSYST code for supporting with nuclear constants main calculation codes on the basis of diffusion, kinetics and Monte-Carlo methods;
- Development within the framework of CONSYST code of the module for preparation of constants for nuclei of fission products required for solving problems of calculation of reactor fuel residence time, isotopic kinetics and fuel burnup, accumulation of fission products and incineration of minor actinides;
- Development of code for preparation of problem-oriented few-group constants for implementation of high-speed multiple-choice and dynamic calculations and preparation of appropriate problem-oriented few-group libraries of nuclear constants;
- Development and preparation for wide dissemination of the verification data bases covering representative sets of benchmark experiments for verification of systems of computer codes and nuclear constants;
- Development and implementation of the methodology and calculation code for evaluation and ranking of calculation uncertainties. Evaluation of contributions from different sources of uncertainties and analysis of permissible uncertainties in the calculations of nuclear installation to focus further efforts on the most significant directions;
- Verification of the CONSYST/ABBN-2020 system of codes and libraries of nuclear constants using their group and detailed dependences. Their certification as a standard reference data.

Development of new generation of CONSYST/ABBN system of software tools and data libraries for supporting calculations of fast reactor neutronics and fuel cycles, using ROSFOND nuclear data files and libraries of multi-group constants developed on the unified methodological basis, offers realistic chances to enhance reliability and safety of reactor facilities, ensure their licensing compatibility and competitiveness, and independence from foreign products.

Development of the unified nuclear constant support system and its implementation in the calculation codes will ensure not only the unification of the procedure for preparation of constants which will enhance reliability of their verification, but, as well, will enhance accuracy and reliability of calculation prediction of all most important characteristics of the designed reactors.

References


