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*Institute for Nuclear Research, National Academy of Sciences of Ukraine, Kyiv, Ukraine*\*Corresponding author: [vistaldi@gmail.com](mailto:vistaldi@gmail.com)**DEVELOPMENT OF NEUTRON AND PHOTOATOMIC DATA LIBRARIES  
FOR THE MCPV AND MCSS CODES**

The paper presents experience gained in the development and verification of neutron and photoatomic libraries for the specialized computational codes MCPV and MCSS, which are used for the analysis of radiation exposure of VVER reactor pressure vessels, irradiation parameters of reactor internals, and irradiation conditions of surveillance specimens. Approaches to the generation of multigroup neutron libraries with different nuclide compositions and energy coverage, as well as neutron and photoatomic libraries in continuous-energy representation in the ACE format, are discussed. The verification of the developed libraries was performed by comparing calculation results obtained using different Monte Carlo codes in benchmark problems of neutron and photon transport in a simple spherical geometry.

*Keywords:* reactor dosimetry, neutron and photoatomic data libraries, Monte Carlo method, MCPV, MCSS.

**1. Introduction**

The operational safety of a reactor facility is largely determined by the reliability of barriers that prevent the release of fission products. For VVER reactors, one of the keys such barriers is the reactor pressure vessel, which must maintain its integrity under both normal operating conditions and design-basis accident conditions. Therefore, monitoring the condition of the vessel material throughout its entire service life is of fundamental importance.

An important source of information on changes in the material properties of the reactor vessel is provided by numerical neutron transport calculations in the near-vessel region and in the locations of surveillance specimens, performed using the Monte Carlo method. To solve these problems, the following specialized computational codes have been developed at the Institute for Nuclear Research of the National Academy of Sciences of Ukraine (INR NASU):

1) MCPV [1] – intended for the calculation of neutron flux functionals in the near-vessel region of VVER reactors for reactor pressure vessel dosimetry;

2) MCSS [2] – used for determining irradiation conditions of surveillance specimens in VVER-1000 reactors.

For the above-mentioned codes, a multigroup neutron data library [3] was developed at the Ukrainian Nuclear Data Center of the INR NASU by Dr. O. Gritzay. This library provided a description of the material composition of the principal structural components of VVER reactors. It is subsequently used as the basic library.

With the evolution of the problems addressed using the MCPV code, its field of application has

significantly expanded. In particular, the need arose to determine neutron fluence at reactor internals and supporting elements of the reactor pressure vessel, as well as to evaluate radiation heating of the VVER-1000 core baffle. In addition, modern reactor cores incorporate new materials requiring a more detailed neutronic description.

This necessitated the development of new neutron data libraries. At present, in addition to the basic multigroup library, two additional multigroup libraries have been generated – one with an extended nuclide set and another covering the full energy range. Furthermore, neutron and photoatomic libraries in continuous-energy representation in the ACE format have been prepared, compatible with computational codes such as MCNP [4], Serpent [5], and others.

Beyond its practical relevance, the work also has methodological significance. Although in most reactor analyses the dominant contribution to overall uncertainty arises from geometric and material parameters of the computational model, the proper selection and preparation of neutron and photoatomic data libraries remain an important factor in ensuring the reliability of calculation results. In practice, situations may arise where standard libraries supplied with computational codes prove insufficient – particularly in cases involving non-standard materials, specific spectral conditions, or temperature regimes characteristic of research reactors or advanced nuclear systems.

Accordingly, this work considers approaches to the development and modernization of neutron and photoatomic data libraries for the MCPV and MCSS codes and outlines the principal methodological aspects of their preparation and verification.

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## 2. Basic principles and requirements for the development of multigroup neutron libraries

The basic principles and requirements for the development of new multigroup neutron libraries are based on the principles used in constructing the basic library, and ensure at least the same level of detail and computational accuracy.

The nuclide composition of the new libraries is determined by the requirement to provide a descrip-

tion of materials that is at least as complete as that of the basic library. Table 1 presents the minimally required set of nuclides and elements for reactor pressure vessel dosimetry applications. Considering current trends in neutronic modeling and the increasing demands on calculation accuracy, natural elemental mixtures should preferably be replaced with explicit isotopic representation.

Table 1. Nuclide and elemental composition of the main components of the computational model and primary nuclear data sources

Model component	Nuclides / Elements	Primary nuclear data sources
Water	$^1\text{H}$ , $^{16}\text{O}$ , $^{17}\text{O}$	JENDL-3.2
Fuel assemblies (fuel, cladding) and burnable absorber rods	$^{235}\text{U}$ , $^{238}\text{U}$ , $^{\text{nat}}\text{Zr}$ , $^{\text{nat}}\text{Nb}$ , $^{\text{nat}}\text{Hf}$ , $^{10}\text{B}$ , $^{11}\text{B}$	JENDL-3.2, JEF-2
Steel structural components (core baffle, core barrel, reactor pressure vessel, etc.)	$^{\text{nat}}\text{Fe}$ , $^{\text{nat}}\text{Cr}$ , $^{58,60-62,64}\text{Ni}$ , $^{55}\text{Mn}$	JENDL-3.2, ENDF/B-VI
Dry biological shield	$^{130,132,134-138}\text{Ba}$ , $^{\text{nat}}\text{Ca}$ , $^{\text{nat}}\text{Si}$ , $^{\text{nat}}\text{S}$ , $^{27}\text{Al}$	JENDL-3.2

The energy range of the basic library covers the interval 0.11109–18.221 MeV and is divided into 51 energy groups of equal width in lethargy. When developing new libraries, the energy range may be refined or extended depending on the specifics of the computational problems. However, the number of energy groups must remain unchanged (51 groups), which is required to preserve consistency with the algorithms of the computational codes.

The neutron weighting function is adopted to be the same as that used in the basic library, as it corresponds to the characteristic spectrum of PWR reactors. It has a combined form: in the epithermal region, a Fermi spectrum proportional to  $\sim 1/E_n$  (up to 0.8208 MeV) is used, whereas in the fast energy region, a fission spectrum of the form  $\sim E_n^{1/2} \cdot \exp(-E_n/E_0)$  with the parameter  $E_0 = 1.273$  MeV (above 0.8208 MeV) is applied.

The allowable relative errors for resonance reconstruction, linearization, Doppler broadening, and integration do not exceed 1%, which corresponds to the accuracy level of the basic library.

The set of neutron constants in the multigroup libraries includes:

1) group-wise effective microscopic cross sections for the main reaction types, including total cross section, elastic and inelastic scattering, threshold reactions of the (n, xn) type (in particular (n, 2n), (n, 3n), etc.), fission, as well as non-fission absorption reactions ((n,  $\gamma$ ), (n, p), (n,  $\alpha$ ), etc.);

2) effective inelastic interaction cross sections formed taking into account the multiplicity of secondary neutron production in threshold (n, xn) reactions and intended for the correct description of neutron balance in the multigroup transport representation;

3) inelastic scattering kernels defined by group-to-group transfer matrices and the average cosine of the scattering angle (first angular moment);

4) elastic scattering kernels defined by group-to-group transfer matrices and angular moments of the scattering distribution up to the fifth order;

5) resonance self-shielding factors for the total cross section, elastic and inelastic scattering, fission, and radiative capture.

For all nuclides, except hydrogen, resonance self-shielding factors shall be calculated for nine background cross-section values: 0,  $10^{-1}$ , 1, 10,  $10^2$ ,  $10^3$ ,  $10^4$ ,  $10^5$ , and  $10^6$ . For hydrogen, only the infinite-dilution case is permitted.

## 3. Multigroup neutron data library with extended nuclide set

The purpose of developing this library was not only to update the neutron constants compared to the basic library, but also to extend the nuclide composition with regard to the specific features of the computational problems. In particular, gadolinium isotopes ( $^{152,154-158,160}\text{Gd}$ ), which are important for modeling burnable neutron absorbers, were added to the library. In addition, all elements that were represented in the basic library in their natural form (see Table 1) are represented on an isotopic basis in the new neutron libraries.

The multigroup library with an extended nuclide set was generated using the NJOY2016 code [6] based on the ENDF/B-VII.1 evaluated nuclear data files. The choice of ENDF/B-VII.1 is due to the need to ensure consistency of nuclear data within the MCPV and MCSS computational chain, including the generation of derived constants (in particular,

neutron source data) using the WIMSD-5B code with a library based on ENDF/B-VII.1 [7].

The energy range and group structure were preserved as in the basic library and include 51 energy groups of equal lethargy width, ensuring consistency of calculation results when different variants of multigroup libraries are used.

When generating multigroup neutron constants with NJOY, the evaluated nuclear data are processed through a sequence of independent modules, each responsible for a specific processing stage. The structure of the NJOY input file defines the order of module execution and their operating parameters. The following module sequence was used for the generation of the multigroup libraries: MODER → RECONR → BROADR → GROUPE → CCCCR.

At the initial stage, the MODER module was used to copy the original ENDF library and create a working version of the data in either text or binary format. The RECONR module then reconstructed the resonance cross sections and produced pointwise tabulated cross sections based on resonance parameters and specified interpolation schemes. At the next stage, the BROADR module performed Doppler broadening of the cross sections for the specified temperatures.

The generation of multigroup neutron constants was carried out using the GROUPE module, which produced multigroup cross sections, scattering kernels (group-to-group transfer matrices and the corresponding angular moments), as well as resonance self-shielding factors in the GENDF (groupwise ENDF) format. At the final stage, the CCCCR module was used to generate libraries in the CCC format suitable for subsequent use in the computational codes.

During library generation, the relative error tolerances for resonance reconstruction and Doppler broadening were set to 0.1 %, while the maximum integral error was limited to 0.3 %. These tolerances are stricter than those applied in the basic multigroup library. All cross-section processing steps were performed at 575 K, corresponding to the assumed operating temperature of the reactor model.

#### 4. Multigroup neutron data library with full energy range

In problems related to the analysis of irradiation of reactor internals and the assessment of radiation damage to materials, an accurate description of the neutron spectrum over the entire energy range – from the thermal region to fast neutrons – is required. In particular, when evaluating displacements per atom (dpa), both low-energy and high-energy components of the spectrum may provide a significant contribution. For this reason, a mul-

tigroup library with full energy range coverage was developed.

The library was generated using the NJOY code with the same sequence of modules as applied for the extended-nuclide library, based on the evaluated nuclear data files ENDF/B-VII.1. It covers the full neutron energy spectrum – from  $10^{-5}$  eV to 19.64 MeV – thus enabling consideration of all principal neutron interaction mechanisms within the computational model.

For the multigroup representation of the energy spectrum, a 51-group structure was adopted, with group boundaries consistent with the VITAMIN-B7 library structure [8]. This energy structure has been widely used and validated in reactor dosimetry and radiation shielding applications employing deterministic methods (in particular, the DORT and TORT codes), stochastic methods (the Monaco code), and hybrid approaches (the MAVRIC sequence within the SCALE system) [9].

The neutron weighting function had a combined form reflecting the spectral behavior in different energy regions. In the low-energy region, a Maxwellian spectrum proportional to  $\sim E_n \cdot \exp(-E_n/E_0)$  with parameter  $E_0 = 0.05$  eV was used (up to 0.1 eV). In the epithermal range, a Fermi spectrum proportional to  $\sim 1/E_n$  was applied (up to 0.8208 MeV), whereas in the fast energy region, a fission spectrum of the form  $\sim E_n^{1/2} \cdot \exp(-E_n/E_0)$  with parameter  $E_0 = 1.273$  MeV was used (above 0.8208 MeV).

#### 5. Neutron and photoatomic data libraries with continuous-energy representation in ACE format

Within the framework of studies aimed at determining energy deposition in the VVER-1000 reactor core baffle, the need arose to perform neutron and photon transport calculations in a continuous-energy representation.

The neutron library with continuous-energy representation in the ACE format was generated using the NJOY code based on the evaluated nuclear data files ENDF/B-VII.1. The library is compatible with Monte Carlo codes such as MCNP, Serpent, MCPV, MCSS, and others.

The library was generated using the following NJOY module sequence: MODER → RECONR → BROADR → HEATR → PURR → THERMR → GASPR → ACER.

The initial data processing stages (MODER, RECONR, BROADR), including resonance reconstruction and Doppler broadening, were performed using the same accuracy criteria as those applied in the development of the multigroup libraries.

Using the HEATR module, total kinematic KERMA cross sections (MT = 443) and total damage energy production cross sections (MT = 444) were generated for energy deposition and radiation damage assessments. In the unresolved resonance region, probability tables were generated using the PURR module with 20 probability bins and 64 resonance ladders for nine background cross-section ( $\sigma_0$ ) values.

The generation of thermal neutron scattering cross sections and angular distributions was carried out using the THERMR module in the free-gas approximation with 16 equiprobable angular bins; the tolerance was set to 0.1 %, and the upper energy limit for thermal treatment was 5 eV. The GASPR module was used to include charged-particle production (p, d, t,  $^3\text{He}$ , and  $\alpha$ -particles) in the library. At the final stage, the ACER module was used to generate the output files in the ACE format.

The parameters of the PURR and THERMR modules, governing the construction of probability tables in the unresolved resonance region and the generation of thermal neutron scattering data, were selected in accordance with the recommendations provided in the validated report [10].

The photoatomic library with continuous-energy representation in the ACE format was generated based on ENDF/B-VII.1 evaluated data for application in the MCPV code. The photoatomic library was prepared using the ACER module of NJOY. In its preparation, photoatomic cross sections and atomic relaxation data were employed, ensuring that both primary photon interactions with atoms and secondary processes associated with electron shell relaxation were properly taken into account.

## 6. Verification of neutron and photoatomic data libraries

A direct approach to verifying the developed libraries is to apply them in particle transport calculations, followed by an analysis of the obtained results. The verification of the developed neutron and photoatomic data libraries was carried out by comparing the results of neutron and photon spectral flux calculations obtained using different Monte Carlo codes.

Within the verification problem, particle transport was modeled in a simple spherical geometry with a point source at the center. Such a setup allows focusing directly on verifying the correctness of the developed libraries while minimizing the influence of factors related to geometrical complexity. The use of multiple codes additionally makes it possible to identify potential deviations associated with the specifics of individual computational models.

The calculations were performed using the MCPV, MCNP, Serpent 2, and OpenMC codes [11]. The

MCNP and Serpent 2 codes use libraries in the ACE format, whereas OpenMC employs the HDF5 format, which can be obtained by converting ACE data. The official OpenMC library based on ENDF/B-VII.1 was used in the verification calculations.

Since the developed ACE libraries are compatible with the MCNP and Serpent 2 codes, they are used in these codes to perform verification calculations. The MCNP and Serpent 2 codes are well established and widely used for neutron and photon transport problems. This provides an additional independent verification of the developed libraries.

On the other hand, the multigroup libraries can only be used with the MCPV code. Since the energy range of the multigroup neutron data library with full energy range covers that of the library with the extended nuclide set, only the multigroup neutron data library with full energy range is considered in the following analysis.

The OpenMC results are taken as reference, since the code uses the official library based on ENDF/B-VII.1 in a continuous-energy representation. The deviations of the results obtained with other codes are defined as the relative difference:

$$\delta = \frac{X - X_{ref}}{X_{ref}} \cdot 100\% ,$$

where  $X$  is the calculated value (MCPV, MCNP, or Serpent), and  $X_{ref}$  is the reference value obtained with OpenMC.

Table 2 presents selected results of the neutron library verification, namely the relative deviations of neutron spectral flux calculations obtained with different codes in spherical geometries of radius 27 cm, each filled with one of the main reactor materials. In the multigroup calculations, the source is defined as uniform over the energy groups, whereas in the continuous-energy calculations, a discrete representation is used with energies corresponding to the group-averaged values. This approach ensures the equivalence of the integral characteristics of the source in both formulations.

Since the MCPV and MCSS codes are primarily intended for evaluating neutron flux functionals in the fast energy region, in particular for energies above 0.5 MeV, as well as the spectral index (defined as the ratio of the neutron flux above 0.5 MeV to that above 3.0 MeV), Table 2 presents results for the corresponding energy ranges of 0–0.5, 0.5–3, and 3–20 MeV.

As can be seen from Table 2, the results obtained using the MCNP code are in very good agreement with the reference OpenMC values: the deviations do not exceed fractions of a percent, which confirms the reliability of the developed ACE libraries.

**Table 2. Relative deviations of energy-integrated neutron fluxes calculated using MCPV (multigroup) and MCNP (continuous-energy) relative to OpenMC results**

Material	Energy range, MeV	$\delta_{\text{MCPV}}$ , %	$\delta_{\text{MCNP}}$ , %
H <sub>2</sub> O	0–0.5	–6.94	0.31
	0.5–3	0.68	–0.03
	3–20	–1.22	–0.03
Fe 72 wt.%, Cr 18 wt.%, Ni 10 wt.%	0–0.5	3.96	–0.03
	0.5–3	1.28	0.01
	3–20	–1.59	0.01
UO <sub>2</sub> (4.4 wt.% <sup>235</sup> U)	0–0.5	–0.63	0.00
	0.5–3	0.39	–0.08
	3–20	–0.60	0.00
Zr (1 wt.% Nb)	0–0.5	4.03	0.02
	0.5–3	0.79	0.00
	3–20	–0.89	–0.02

For multigroup calculations performed with the MCPV code, somewhat larger deviations are observed, which is an expected consequence of the group-wise representation of nuclear data. In the fast energy region (0.5–20 MeV), the deviations generally do not exceed 1–2 %, whereas in the low-energy region (0–0.5 MeV) they may reach several percent. The largest deviations are observed for water, which is typical for multigroup models and is associated with the specifics of neutron slowing-down processes.

Overall, the obtained results demonstrate good agreement between the multigroup and continuous-energy libraries and confirm the suitability of the developed libraries for reactor dosimetry applications.

For the verification of the photoatomic libraries, calculations were performed using the MCNP code (in photon mode) and in Serpent 2. The OpenMC results obtained using the photoatomic library based on ENDF/B-VII.1 were taken as reference.

For the verification of the photoatomic library, a photon transport problem was considered in concentric spherical shells with radii from 1 to 10 cm and a point source at the center. The source was defined as a discrete energy spectrum with uniform probability, where the energy values correspond to the group-averaged energies of the tally bins. The energy grid for tallying was based on the MCPV group structure with equal lethargy width, but with a lower bound of 1 keV instead of 0.11109 MeV; the total number of energy intervals was 99.

Table 3 presents the results of the photoatomic library verification, namely the relative deviations of the photon spectral flux calculated using different codes in spherical shells with radii from 3 to 10 cm, filled with the materials listed in Table 2. The spectral flux results were integrated over the following

energy ranges: 0.001–0.1, 0.1–1, and 1–18.2 MeV. The selected ranges correspond to a coarse grouping of the equal-lethargy energy grid and provide representation of the low-, intermediate-, and high-energy regions of the photon spectrum.

**Table 3. Relative deviations of energy-integrated photon fluxes calculated using MCNP and Serpent with photoatomic data libraries relative to OpenMC results**

Material	Energy range, MeV	$\delta_{\text{MCNP}}$ , %	$\delta_{\text{Serpent}}$ , %
H <sub>2</sub> O	0.001–0.1	0.07	–0.14
	0.1–1	–0.01	0.01
	1–18.2	0.03	0.01
Fe 72 wt.%, Cr 18 wt.%, Ni 10 wt.%	0.001–0.1	2.14	–0.25
	0.1–1	1.21	0.29
	1–18.2	0.80	0.06
UO <sub>2</sub>	0.001–0.1	4.28	0.78
	0.1–1	6.78	1.30
	1–18.2	4.60	0.75
Zr (1 wt.% Nb)	0.001–0.1	0.56	–0.37
	0.1–1	2.18	0.41
	1–18.2	1.39	0.12

As can be seen from Table 3, the results obtained using the Serpent code are in good agreement with the reference OpenMC values, with deviations generally not exceeding ~1 %. The MCNP results also demonstrate overall satisfactory agreement; however, for some materials, in particular UO<sub>2</sub>, larger deviations (up to several percent) are observed, especially in the intermediate energy range. Since such deviations are not observed for Serpent, this indicates that the discrepancies are not related to the quality of the photoatomic libraries, but rather to differences in the implementation of physical models and photon transport methods in the codes, which become more pronounced for high-Z materials. Overall, the obtained results confirm the reliability of the developed photoatomic libraries and their suitability for photon transport applications.

## 7. Conclusions

The paper summarizes the experience gained in the development and modernization of neutron and photoatomic data libraries for the specialized computational codes MCPV and MCSS, which are used for the analysis of radiation exposure of VVER reactor pressure vessels, irradiation parameters of reactor internals, and irradiation conditions of surveillance specimens.

Based on the principles used in constructing the basic multigroup library, additional multigroup neutron data libraries were developed, differing in nuclide composition and energy coverage, including

a library with an extended nuclide set and a library covering the full energy range.

In addition to the multigroup libraries, neutron and photoatomic libraries in continuous-energy representation in the ACE format were prepared, suitable for neutron transport, photon transport, and coupled neutron-photon transport calculations. This ensures their applicability both in the specialized MCPV and MCSS codes and in widely used Monte Carlo codes.

The verification of the developed libraries was carried out by comparing neutron and photon spectral fluxes calculated using multiple Monte Carlo

codes (MCPV, MCNP, Serpent 2, and OpenMC) in benchmark problems of particle transport in a simple spherical geometry. The results demonstrate good agreement between multigroup and continuous-energy approaches and confirm the reliability of the developed neutron and photoatomic libraries, as well as their suitability for reactor dosimetry applications.

The proposed approaches may be used to adapt computational models to specific materials, spectral conditions, and temperature regimes characteristic of power and research reactors, as well as advanced nuclear systems.

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#### СТВОРЕННЯ БІБЛІОТЕК НЕЙТРОННИХ І ФОТОАТОМНИХ КОНСТАНТ ДЛЯ КОДІВ MCPV І MCSS

У роботі представлено досвід створення та верифікації бібліотек нейтронних і фотоатомних констант для спеціалізованих розрахункових кодів MCPV і MCSS, що застосовуються для аналізу радіаційного навантаження на корпус реакторів типу ВВЕР, параметрів опромінення внутрішньокорпусних пристроїв та умов опромінення зразків-свідків. Розглянуто підходи до формування багатогрупових бібліотек нейтронних констант з різним нуклідним складом і енергетичним охопленням, а також нейтронних і фотоатомних бібліотек з неперервним енергетичним представленням у форматі ACE. Верифікацію підготовлених бібліотек здійснено через порівняння результатів розрахунків, отриманих з використанням різних Монте-Карло кодів, у тестових задачах переносу нейтронів і фотонів у простій сферичній геометрії.

*Ключові слова:* реакторна дозиметрія, нейтронні та фотоатомні бібліотеки, метод Монте-Карло, MCPV, MCSS.

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