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From Basic Nuclear Data to Applications

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FROM BASIC NUCLEAR DATA TO APPLICATIONS

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Reaction rates of neutron interactions with matter are parametrised by the neutron flux, which describes the neutron population and the nuclear data, which define the properties of the medium. Reaction rates determine other parameters of interest. To determine these parameters, a long chain of calculations needs to be performed. It requires on input a set of complex nuclear data and the accuracy of the calculations depends on them. To make calculations feasible, techniques have been developed to reduce the amount of information in several steps. In the lecture notes the data reduction techniques are briefly described, with emphasis on the classifications of the data resulting from individual steps.

1 Introduction

Reaction rates of neutron interactions with matter are the key parameters of interest in nuclear applications such as reactor core design calculations, shielding problems, etc. They are parametrised by the neutron flux, which describes the neutron population and the nuclear data, which define the properties of the medium. Reaction rates determine other parameters of interest like the neutron fluence at a point in shielding problems, the multiplication factor and the power distribution in nuclear reactors, etc. Consider for illustration a nuclear core design calculation. The neutron multiplication factor and the neutron flux distribution under various operating conditions need to be calculated repeatedly. A long chain of calculations needs to be performed, with input parameters governed by the geometry, the material composition and the *neutron nuclear data* (i.e. the cross sections, their energy dependence, energy spectra and angular distributions of secondary particles etc. for all nuclides of each material that constitutes the assembly). For shielding calculations the same data are used except that, in addition, photon interaction and coupled neutron-photon interaction data are sometimes required.

The nuclear data for individual isotopes at particular energies of incident particles can be measured experimentally, or else they can be predicted by nuclear model calculations. Usually an experiment provides a single parameter value (i.e.: the cross section at a particular energy) or at most, the cross section behaviour over a rather limited energy range. For each reaction rate the cross sections are strongly energy dependent and very difficult to model or

predict analytically. Also in a realistic situation one needs to consider a mixture of a number of materials. Therefore the necessary amount of information increases enormously. This immediately raises the following points:

- in order to obtain sufficient data, a very large number of experiments must be performed. International collaboration and data exchange are essential,
- since the amount of data is large, it must be presented in computer-readable form,
- when no experimental data in a certain energy range exist, one must resort to theoretical model calculations and the systematics (if any) in the cross-section behaviour of nuclei with similar characteristics (i.e. similar parity in the number of neutrons and protons, etc.),
- when more than one measurement exist for a quantity, each measured with a certain error, an evaluation is necessary to obtain the "best estimate" value,
- routinely used computer codes for solving reactor core and shielding problems can not cope with energy dependence of parameters in full detail, therefore data reduction techniques are necessary.

In view of the above, the following tasks associated with the nuclear data can be identified:

1. basic nuclear data production,
2. nuclear data evaluation,
3. evaluated nuclear data processing, verification, validation and benchmarking,
4. nuclear data applications.

The flow of information is displayed schematically in Figure 1.

These tasks will be discussed in more detail, so that the link between the data produced by an experimentalist and the results of reactor core and shielding calculations can be further elucidated.

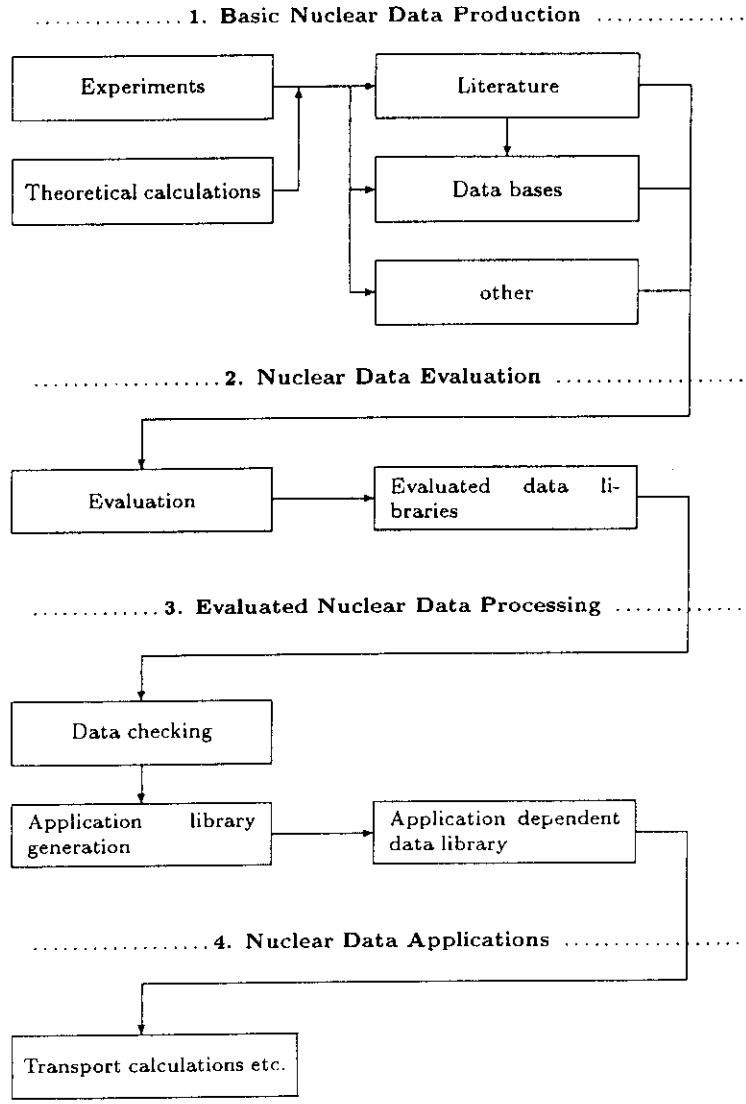

Figure 1. Activities associated with Nuclear Data

2 Activities Associated with Nuclear Data

2.1 Basic nuclear data production

Experimental measurements: The required effort on experimental measurements is enormous. By international collaboration (through regular scientific meetings between the data producers and the users, and through national, regional and international nuclear data committees) the task of data production is fairly well coordinated. The users assess the needs for new or more accurate data, which are published periodically by the IAEA in the World REquest list for Nuclear DAta WRENDA [1]. In this way the laboratories, which can perform experimental measurements have guidelines, which can help them to plan their activities, so as to make their results directly useful to the data users. Current and planned activities of some laboratories are compiled by the NEA Data Bank [2].

Nuclear model calculations: In recent years a considerable improvement has been achieved in the capabilities of theoretical models [3] to predict the cross-sections. However, experimental data are to be preferred because the nuclear models are still not sufficiently accurate, but there are cases where experimental data are not available (for example, for isotopes which are difficult to obtain in sufficient purity, rapidly decaying isotopes and data in energy ranges which make experiments more difficult and less reliable). In such cases nuclear model calculations are used to interpolate or extrapolate experimental data, to resolve discrepancies between different experimental data and to provide some data (although with greater uncertainty) for materials, for which the experimental data are lacking altogether.

Data compilation: As produced, the results of experimental measurements and nuclear model calculations are scattered in various publications and hence inconvenient to access by a user. There is a need for a data base which would include all available experimental values, measured in all the laboratories in the world. Nuclear data centres, which regularly compile and update such a data base already exist:

NNDC	for USA and Canada (at Brookhaven National Laboratory, USA),
CJD	for Russia and former USSR countries (at Obninsk, Russia),
NEA DB	for West European countries and Japan (at Issy-Les-Moulineaux, France),
IAEA-NDS	for all other countries (in Vienna, Austria).

Each of these centres compiles the nuclear data published in its area and then the centres exchange the data on a regular basis.

Data base formats: Due to the large amount of information, the data bases must be managed in a computerized way. Also, the formats for data storage must be well defined to allow automatic data maintenance and data retrieval. For this purpose, special formats exist which can accommodate all relevant information about experimental measurements and analytical model calculations. The CINDA file is a compilation of the references related to neutron nuclear data and is kept up-to-date by each of the four data centres. It is published annually in printed form by the IAEA [4]. It is also available on the Internet, following the path to the Nuclear Data Information System on the IAEA's Nuclear Data Centre homepage at "`http://www-nds.iaea.org/`". The EXFOR file [5] contains the actual experimental results and other important information to allow an evaluation of the experimental data. This information is also available on the same Internet address.

The four neutron data centres maintain identical master data files. The CINDA file serves as an index for the EXFOR file, so the two data bases complement each other.

2.2 Nuclear data evaluation

All available data must be critically reviewed because some measurements may be unreliable due to obsolete methods used or due to systematic errors. It is the work of the evaluator to gather all available experimental information for a particular nuclide, make a critical review and decide on the "best estimate" value of the parameters. This is often done using sophisticated numerical procedures. Especially in recent years an evaluator is not a single person but a group of people, possibly from different laboratories and even different countries, each being a specialist in some particular data type and energy range. Partial evaluations obtained in such a way are then checked for consistency and combined to form a complete set. Compared to other stages of data processing, the evaluator's work requires a particularly broad knowledge and a vast amount of experience ranging from experimental techniques to application aspects of nuclear data.

Evaluated data files are a rather large and highly ordered data set, grouped by materials and by data types. They must be computer-readable and in the past a number of formats evolved. One of the oldest is the British UKNDL format [7]. In Germany the KEDAK format [8] was designed. In the USA the ENDF series of formats were developed [9,10,11], version ENDF-6 be-

ing the most recent. Apart from the USA, it has now been adopted for the evaluated data files in the OECD countries, in Russia, in China and in Japan. The UKNDL and KEDAK formats are being phased out, since Britain as well as Germany participate in the joint effort of the OECD countries to produce a general purpose evaluated data library, for which the ENDF-6 format has been adopted. Some of the more recent libraries, their formats and the country of origin are presented in table 1.

Table 1. Some of the more recent evaluated data libraries, their formats and country of origin

Country	Data file	format	Comments
Russia	BROND-2.2	ENDF-6	Available.[14]
China	CENDL-2	ENDF-5	Available.[15]
U S A	ENDF/B-IV	ENDF-4	(Old but useful for reference), available[12]
	ENDF/B-V	ENDF-5	Restrictions lifted recently.[13]
	ENDF/B-VI	ENDF-6	Including Rev.6, 1999, available.[16]
	ENDL-84	ENDF-5	Livermore laboratory evaluations, available.[21]
OECD/	JEF-2.2	ENDF-6	Available.[17]
NEA	EFF-2.4	ENDF-6	European fusion file.[18]
	JEFF-3	ENDF-6	European file, in preparation.[19]
Japan	JENDL-3.2	ENDF-6	Available.[20]

The ENDF format (particularly ENDF-6) has received the most widespread acceptance. It has been adopted for the Japanese JENDL data library, the Chinese CENDL library, the Russian BROND library, the joint European JEF file and also by the IAEA as the format for the exchange of nuclear data. The deficiencies of the older versions of the format have been discussed internationally [23]. As a result, version ENDF-6 of the format has been designed. Practically, it became the standard format for evaluated data.

The above mentioned evaluated data libraries and several others are available from the IAEA [6].

2.3 Evaluated nuclear data processing

Basis for data reduction: The detailed information contained in the evaluated data files exceeds the capacity of the calculational tools (i.e. computer programs) for practical neutron transport applications. Some statistical Monte-Carlo programs can in principle use the detailed information contained

in the evaluated data files (reformatted for compatibility and better computational efficiency) but such codes require very fast modern machines and are generally very expensive to run. They are mainly used for verification of results, for very difficult geometries and for setting up benchmarks.

Deterministic methods solve the differential or the integral forms of the transport or the diffusion equation using one of the standard methods. They usually solve the one-neutron-speed form of the equation in the spatial domain (i.e. a one group equation) but the calculations can be done for several groups - one at a time. The equations are coupled through the neutron transfer cross sections (scattering matrices) and the fission source. This means that the entire energy interval is divided into a number of subintervals - groups. Within a group, each energy dependent parameter takes some average value. The accuracy of the calculation depends on the number of groups and the group averaging method. Usually a compromise must be made between the complexity in geometry and the number of groups. The accuracy of the calculations can be retained even when the entire energy interval is divided into only a few groups, provided that a proper cross section averaging method is implemented.

Data verification and validation: Automatic data processing is not possible unless the file is free of formal formatting errors. Next, the data in a file must be self-consistent. Before an evaluated data library can be used for practical applications it must undergo thorough checking to avoid processing code failure due to format rule violation, to ensure that the data on the file correspond to what the evaluator intended them to be and that they are consistent with integral experimental measurements, when they are available. The following stages of data testing can be identified:

- removal of data formatting errors,
- removal of data inconsistency errors,
- visual inspection of the graphical representation of the data,
- comparison of the data on the file with the measured values (for example, from the EXFOR database),
- integral (spectrum averaged) cross section comparison with measured values,
- comparison with simple, *"clean"* experimental benchmarks.

Extensive programmes have been undertaken to validate the ENDF/B-IV and ENDF/B-V libraries. Some reports on the testing of JENDL-3, JEF-2 and ENDF/B-VI have also been released, but the user must be aware of the diversity of data application. Suitable benchmark experiments are not always available and exhaustive data testing can not be performed for all areas of interest. Compilations of benchmark experiments are available for some cases. A good example are the *CSEWG Benchmark Specifications*[24], but these are rather old and in some cases doubts are raised whether the benchmark model description is adequate to reproduce the quoted measured values. New compilations for some applications exist, like the *Criticality Safety Benchmarks* [25], *SINBAD Shielding Benchmarks* [27] and a compilation related to the fusion activity [26]. Internet is again a useful and comprehensive source of information on the bechmarking activity, such as the appropriate sections in the RSICC home page at "`http://www-rsicc.ornl.gov/rsic.html`" or the FENDL benchmarks, to which links can be found from the above mentioned IAEA's Nuclear Data Centre homepage. Some of the codes which are useful for evaluated nuclear data checking and for multigroup constants library generation are mentioned briefly in Section 5.3.

Multigroup constants library generation: In updating or preparing a new multigroup constants library the following pre-requisites are important:

- to use a verified and validated evaluated data library,
- to use validated processing codes.

The structure of a multigroup constants library is governed by the computer code which uses it. The procedures have to be considered on a case-by-case basis, such as suggested in the example in Section 5.

2.4 Nuclear data applications

In nuclear data applications one normally starts from a selected multigroup constants library. Further data reduction is often performed by group condensation and spatial homogenization (see Section 4) to produce few-group parameters. The processed nuclear data are used in a large variety of applications. Some examples are listed below:

- small experimental thermal reactors,
- thermal power reactors,
- fast reactors,

- nuclear fusion applications,
- shielding problems,
- radiotherapy,
- radioactive isotope production, inventory estimation, transport etc.

3 Nuclear Data Classification

The terms "nuclear data" or "cross section data" are applied to a wide range of specific data types appearing at different stages of data processing and reactor calculations (described in Section 2). To avoid ambiguity it is useful to have precise definitions of these data types and the relation between them.

3.1 Basic nuclear data

Data resulting directly from experimental measurements or nuclear model calculations are implied. They include differential cross sections in energy and angle for neutrons and photons, resonance parameters, integral cross sections measured in various spectra and other data types. They were already discussed in Section 2.1.

3.2 Evaluated nuclear data libraries

Evaluated nuclear data are constructed by an evaluation process (see Section 2.2) from the data base containing the basic nuclear data. Evaluated nuclear data libraries consist of evaluated data files for individual isotopes, elements and/or compounds (at thermal energies, evaluations are made for the scattering properties of compounds where molecular and crystal lattice binding effects are significant). The data base of the basic nuclear data may contain several data points at a particular energy or it may contain gaps where no data are given (subject to the availability of experimental data or nuclear model calculations). On the contrary, in an evaluated data file a single parameter value must be prescribed at each point, with a precisely defined interpolation law in between points. The data must cover the full range (usually $10^{-5}\,eV$ to $20\,MeV$). Each parameter must be evaluated and checked for consistency with other parameters and with integral measurements. The data are then entered on a file in a strictly defined format. Examples of evaluated data libraries were discussed in Section 2.2.

The energy dependence of cross sections is rather complex (some reactions may require more than 100 000 data points for accurate representation).

Except for some Monte-Carlo programs which can read evaluated data in pointwise cross section representation directly, a data reduction technique (i.e. group averaging) is normally applied.

3.3 Problem-Independent Group Constants Libraries

Problem-Independent Group Constants Libraries are derived from the evaluated data files. The parameters are averaged on a fine energy group structure, typically between 2000 and 200 groups (for example the SAND II extended energy grid with 640 groups between 10^{-4} and $20 \times 10^{6} eV$). A flat weighting function is normally sufficient. The group constants definitions are given in Section 4. The so constructed library is used as a source for group constants condensation into a coarser group structure (i.e. into multigroup constants) using some rough approximation to the problem dependent neutron averaging spectrum as the weighting function. At this stage the energy mesh is sufficiently fine so that local variations in the neutron spectrum can be disregarded.

3.4 Multigroup Constants Libraries

Multigroup constants libraries can be derived from the problem-independent group constants libraries by group condensation (see Section 4.4) or else they can be calculated from the evaluated data libraries directly by using an appropriate weighting function. The multigroup constants are broadly problem oriented - such as: thermal reactors, fast reactors, fusion problems or shielding calculations. The criterion which defines a group of problems for which a data set is valid is the similarity in the *smooth* neutron spectrum (i.e. spectrum in which detailed structure is neglected), Such a spectrum is used for weighting in the cross section averaging process.

Consider for example an idealized infinite homogeneous reactor with hydrogenous moderator and a $1/v$ absorber at thermal energies (i.e. the absorption cross section is inversely proportional to the neutron velocity). The neutrons are born with the fission spectrum distribution. Assuming an idealized hydrogen-like medium with no absorption and a constant scattering cross section, the slowing down neutrons have a $1/E$ distribution. With weak $1/v$ absorption at thermal energies, the resulting neutron spectrum has approximately a Maxwellian distribution. A spectrum having a fission neutron spectrum shape in the fast energy range, a $1/E$ shape in the intermediate range and a Maxwellian shape in the thermal range is representative of thermal reactor problems over limited energy intervals, and is a candidate for the weighting function in the multigroup library preparation. Spatial variations

of the neutron spectrum are not considered. For a desired accuracy in the calculations, the deviation of the local *true* neutron spectrum from the assumed one determines the required energy discretisation which ranges typically from about 400 to 26 groups. Finer discretisation is required at energies where higher rates of reactions of interest are expected. Furthermore, inside each group, the smooth spectrum exhibits the general trend but not the detailed structure. Allowance must be made for a detailed treatment, especially of the resonance self-shielding and Doppler broadening (usually in the form of separate tables). Interference between resonances of different nuclide constituents of a mixture is frequently neglected or treated very crudely.

To illustrate the cross section representation in group averaged form under different group structures, ^{240}Pu from the ENDF/B-VI evaluated data library [11] has been processed. The radiative capture cross section represented in four different group structures is shown in Figure 2.

For shielding problems where neutron spectra vary significantly with material composition it is not normally possible to obtain general multigroup libraries with fewer than about 50 groups (most of them being in the fast and intermediate energy region) whereas for reactor core calculations one can sometimes do with as few as 26 groups, with emphasis in the thermal energy region.

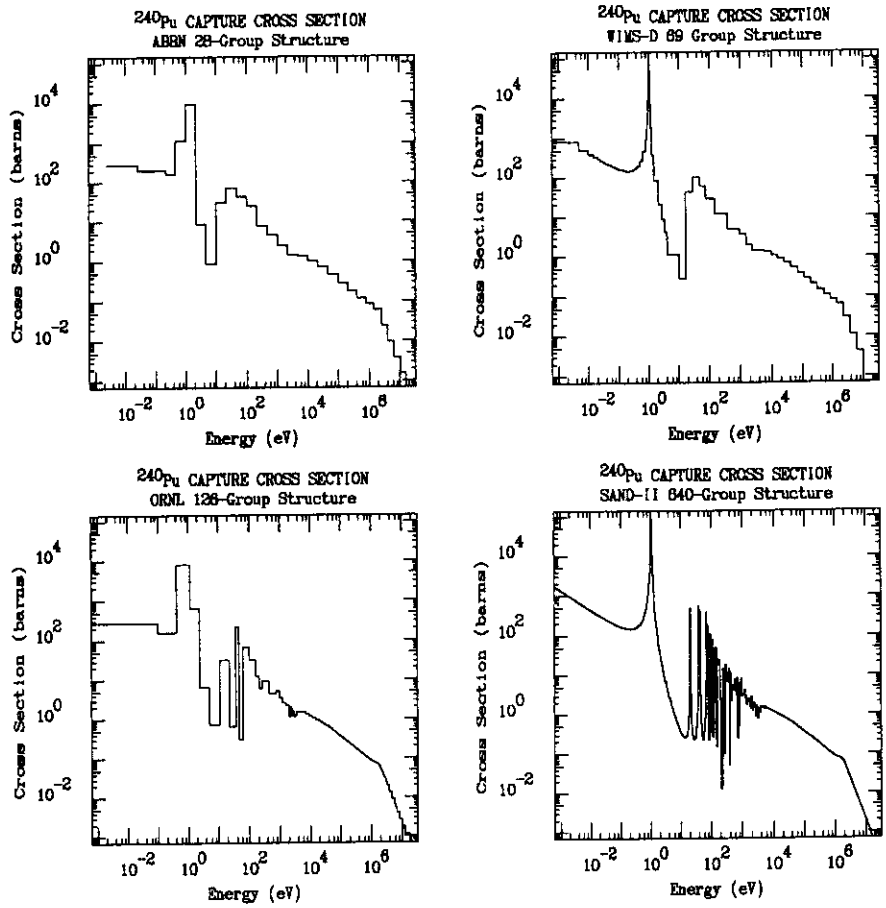

Figure 2. ^{240}Pu radiative capture cross section from the ENDF/B-VI evaluated data library represented in various group structures.

3.5 Problem Dependent Few-Group Constants

Problem Dependent Few-Group Constants are the result of the final stage of the data reduction process, starting from the multigroup data and using the neutron (and gamma) transport methods. The number of groups varies from 1 to 18 and spatial homogenization is also performed. Equivalent diffusion equation parameters (macroscopic cross sections and diffusion constants) can be deduced. Such data are highly problem oriented. They are calculated on a case-by-case basis and are normally considered as an application of nuclear data, according to the classification in Section 2.

Usually, multigroup data sets prove to be too large for the deterministic methods of solving the transport equation, so it is a common practice to reduce the number of groups in two steps. Starting from the multigroup constants library, a zero dimensional (or approximate one-dimensional) calculation is performed, with appropriate material composition in individual homogeneous zones, to get an estimate of the local neutron spectra. These spectra are used to collapse the group constants (specific for each zone) down to typically 32 or 18 groups. With such a group structure it is feasible to perform full scale transport calculations, to obtain few-group constants (usually from 1 to 12 groups) by group collapsing and spatial homogenization (for example effective diffusion equation parameters for a pin cell or a fuel assembly at a specific power, temperature and burnup). Data obtained from this step form the input to 2D and 3D neutron flux distribution solution algorithms used in reactor core design and fuel management calculations.

4 Definition of Group Averaged Constants

4.1 Single valued energy dependent parameters

Group averaged values of simple energy dependent parameters such as the cross sections are defined by the following equation:

$$\langle \sigma_x \rangle_g = \frac{\int_{E_{g+1}}^{E_g} \sigma_x(E)\, w(E)\, dE}{\int_{E_{g+1}}^{E_g} w(E)\, dE} \tag{1}$$

where: σ_x is the parameter to be averaged,
w is the weighting function,
E_g are the energy group boundaries,
g group index

The weighting function can be chosen arbitrarily, but from the aspect of the reaction rate conservation when going from fine to broader group structures it can easily be seen, that the weighting function for averaging the cross sections must be the incident particle spectrum (i.e. the neutron or the gamma spectrum). Different weighting functions may be applied to other parameters, based on physical considerations.

For the construction of problem-independent group constants on a fine energy mesh the weighting function is unimportant and can be assumed constant. In the case of the multigroup data it is chosen as the smooth weighting spectrum which approximately follows the behaviour of the real spectrum. For thermal reactor applications it may consist of the Maxwellian form in the thermal energy range, the $1/E$ form in the intermediate range and the fission spectrum in the fast range. Other applications (such as fusion or shielding problems) require a different weighting spectrum. Furthermore, each class of problems requires energy mesh refinement in different energy ranges, therefore it is not be possible to construct a general purpose multigroup library which is reliable in all areas of application and have a reasonably small number of groups.

4.2 Differential energy-angle dependent parameters

The differential energy and angle scattering cross sections (the elastic and the inelastic cross section in the fast and the thermal energy range) can be group-averaged into the scattering matrix. The angular dependence can be taken into account through Legendre polynomial expansion. The elements of the ℓ^{th} Legendre moment of the scattering matrix are defined by the following equation:

$$\langle \sigma_{s,l}^{g \to h} \rangle_g = \frac{\int_{-1}^{1} d\mu \int_{E_{g+1}}^{E_g} dE\, w(E) \int_{E_{h+1}}^{E_h} dE'\, \sigma_s(E \to E', \mu)\, P_l(\mu)}{\int_{E_{g+1}}^{E_g} w(E)\, dE} \qquad (2)$$

where: μ is the cosine of the scattering angle in laboratory system,

$P_l(\mu)$ Legendre polynomial of degree l

$\sigma_s(E \to E', \mu)$ cross section for scattering from energy E into energy E' at an angle μ.

For elastic scattering and for inelastic scattering into discrete levels the angle μ and and the secondary particle energy E' are not independent. They are

related through the laws of conservation of momentum and energy and defined by the mass ratio of the target nucleus to that of the secondary particle (for elastic scattering) and the reaction Q-value (for the inelastic scattering into discrete energy levels). This considerably simplifies the technical process of producing scattering matrices. For inelastic scattering into the continuum and for inelastic scattering at thermal energies additional data need to be processed (secondary neutron distributions and the scattering law data respectively). Alternatively, some approximations can be introduced such as the "evaporation spectrum" to represent the secondary neutron distribution for inelastic scattering into the continuum and the "free gas" approximation for inelastic scattering at thermal energies.

4.3 The Resonance region

The resonance integral is commonly defined by an equation similar to Equation (1).

$$\text{R.I.} = \int_{E_{g+1}}^{E_g} \sigma(E)\, w^*(E)\, dE \tag{3}$$

At infinite dilution (i.e. at small absorber concentrations which offer no perturbation to the neutron spectrum), the weighting function w^* is the usual smooth neutron weighting spectrum. In well moderated weakly absorbing systems it has a $1/E$ form.

When a strong resonance absorber is present in an *infinite medium* at a high concentration, a large fraction of the neutrons is absorbed and produces a "hole" in the neutron spectrum at the resonance energy, thus reducing the reaction rate. When the absorber of *finite dimensions* is surrounded by a moderator, the neutrons from the moderator tend to fill this hole. This is approximately analogous to the dilution of the absorber nuclei. However, this effect can not propagate deeply into the absorber because the nuclei in the centre are shielded by the absorber nuclei on the surface, which remove the neutrons entering the absorbing medium at the resonance energy. The degree of the *effective* absorber dilution therefore depends on the material composition and on the geometry.

Average cross sections of strong absorbers can be calculated by rigorously solving the slowing down equation for mixtures of the absorber with an idealized hydrogenous moderator of constant scattering cross section and different concentrations. In this way the self-shielded absorber cross sections can be parameterized as a function of the the Bondarenko background cross section σ_0, which is the macroscopic "moderator" cross section per absorber atom

(note that it is expressed in *barns* units).

A rigorous solution of the neutron slowing down equation is rather tedious. Relatively simple approximations are available which produce satisfactory results, such as the Intermediate Resonance approximation (IR), introduced by Goldstein and Cohen [31]. A parameter λ is defined so that the cross section weighting function is:

$$w^*(E) = \frac{\sigma_0 + \lambda\sigma_p(E)}{\sigma_0 + \lambda\sigma_a(E) + \sigma_s(E)}\, w(E) \tag{4}$$

where: σ_0 is the Bondarenko background cross section,

σ_a is the absorption cross section,

σ_s is the scattering cross section,

σ_p is the potential scattering cross section,

λ is the Goldstein - Cohen parameter. It is a "measure" of the resonance width.

When $\lambda = 1$ the well known Narrow Resonance (NR) approximation is obtained and when $\lambda = 0$ the equation reduces to the Wide Resonance (WR) approximation. Goldstein and Cohen used a variational technique to determine λ but Forti proposed a very simple approximation [32], which relates λ to the resonance width:

$$\lambda = \begin{cases} 1 - \frac{\Gamma_{p,r}}{2\alpha E_r} & ; \alpha > \frac{\Gamma_{p,r}}{E_r} \\ \frac{\alpha E_r}{2\Gamma_{p,r}} & ; \alpha \leq \frac{\Gamma_{p,r}}{E_r} \end{cases} \tag{5}$$

where: E_r is the energy of resonance r,

$\alpha = 1 - ((A-1)/(A+1))$

A is the ratio of the mass of the target nucleus to that of the neutron,

$\Gamma_{p,r}$ is the "practical" width [33] of resonance r which measures the energy range over which the resonance contribution exceeds the non-resonance part of the cross section,expressed approximately by

$$\Gamma_{p,r} = \Gamma_{t,r}\sqrt{\frac{\Sigma_0}{\Sigma_p}}$$

$\Gamma_{t,r}$ is the total width of the resonance,

Σ_0 is the macroscopic cross section at the resonance peak,

Σ_p is the macroscopic potential scattering cross section of the absorber and the admixed moderator.

Alternative approaches to the definition of the λ parameter are based on empirical derivations, based on matching the slowing down properties for an absorber diluted in an arbitrary medium, compared to the same dilution in an idealised hydrogenous medium.

4.4 Group condensation

As mentioned in Section 3 the number of groups over which the cross sections are defined is often reduced by group condensation (or group collapsing). Assume that the data are given on a fine energy grid. We require a weighting function which is averaged over the same energy grid. A number of fine groups can be collapsed into one coarse group by a procedure similar to the one defined by equations (1) to (3), except that the integral sign is replaced by a summation over the fine groups g which constitute the coarse group h:

$$\langle \sigma_x \rangle_h = \frac{\sum_g \langle \sigma_x \rangle_g \langle w \rangle_g}{\sum_g \langle w \rangle_g} \tag{6}$$

and similarly for the scattering matrices and the resonance integrals.

4.5 Spatial homogenization

Spatial homogenization can be performed using the same criterion of reaction rate conservation, using the spatial neutron flux distribution for weighting. Consider an energy group g and a homogenization volume V where $\boldsymbol{r}$ is the position vector inside V. For clarity the group index is omitted. The average cross section is given by:

$$\langle \sigma_x \rangle = \frac{\int_V \sigma_x(\boldsymbol{r})\, w(\boldsymbol{r})\, dV}{\int_V w(\boldsymbol{r})\, dV} \tag{7}$$

The scattering matrices and the resonance integrals can be averaged in a similar way.

Such simple flux and volume weighting procedure is valid when there is no leakage from the region which is homogenized. In general, averaged cross sections homogenized by the simple flux and volume weighting satisfy the

condition of average reaction rate conservation, but do not reproduce the partial neutron currents on the region boundaries. Recently, new homogenization methods have been developed [34] which to a large extent remove this deficiency and help to improve the results of global calculations.

5 A Multigroup Library Update - An Example

5.1 Multigroup library format

Consider the WIMS multigroup constants library [35] because the WIMS code [36] is extensively used in various laboratories throughout the world and for different reactor types.

First of all one must get familiar with the format of the library. Once this is done, the definitions of individual quantities must be carefully reviewed. The library documentation is not always adequate because it is scattered in several publications and internal notes. Below, a few hints are given which might be useful:

- The fission spectrum contains some adjustments which are not supported by experimental measurements of the spectra but they improve the agreement between the calculations and the integral measurements on a variety of simple "benchmark" core configurations. The same fission spectrum is used for all fissile isotopes.

- Care must be taken with regard to the fission product yields per fission event, since some precursors are lumped with the fission yield value for a particular fission product.

- While the definition of the potential cross-section and the slowing down power per lethargy width is fairly straightforward, the definition of the transport cross-section is quite tricky. Transport cross section is defined in the usual way at thermal energies as

$$\langle \sigma_{tr} \rangle_g \;=\; \langle \sigma_a \rangle_g + \langle \sigma_{s0} \rangle_g - \langle \sigma_{s1} \rangle_g \tag{8}$$

where: $\langle \sigma_{tr} \rangle_g$ is the transport cross section,

$\langle \sigma_a \rangle_g$ is the absorption cross section,

$\langle \sigma_{s0} \rangle_g$ is the zero-th moment of the scattering cross section $= \sum_h \langle \sigma_{s0} \rangle_{g \to h}$

$\langle \sigma_{s1} \rangle_g$ is the first moment of the scattering cross section
$= \sum_h \langle \sigma_{s1} \rangle_{g \to h}$

$\langle \sigma_{sl} \rangle_{g \to h}$ is the l^{th} moment of the cross section for scattering from group g into group h.

In the fast and the resonance region the equations incorporated into WIMS require a different definition of the transport cross section. The 1^{st} moments of the scattering cross section is defined by:

$$\langle \sigma_{s1} \rangle_g = \frac{\sum_h \langle \sigma_{s1} \rangle_{h \to g} \langle J \rangle_h}{\sum_h \langle J \rangle_h} \tag{9}$$

and $\langle J \rangle_h$ is the group average neutron current spectrum. When no better approximation is available, the $1/E$ form can be used.

The difference between the two definitions of the transport cross section is small for heavier nuclei, but for moderators the incorrect definition of the transport cross section can lead to significant errors.

- The absorption cross section is the sum of the fission cross section and all other cross sections for reactions which produce no neutrons. In the fast energy range a correction is made to approximately conserve the neutron balance due to reactions which produce multiple neutrons.

- The parameter χ is only used in some old versions of the WIMS program.

- The Goldstein-Cohen parameter defined in Section 4.3 must be included in the library. It accounts for the resonance widths which are neither wide nor narrow and it partly compensates for the moderators which are not ideally hydrogen-like.

- Standard definition applies to fission cross section Σ_f and the fission neutron yield $\nu\Sigma_f$.

- The scattering matrices are defined in the usual way except for one modification: for nuclides which do not have a P_1 scattering matrix tabulated, the diagonal elements of the P_0 scattering matrix are modified so that the row-sum of the matrix (i.e. the $\langle \sigma_{s0} \rangle$ cross section) and the absorption cross section reproduce the transport cross section and not the total cross section. Note that the information on the true total cross section is thus lost. Also, the P_1 scattering matrix is defined without the $(2l + 1)$ term in the numerator, which is required in some codes.

- The resonance integral tables are as defined in Section 4.3 but they are normalized with the lethargy width. They must not be confused with the self-shielded cross section since this would cause errors especially in the lower energy groups.

5.2 Library update strategy

In performing the update, two approaches are possible:

- to create the library from scratch using new evaluated data,
- to selectively replace individual material data or to add the data which are missing from the library.

For the first option it is recommended to use a well tested evaluated data library so that the results can be compared against the benchmark test cases for the library. The use of other data may give unsatisfactory results since the existing multigroup libraries are usually tested and adjusted to give good agreement with integral benchmark experiments.

The second option is attractive because the test results with the original library can serve as reference and the effects of the changes in the library can be tested individually. The applicability of the library can be extended by adding materials which were not included originally, without seriously affecting the performance of the library for the test problems on which the library designer adjusted the data.

5.3 The choice of the processing codes

Although in principle the averaging process is very straightforward (see Section 4), the computer programs are usually very complex because they have to consider several data types and many different forms of data representation [11]. For this reason, producing a bug-free program is not trivial as illustrated by the IAEA Cross Section Processing Code Verification Project [28].

In recent years an enormous effort has been placed in removing the processing errors from the multigroup constants. Listed below are a few examples of the computer codes which are generally useful for handling nuclear data:

- ENDF Utility Codes [30] consist of a package of codes which check ENDF formatting rules, data consistency and provide graphical display. The codes are also available on the Internet from the IAEA's Nuclear Data Centre homepage.

- ENDF Pre-Processing Codes [29] are designed as a series of relatively short, simple to use codes which allow step-wise operations on evaluated data such as linearization, resonance reconstruction, group constants preparation, graphical display and others. The codes are very useful for data checking and display but they were not designed for general multigroup library preparation because they lack the processing capabilities of certain data types (such as scattering matrices) and the interfaces to the desired multigroup libraries. The codes are also available on the Internet from the IAEA's Nuclear Data Centre homepage.

- The `NJOY` system was designed for general purpose applications. It can handle practically all the information available in the evaluated data files and has been continually upgraded to conform with the adopted changes in the ENDF formatting rules. It includes interfaces to a number of widely used multigroup constants libraries. Due to its international support it is likely to become the standard nuclear data processing code. Version `NJOY99` has just been announced. The source code must be obtained from a U.S. distribution centre such as the Radiation Safety Information Computational Center (`"http://www-rsicc.ornl.gov/rsic.html"` Internet address), but the updates and additional information is available on the Internet at `"http://t2.lanl.gov/"`.

- Possible alternatives to `NJOY` exist [37], such as `AMPX77`, `GRUCON`, `MC`^{2}`-II`, `GROUCH-G/B`, etc. The `AMPX77` system most nearly covers the functions of `NJOY` but does not include production of Monte Carlo data. In addition there are other codes (such as `FOURACES`, `FEDGROUP-C` etc.). The main problem with these codes is that they were not fully upgraded to handle the format extensions which are provided for in the ENDF-6 format.

5.4 Possible sources of error

When making changes in the multigroup libraries one must be aware of the possible sources of errors:

- **Errors in the basic data** - these are gradually removed as new evaluations, which include new highly accurate measurements, replace the older ones.

- **Errors in the adjusted libraries** - the adjustments may prove to be physically unjustified (i.e. to achieve agreement with integral measurements, the library designer should have adjusted another parameter).

Consequently, partial data improvement in an adjusted library may actually produce worse results.

- **Nuclear data processing errors** can be eliminated to a large extent by using verified codes [28].
- **Inconsistencies in the definitions** of the parameters in the library can result from inadequate library documentation or from misinterpretation of the library description.
- **Rigidity of the multigroup library format** may not allow exact data representation for all cases.

Before an updated library is used for routine applications it requires extensive benchmarking to verify that it produces satisfactory results for the type of problem considered.

6 Summary

The tasks associated with the nuclear data activities involve:

- basic nuclear data production,
- nuclear data evaluation,
- evaluated nuclear data processing,
- nuclear data applications.

The data types which result from the individual data processing steps can be classified as follows:

- basic nuclear data,
- evaluated nuclear data libraries,
- problem independent group constants libraries,
- multigroup constants libraries,
- problem dependent few-group constants.

To update a multigroup constants library for a particular transport code, one must understand well the structure of the library and the precise definitions of the parameters which it contains. In performing the update, two approaches are possible:

- to create the library from scratch using new evaluated data,
- to replace selectively individual material data or to add the data which are missing from the library.

The selection of the source evaluated data library depends on the approach adopted. Thoroughly tested and well documented evaluated data libraries are convenient to use, but in any case, careful data checking at every stage of a multigroup library preparation is essential.

For the convenience of the user, the choice of the evaluated data processing code is often application dependent. Past experience has shown, that the codes which have not been thoroughly checked and compared against the results of other codes (whenever possible) can produce significant processing errors and should be avoided.

Finally, when making changes in the multigroup libraries one must be aware of the possible sources of errors. Good documentation and careful work are the prerequisites for satisfactory results.

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