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# Group-averaged neutron and gamma-ray cross sections for radiation protection and shielding calculations for nuclear reactors

*Sections efficaces multigroupes neutrons et gammas pour les calculs de radioprotection associés aux réacteurs nucléaires*



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# Foreword

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This document was prepared by Technical Committee ISO/TC 85, *Nuclear energy, nuclear technologies, and radiological protection*, Subcommittee SC 6, *Reactor technology*.



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# Group-averaged neutron and gamma-ray cross sections for radiation protection and shielding calculations for nuclear reactors

## 1 Scope

This document provides guidance in the preparation, verification, and validation of group-averaged neutron and gamma-ray cross sections for the energy range and materials of importance in radiation protection and shielding calculations for nuclear reactors1), see also Annex A.

## 2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 12749-5, *Nuclear energy, nuclear technologies, and radiological protection — Vocabulary — Part 5: Nuclear reactors*



## 3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 12749-5 and the following apply.



ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at https://www.electropedia.org/

**3.1**
**cross-section processing code**
computer code that converts evaluated nuclear data in a specified format and procedure into a form that is appropriate for use in applications

Note 1 to entry: A cross-section processing code performs calculations such as resonance reconstruction, Doppler broadening, and multigroup averaging.

**3.2**
**ENDF/B**
United States of America *evaluated nuclear data file* (3.3) prepared and reviewed by subject matter experts that is coordinated and maintained by CSEWG and NNDC at Brookhaven National Laboratory

**3.3**
**evaluated nuclear data file**
nuclear reaction database stored using a specified format and procedure

EXAMPLE ENDF/B[2], JEFF[3], and JENDL[4].

1) This edition is based on ANSI/ANS-6.1.2-2013[1].

 

**3.4**
**experimental benchmark**
experiment for which conclusions can be drawn as to the accuracies of computational models and the underlying nuclear data

Note 1 to entry: An experimental benchmark contains the following:

— a complete description of the conditions under which the experiment took place, including input data such as reactor geometry, material compositions, core power distribution, relevant material temperatures, and experimental conditions specified in sufficient detail to model or to replicate the experiment;

— measured data and their associated uncertainties.

Note 2 to entry: An experimental benchmark can provide “integral” or “differential” metrics; ”integral” pertains to integral quantities such as reaction rates, while “differential” provides energy-dependent spectral information such as time-of-flight measurements.

**3.5**
**group-averaged cross section**
cross section averaged over energy groups (intervals) as weighted by specified functions

**3.6**
**JEFF**
*evaluated nuclear data file* (3.3) produced via an international collaboration of NEA Data Bank participating countries



**3.7**
**JENDL**
Japanese *evaluated nuclear data file* (3.3) for fast breeder reactors, thermal reactors, fusion neutronics and shielding calculations, and other applications



**3.8**
**neutron and gamma-ray cross section**
cross section for the interactions of neutrons and gamma-rays with matter, including cross section for the secondary emission of neutron and gamma-ray as well as cross section for the effects of neutron and gamma-ray on materials (e.g. heating or helium generation)

**3.9**
**numerical benchmark**
specification of a set of input quantities (e.g. composition and geometry of bulk material and radiation sources) and of reference calculated output quantities relevant to the benchmark (e.g. spatial and energy dependence of neutron or gamma-ray fluence profiles) in detail sufficient to determine the accuracies of a specified computational method when applied to modelling of the same input specifications

## 4 Abbreviations and acronyms

| | |
|---|---|
| CSEWG | Cross Section Evaluation Working Group |
| KERMA | Kinetic Energy Released per unit Mass |
| LWR | Light Water Reactor |
| NEA | Nuclear Energy Agency |
| NNDC | National Nuclear Data Center |
| OECD | Organisation for Economic Co-operation and Development |
| ORNL | Oak Ridge National Laboratory |
| RSICC | Radiation Safety Information Computational Center |

# 5 Preparation of group-averaged neutron and gamma-ray cross sections

## 5.1 Evaluated nuclear data files

Evaluated nuclear data files shall be derived from documented and reviewed information, including basic experimental data, nuclear models, and systematics. The evaluated microscopic cross sections shall be expressed as unique physical parameters and piecewise-continuous functions of incident particle energy, of secondary particle energy, and of secondary particle angle with respect to the incident particle direction. The evaluation shall be in sufficient detail for shielding applications, shall be reviewed and documented, and should be tested against benchmark experiments.

## 5.2 Checking of evaluated nuclear data files

Before processing an evaluated nuclear data file, it should be checked for format conformation, data validity, recommended procedure conformation, and physics content (e.g. using ENDF Utility Codes[5]). If KERMA values are computed for response functions, cross-section processing code outputs (showing kinematics limits from the total momentum conservation) should be analysed to avoid KERMA calculation problems[6].

## 5.3 Energy ranges and materials of importance

The evaluated nuclear data files should cover energy ranges (~$10^{-5}$ eV to ~20 MeV for neutrons and ~1 keV to ~30 MeV for gamma-rays), and materials (shield materials as well as other materials required for calculation of radiation sources) of importance in radiation protection and shielding calculations for nuclear reactors.



## 5.4 Group-averaging techniques



### 5.4.1 General

Evaluated nuclear data files shall be averaged over energy groups by numerical techniques that do not significantly degrade the accuracy of the evaluated nuclear data files for the application of interest. Weighting functions and energy group structures should be appropriate for the application. The group-averaging process should be carried out by tested, verified, and validated computer codes that have been documented and reviewed.

### 5.4.2 Fine-group structures

The number and energy boundaries of fine energy groups shall be specified in detail sufficient to yield adequate accuracy for radiation protection and shielding calculations, even if the number of fine groups would impose significant computation time, memory, and hard disk space requirements. A fine-group structure shall be used to determine the sufficiency of a coarser collapsed-group structure derived from that fine-group structure. The fine-group structure shall accommodate weighting functions that will be applied to the collapse of the fine-group data to coarse groups. The fine-group structure should be insensitive to the weighting functions used for specific applications.

### 5.4.3 Pointwise weighting function

The pointwise weighting function applied to the calculation of averaging neutron and gamma-ray cross sections for an isotope of interest should be representative of the spectrum for the energy range and application of interest. If the fine-group structure contains sufficiently small groups, the shape of the weighting function within a fine group will not be important. If the weighting function does not explicitly account for resonance effects, energy self-shielding calculations, such as Bondarenko factors[7], shall be used to correct cross sections in resonance regions.

### 5.4.4 Self-shielding treatment

Self-shielding effects can be very significant in deep-penetration problems. If systems containing pure iron or other structural materials are of interest and Bondarenko factors are used, Bondarenko data at sufficiently low-background cross sections (i.e. low dilution), such as 0,1 b or lower, should be provided. Studies have shown that insufficient self-shielding correction of the scattering matrix can cause a noticeable effect in some cases[8]. Most available shielding libraries do not currently treat these effects.

### 5.4.5 Collapsed-group cross sections

A set of group-averaged neutron and gamma-ray cross sections for practical shielding analysis shall be obtained by the collapse of a fine-group set to a smaller number of groups. The fine-group set shall have been prepared in accordance with 5.4.2, 5.4.3, and 5.4.4. Collapsing from the fine groups to the coarse groups shall be performed with a fine-group weighting function appropriate to the shield configuration to which the collapsed-group set is to be applied. The number of the collapsed energy groups and the group boundaries should represent a balance between the objectives of avoiding impractical computing requirements and yielding acceptable accuracy in the shielding analysis. Examples of fine-to-coarse group averaging techniques are scalar flux weighting, consistent $P_N$[9], and bi-linear adjoint weighting[10].

## 5.5 Upscattering cross sections

The thermal energy range (e.g. energies less than 5 eV) of a fine-group cross-section library should include upscattering cross sections. Upscattering cross sections provide more accurate thermal fluence rate calculations compared to cross-section sets that do not include upscattering. The inclusion of upscattering cross sections will also improve the accuracy of photon production from thermal neutrons in a coupled neutron and gamma-ray calculation.



In collapsed-group cross section sets, upscattering cross sections should be retained if thermal neutrons contribute to the results of the analysis. In order to decrease the computational time in treating upscattering cross sections, an upscattering truncation method may be used. For upscattering truncation, the ANISN method should be used, which preserves the cross-section balance in energy groups[11]. The accuracy of a calculation using the ANISN method of upcattering truncation should be verified by comparing with a calculation using a cross section set that contains upscattering.

## 5.6 Legendre order of scattering

The order of scattering cross sections for both neutrons and gamma-rays should be available as $P_7$ or higher order for nuclides with atomic numbers 1 through 29 and $P_5$ for the remainder of the nuclides. A minimum of a $P_3$ Legendre expansion of the scattering cross section shall be used in particle transport calculations[12]. The order of Legendre polynomials also depends on the geometry of the problem.

# 6 Verification and validation of cross sections

## 6.1 Verification of cross-section sets

The choice of energy group structure, the averaging technique employed, and the choice of weighting function should be verified by the calculation of appropriate numerical benchmarks. Differences should be considered acceptable based on the energy group structure and weighting functions used in preparation of the fine-group and coarse-group cross-section set. The analyses performed for numerical benchmarking shall be documented in sufficient detail to allow an experienced shielding analyst to duplicate the results. The results of collapsed-group calculations shall be compared with fine-group results to determine the adequacy of the coarse-group structure and weighting function used in the collapse. If the differences between the fine-group results and the collapsed-group results are considered to be unacceptable, the coarse-group energy structure shall be refined until the differences are acceptable.

### 6.2 Validation of cross-section sets

The fine-group and coarse-group cross sections shall be used in calculations of appropriate experimental benchmarks. The experimental benchmarks shall conform to formats approved by national or international bodies such as CSEWG, OECD/NEA/Nuclear Data Bank, or the Sigma Advisory Committee in Atomic Energy Society of Japan. The agreement between the experimental and the calculated metrics shall be documented.

# Annex A
(informative)

# Information on group-averaged neutron and gamma-ray cross section verification, validation, libraries, and generation

## A.1 Example of numerical benchmark guidelines

ORNL-RSIC-25[13] provides guidelines for a numerical benchmark so that it is reproducible and contains sufficient documentation.

## A.2 Examples of experimental benchmarks

Examples of appropriate experimental benchmarks are the ORNL Pool Critical Assembly benchmark[14][15], H. B. Robinson Unit 2 in-vessel and ex-vessel neutron dosimetry benchmark[16], and Venus benchmarks[17]. Experience demonstrates that ±20% agreement between measured and calculated reaction rates can be achieved for reactor pressure vessel surveillance capsule dosimetry.



## A.3 Examples of group-averaged cross-section libraries

Examples of group-averaged cross-section libraries that have been developed are as follows:



a) VITAMIN-B7: A fine-group (coupled 199-neutron- and 42-gamma-ray-group) cross-section library based on ENDF/B-VII.0 for radiation transport applications; generated at ORNL; distributed by RSICC as DLC-245 and NEA as DLC-0245/02[18];

b) BUGLE-B7: A coarse-group (coupled 47-neutron- and 20-gamma-ray-group) cross-section library based on ENDF/B-VII.0 for LWR shielding and pressure vessel dosimetry applications; data were collapsed from VITAMIN-B7; generated at ORNL; distributed by RSICC as DLC-245 and NEA as DLC-0245/02[18];

c) ENDF/B-VI.8–based and ENDF/B-VII.0–based coupled 200-neutron and 47-gamma-ray-group cross-section libraries: Cross-section data sets created for radiation transport applications; nuclides were processed using the AMPX code system; data sets were generated by ORNL[19];

d) VITAMIN-B6 (RSICC) / ZZ-VITAMIN-B6 (NEA): A fine-group (coupled 199-neutron- and 42-gamma-ray-group) cross-section library based on ENDF/B-VI.3 for radiation transport applications; nuclides were processed with NJOY 94 or NJOY91.94m and the AMPX code system; distributed by RSICC as DLC-184 and NEA as DLC-0184/01[20];

e) BUGLE-96 (RSICC) / ZZ-BUGLE-96 (NEA): A coarse-group (coupled 47-neutron- and 20-gamma-ray-group) cross-section library based on ENDF/B-VI.3 for LWR and pressure vessel dosimetry applications; data were collapsed from VITAMIN-B6; distributed by RSICC as DLC-185 and NEA as DLC-0185/01[20];

f) ZZ-VITJEFF32.BOLIB (NEA): A coupled 199-neutron- and 42-gamma-ray-group pseudo-problem-independent cross-section library in AMPX format for nuclear fission applications based on JEFF-3.2, processed through the NJOY2012.53 nuclear data processing system and the ENEA-Bologna 2007 revision of the ORNL SCAMPI nuclear data processing system in the VITAMIN-B6 energy group structure using the same methodology and calculation procedures; distributed by NEA as NEA-1891/01;

 