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Research Article

ROCOCO system of combined neutron constants – current status and results of testing using geometrical module of the MMK code*

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Abstract

Results of studies aimed at the further refinement of the ROCOCO system (routine for calculation and organization of combined constants including cross-sections in group and subgroup representation with detailed description of energy dependence of neutron cross-sections) (Zherdev et al. 2018, Kislitsina and Nikolaev 2016) are presented in the paper. Inclusion of this system as a physical module into a set of Monte Carlo calculation codes with OOBG geometric module from the MMK code (Zherdev et al. 2003) is discussed. OOBG module is designed for calculation of neutron multiplication systems with heterogenous cores arranged as hexagonal grids with different degrees of complexity. The name ROCOCO-MMK was assigned to the complex. Results of testing the complex in the calculations of multi-zone neutron multiplication systems (including those with zones containing neutron moderator, zones with close composition but with different temperature, etc.) are described. Accounting for the dependence of constants for one and the same nuclide in the zones with different compositions and temperatures required substantial modernization of routines for preparation of constants for calculation described in (Zherdev et al. 2018). Algorithm for preparation of subgroup constants was modified, methodology for taking into account resonance self-screening of cross-sections within the range of unresolved resonances was improved, and other changes were introduced in the process of this modernization.

Results of calculations are compared with data obtained using the MCNP-5 precision program (MCNP 1987), which is linked to the same library of evaluated neutron data ROSFOND as that used in ROCOCO. The ROCOCO-MMK includes procedures for registering different neutron flux functionals (also based on ROCOCO data), which allowed including it in the SCALA computation complex (Zherdev et al. 2003, Zherdev 2005), and performing step-by-step calculation of evolution of fuel nuclide composition during the fuel residence campaign. Directions for further development of the system are outlined in conclusion and, in particular, some possibilities of using the created software for further improvement of methods for preparation of few-group constants for calculations in diffusion approximation are examined.

Keywords

New ROCOCO combined system of neutron constant preparation; further refinement; introduction in the practice of calculations; Monte-Carlo method; results of comparative calculations; potential of development

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ROCOCO modernization

As compared with the ROCOCO system presented during the Neutronics Seminar in 2015 (Zherdev et al. 2018) a number of improvements were introduced in the present version of the complex for preparation of nuclear constants. Configuring the data for calculation was simplified. List of nuclides included in the composition of the calculated system is preset in arbitrary order, the procedure for job processing independently constructs from the original arbitrary list the "ordered shortlist" where actinides occupy first places followed by non-fissionable nuclides and, finally, by multi-isotope elements. Let us remind that such arrangement is essential, because the sets of constants for the above-mentioned three types of nuclides needed for modeling the trajectories are different and arrangement of nuclides allows the operating procedures to process the data in the most optimal manner. If the same "detailed" or "subgroup" nuclides are present in the preset calculation job in different zones at different temperatures, they are treated as different nuclides for which respective constants are prepared and, correspondingly, the "ordered longlist" is organized. Data on the cross-sections are calculated according to the addresses indicated in the longlist; data on the energy and angular distributions not dependent on temperature above the thermalization region are calculated according to the addresses indicated in the original "shortlist".

It was discovered that two subgroups are sufficient for describing the effect of self-screening of cross-sections within the range of unresolved resonances. Special simplified algorithm was developed for obtaining two-subgroup parameters of the resonance structure of cross-sections on the basis of the data on self-screening factors. Within the range of resolved resonances two-subgroup approximation fairly often proves to be insufficient and in that case previous universal algorithm (Zhemchugov 2018) determining the parameters for a larger number of subgroups ensuring preservation of self-screening factors within the whole range of variation of dilution cross-section for the nuclide under description in all zones of the system is applied.

A number of ambiguities were identified and eliminated in the process of operation of the ROCOCO complex in subroutines of the complex, number of error messages accompanied with output of information helping to reveal and remove the causes of these errors was increased. Several errors were found as well in the input data and were also removed.

Additional version of the COLIBRY library (combined library) was formed on the basis of ENDF/B-VII evaluated data library. This version includes the data for the most important nuclides, including the data for 15 actinides and 81 non-fissionable isotopes. The version is linked to ROCOCO programs and was successfully tested on a small number of principal tests.

Linking MMK code to the OOBG geometrical module

Geometrical modules of the MMK code were earlier combined with KENO-VA code (Petrie and Landers 1984) in order to use the module for preparation of multi-group constants for calculation incorporated in the above code. The constants per se were prepared by CONSYST code. Thus obtained conglomeration was used under the name of MMKKENO (Blyskavka et al. 2014a) in the SCALA computational system (Zherdev et al. 2003). In 2015 group headed by K.F. Raskach separated the most important in the practice geometrical module OOBG and linked it to the library of neutron data in ACE format (NJOY99.0 2000) which resulted in the creation of MMKC code (Blyskavka et al. 2014b). It was the OOBG geometrical module that was taken as the basis in the development of the ROCOCO-MMK complex. Conservation of energy and energy group of the neutron as the indicators of neutron state were introduced in the geometrical module. New control module was written using which subroutines of the geometrical module could be supplied with all the necessary macro-constants for the given energy and group utilizing ROCOCO – SIGMA (Zherdev et al. 2018) (calculation of micro-constants, macroscopic total cross-section, kerma, etc.) and COLLY (Zherdev et al. 2018) (determination of the nuclide with which collision occurs, nature of the collision, scattering angle and energy of scattered neutron, if scattering takes place, and number of secondary fission neutrons if fission occurs) operational procedures. The module for simulating the source of next generation neutrons was profoundly changed with introduction of GEFIS procedure (Zherdev et al. 2018) calculating spectrum of fission neutrons for the given nuclide induced by neutron from the given group. These procedures are described in details in (Zherdev et al. 2018).

The following registration procedures were also introduced in the ROCOCO-MMK code:

- Microscopic cross-sections of fission, capture (without fission), elastic and inelastic scattering, formation of secondary fission neutrons, formation of secondary neutrons in (n,2n) reactions, etc., energy release averaged by the registration zones;
- Rates of the processes characterized by the above listed constants averaged over the registration zones with uncertainties (only for nuclides identified in the prescribed calculation job);
- Multi-group spectra of neutron and gamma-quanta fluxes averaged over the zones;
- Energy release and contribution of separate nuclides in it;
- Effective fractions of delayed neutrons for precursor groups.

Possibility of registration of a number of other functionals including average neutron lifetime, number of collisions, absorptions, number of neutrons leaking from the system, neutron leakage spectrum, etc., is provided as well. Registration

is performed either "by the free path", or "by the collision", or "by the absorptions". Combined estimations of the above functionals are not provided in the present version.

The complex is designed in the form of two independent program modules – the module of preparation of constants for calculations and module of modeling trajectories and registration. Calculation is performed in two stages. All data required for calculations are prepared during the first stage in accordance with isotopic composition, temperature and other parameters prescribed in the job description in the format and in the order optimal for simulation. All the data are stored in the external library. This library can be both in binary and in text form. The latter simplifies installation of the complex on different platforms and maintenance of the block of constants.

Testing ROCOCO-MMK

Results of calculation of infinite multiplying media performed using ROCOCO in comparison with calculations performed using precision MCNP-5 code tied to the same ROSFOND library were presented in (Zherdev et al. 2018). Testing was performed for multiplying systems with different degree of complexity of the geometry and composition, starting from BIGTEN (NEA/NSC/DOC(95)03/III) (for which simple cylindrical model was used) to BFS-97 (NEA/NSC/DOC(95)03/VI) and BFS-80 assemblies (Bednyakov 2018). Calculations were performed using ROCOCO-MMK and MCNP codes. ROSFOND and и ENDF/B-VII libraries of evaluated data were used in the latter case. Results of calculations are presented in Table 1. No statistically significant discrepancies between the results of calculations obtained using ROCOCO-MMK and MCNP-5 were detected. Conversion from ROSFOND to ENDF/B-VII leads in the case of BFS-80-1 to small, but statistically significant discrepancy between the results. Ratio of the running time for MCNP code to that for ROCOCO-MMK is presented in the last column of the table. Calculations were performed using the same computer for the same number of simulated trajectories with disabled registration procedures. Economy of time is fairly significant. Results of calculation where composition of non-fissionable nuclides was preset element by element are presented in the last line of Table 1. It is evident that this led to barely perceptible shift of the result and to the reduction of computing time by approximately 1.5 times.

Results of calculations obtained using ROCOCO-MMK are compared in Table 2 with results of calculations performed using MMK_C code where, as it has been already mentioned, the same geometrical module and physical module similar to those used in MCNP-5 (on the basis of ROSFOND library data represented in ACE format) were used. The cause of small, but statistically significant, overestimation of the result of calculation of k_{eff} for BIGTEN obtained using MMK_C from results obtained using MMK-RF and MCNP-5 has not yet been identified.

Table 1. Results of calculation of keff for multidimensional multiplying systems.

Model	MMK-RF	MCNP5	Discrepancy from MCNP5 (ROSFOND)		Ratio of calculation time using MCNP-5 to that for ROCOCO-MMK
			ROCOCO-MMK	MCNP5 (ENDF/B-VII)	
BIGTEN	0.99430(7)	0.99497(7)	–0.01±0.01%	0.01±0.01%	3.84
BFS-97-1	0.99481(12)	0.99511(12)	–0.03±0.02%	0.02±0.02%	6.56
BFS-80-1	1.00231(18)	1.00216(22)	0.01±0.03%	–0.15±0.03%	2.65
BFS-80-1 (elem.)	1.00265(18)		0.05±0.03%		3.94

Table 2. Comparison with calculation results obtained using MMK_C.

Model	ROCOCO-MMK	MMK_C (ROSFOND)	Discrepancy from ROCOCO-MMK	Ratio of calculation time using MMK_C to that for ROCOCO-MMK
BIGTEN	0.99430(7)	0.99660 (6)	–0.23±0.01%	18.5
BFS-80-1	1.00231(18)	1.00233(57)	0.002±0.03%	21.3

Testing operational modes of ROCOCO in the systems with zones with different temperatures of the medium was performed using calculation model of BN-800 fast reactor. 41 zones with seven temperature values were used in the model. Here, fissionable isotopes were present in the zones with only two different temperatures. Calculation performed using ROCOCO-MMK with detailed description of neutron cross-sections produced the result equal to k_{eff} = 0.99753(18). Multi-group (299 groups) calculation using MMKKENO with constants prepared by CONSYST system on the basis of BNAB-RF produced k_{eff} = 1.00120(14). Although statistically significant, discrepancy of – 0.37±0.22% proved to be of small significance. Expenditures of computation time for calculation with detailed description of cross-sections proved, naturally, to be higher – by 2.3 times. No significant discrepancies in the distribution of energy release for reactor zones were identified, and, thus, this testing also produced positive result.

Temperature dependences of multiplication factor for BN-800 model calculated using MMKKENO and ROCOCO-MMK are compared in Figure 1. The observed discrepancies can hardly be regarded as significant.

ROCOCO-MMK incorporation in the SCALA computational system

For the purpose of expansion of the field of application the MMK-RF code was incorporated in the SCALA system (Zherdev et al. 2003, Zherdev 2005) intended, in particular, for calculation of nuclide kinetics. Functionals calculated using MMK-RF (heat release, multi-group neutron fluxes, group reaction cross-section on actinides, etc.) required for calculation of nuclide kinetics are entered in

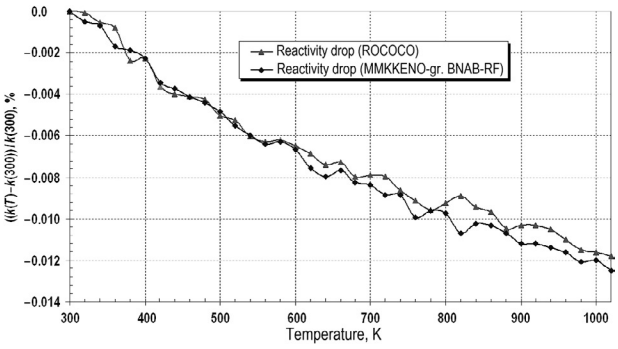

Figure 1. Temperature dependences of multiplication factor for BN-800 model.

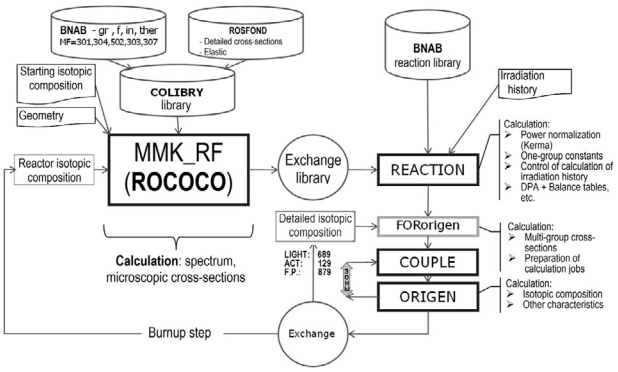

Figure 2. Layout of SCALA-RF computational system.

the SCALA system exchange file from where the data are directed via the REACTION code to the COUPLE-ORIGEN software complex (Zherdev 2015) calculating evolution of nuclide compositions during the preset burnup step. REACTION code (Zherdev et al. 2003) supplements the set of microscopic cross-sections obtained in ROCOCO-MMK with additional data required for calculation of all burnup chains. Setting of the calculated block of constants for calculation of the next burnup step is formed on the basis of calculated compositions (modified in case of necessity to allow for the holding time).

Radiation characteristics of irradiated fuel, dpa numbers, etc., are calculated within the SCALA system simultaneously with calculation of nuclide composition.

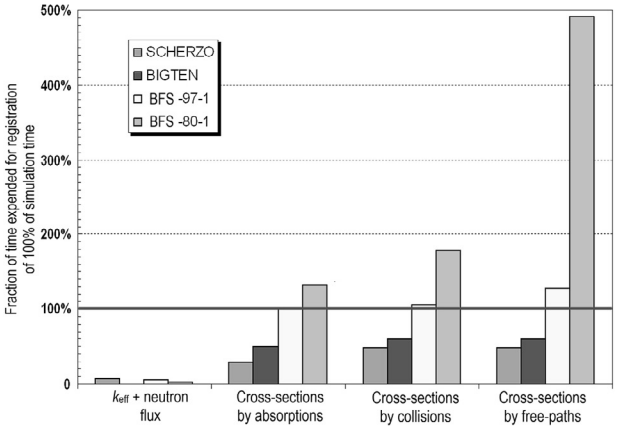

Figure 3. Fraction of time expended for registration relative to the time for modeling the trajectories.

The layout of the SCALA system with incorporated ROCOCO-MMK code is represented in Figure 2. Programs of the nuclear constant and program complex remaining in the composition of the SCALA system are not shown here in order to not overload the figure with information.

Experience of application of ROCOCO-MMK demonstrated that performance of registration procedures occupies significant fraction of total calculation time. Obviously, this effect is manifested especially strongly in the calculations of geometrically complex systems, such as, for instance, BFS-80-1. In such case registration of not only fluxes and energy release, but of micro-constants, reaction rates, etc., required five times more time compared to the time required for calculation of only k_{eff}, energy release and group fluxes for zones. Time expenditures for registration in the calculation of more simple systems are significantly smaller (Table 3.).

It was precisely the time expended for registration that drove us to reject (at least temporarily) from combining registration procedures.

Figure 3 gives clear illustration of time expended for registration, as well as of the possibility to optimize time expenditures.

For the examined models the fraction of time expended for registration of cross-sections can constitute from 30 to 56% and more, i.e. more than half of the calculation time may be spent for registration. For strongly heterogenous system registration time can reach or even exceed the time expended for simulation (by five times for BFS-80-1, see Fig. 3). However, this time can be significantly reduced by registering nuclide cross-sections only by absorptions, which, for geometrically complex systems, allows reducing total calculation time by four-five times. It is obvious, that this leads to increased statistical uncertainties of the calculated results (especially in small-volume zones).

Incorporation of ROCOCO-MMK in the SCALA system allows recording heterogeneously blocked (taking into account the detailed energy dependences) constants calculated using this code in the library in GMF format (Manturov et al. 1999) used by the constant support system of the CONSYST code to replace constants actually prepared by the code itself. Here, matrices of energy and angular transitions in elastic and inelastic scattering on which self-screening produces practically no effect remain to be as before. Thus, possibility appears to move in the preparation of constants away from the main approximations of the applied methodologies:

Table 3. Time (min) expended for execution of calculation job depending on the set of registered functionals.

System	Only k_{eff}	k_{eff}, group fluxes and energy release	k_{eff}, group fluxes, energy release and micro-constants for nuclides		
			By collisions	By absorptions	By free-paths
BIGTEN	41.2	41.4	61.8	66.1	66.2
BFS-97-1	68.2	72.1	136.8	140.7	155.9
BFS-80-1	63.8	65.9	148.7	177.6	377.6

– Narrow resonance;
– "Weak diffusion", i.e. neglecting the effects of current on the resonance structure of the flow;
– "Standard spectrum" according to which group sections are averaged по.

Development potential

1. Testing ROCOCO-MMK performance in solving (n, γ)-problems appears to be one of the first priority tasks. Let us remind, that ROCOCO complex supplies all the constants necessary for that. Gamma-quanta are described in ROCOCO in 127-group approximation with the use of macro-constants. They are assigned group numbers from 301-st to 427-th. Simulation of free path, collisions of the gamma-quantum and consequences of this collision are already incorporated in ROCOCO operational procedures.
2. The necessity of modernization of 127-group system of BNAB constants for the purpose of accounting for X-ray radiation emitted during deceleration of photoelectrons, Compton electrons and positron-electron pairs should also be mentioned in connection with gamma-task. The necessity of accounting for the bremsstrahlung became apparent in the calculations of radiation environment in SNF storage facility of the Bilibino NPP. Since generation of hard bremsstrahlung is mainly determined by the atomic number of the medium in which electrons are decelerated, inclusion of these data in the library for gamma-quanta will not require modernization of the structure of this library.
3. For the purpose of further reduction of calculation time we intend as well to anticipate the possibility of combining all "group" nuclides, i.e. nuclides for which resonance self-screening is not significant, in one macro-nuclide. Energy-angular distributions of elastically scattered neutrons for this nuclide can be described in P5-approximation using three discrete scattering angles with preset probabilities, similarly to how it is done in KENO-Va and in ROCOCO in the description of gamma-quanta scattering.
4. Algorithm for generating two-subgroup parameters tested in ROCOCO-MMK could find its application in the anticipated modernization of CONSYST for obtaining two-subgroup macro-constants. Transition to two-subgroup approximation would allow correct accounting for the boundary resonance effects and angular dependence of resonance structure of the flux inside the group and, consequently, group constants as well.
5. Creation on the basis of ROCOCO-MMK (or independently from it) of the program for calculation of BFS assembly cell allowing preparation of heterogeneously blocked (taking into account the detailed picture of cross-sections) homogenized constants including transport cross-sections determined from the condition of conservation of the ratio of neutron flow through the cell and gradient of the flux for its subsequent use in diffusion codes, such as TRIGEX (Kislitsina et al. 2013).

Conclusion

Functionality of the combined ROCOCO nuclear constant supply system as the physical module of the engineering Monte-Carlo nuclear reactor calculation code – the ROCOCO-MMK code – was demonstrated. Difference between the results of calculation performed with detailed follow-up of neutron energy in the description of cross-sections using the above code and the results of calculations using reference MCNP5 code does not exceed the uncertainties caused by the inaccuracy of knowledge of neutron data. Expenditures of CPU time on the calculation in the case of application of ROCOCO-MMK are lower (in many cases significantly lower) then the expenditures of time for similar calculation using MCNP. Certain ways are examined for application of ROCOCO-MMK in engineering calculations. Potential of future development was outlined.

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