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Requirements for an Evaluated Nuclear Data File for Accelerator-Based Transmutation

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Abstract

The importance of intermediate-energy nuclear data files as part of a global calculation scheme for accelerator-based transmutation of radioactive waste systems (for instance with an accelerator-driven subcritical reactor) is discussed. A proposal for three intermediate-energy data libraries for incident neutrons and protons is presented:

- a data library from 0 to about 100 MeV (first priority),
- a reference data library from 20 to 1500 MeV,
- an activation/transmutation library from 0 to about 100 MeV.

Furthermore, the proposed ENDF-6 structure of each library is given. The data needs for accelerator-based transmutation are translated in terms of the aforementioned intermediate-energy data libraries. This could be a starting point for an "International Evaluated Nuclear Data File for Transmutation". This library could also be of interest for other applications in science and technology. Finally, some conclusions and recommendations concerning future evaluation work are given.

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Abstract

The importance of intermediate-energy nuclear data files as part of a global calculation scheme for accelerator-based transmutation of radioactive waste systems (for instance with an accelerator-driven subcritical reactor) is discussed. A proposal for three intermediate-energy data libraries for incident neutrons and protons is presented:

- a data library from 0 to about 100 MeV (first priority),
- a reference data library from 20 to 1500 MeV,
- an activation/transmutation library from 0 to about 100 MeV.

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Contents

1 Introduction

The incineration of long-lived radioactive waste components by means of accelerator-based transmutation, e.g. with a hybrid system of accelerator and subcritical reactor has received growing attention during recent years [1-6]. The main idea behind the accelerator method is the possibility to generate a sufficiently intense neutron spectrum (resulting from proton bombardment of a spallation target), yielding an effective transmutation of unwanted isotopes into non-radioactive and relatively short-lived reaction products. This and other arguments [5] (mainly concerning safety problems) have led to an increasing popularity of the hybrid system concept.

In a series of two reports, we aim to give a contribution to the nuclear data part of accelerator-based transmutation research. In the first report [7], see also [8], we have given a review of the most important nuclear data needs for accelerator-based transmutation and have established the present status of the relevant available experimental data, systematics, theories and model codes. One of the conclusions of this report was that there is a sizeable treasure of nuclear data tools and bibliographic databases containing experimental nuclear data in the energy region 20-1500 MeV that can be employed for the construction of evaluated intermediate-energy nuclear data files. It was argued that the extension of the existing low-energy data files to energies of at least 100 MeV is of great importance for accelerator-based transmutation research. An update of the experimental database (EXFOR) and proper benchmarking of model codes (especially for the energy region between 20 and 100 MeV) was recommended. In the present report, we will focus attention on another action that was proposed in [7], namely the specification of requirements for evaluated data files for energies above 20 MeV. Several aspects of these intermediate-energy data files will be brought up for discussion:

- Necessity of intermediate-energy data files for accelerator-based transmutation.
- Relation of intermediate-energy data files with existing processing and transport codes.
- The proposed variety of intermediate-energy data libraries in relation with their specific purposes.
- Establishment of a consensus on the general approach towards an evaluated intermediate-energy data file.
- Choice of procedures within the ENDF-6 format for intermediate-energy data (for neutrons and other incident particles). This includes the possible transformation of the low energy ($<$ 20 MeV) data as categorized in the usual ENDF-6 files to other MF/MT numbers so that a unified form for all incident energies is obtained.

- Specification of the data needs for accelerator-based transmutation in terms of requirements for evaluated files.

As a guide for the definition of the general structure of a intermediate-energy library, we investigated the recently created intermediate-energy data files of Fukahori and Pearlstein [9, 10] and those of the Los Alamos National Laboratory [11, 12]. A description of the structure of these files is given in Appendices A and B, respectively.

Although the present report has been written to address the requirements for intermediate-energy nuclear data for accelerator-based transmutation, there are also important requests for intermediate-energy nuclear data in other fields of science and technology. A few examples are given below.

- In the medical field data are required for the diagnosis and treatment of cancer and other diseases. Among the required data are neutron interaction cross sections for tissue and related materials in the energy range 20-70 MeV and charged-particle induced spallation reaction cross section in the range of 100 MeV. These nuclear data are critically important to the advancements of these fields.

- For fusion materials research there are proposals to construct accelerators to create an intense neutron source at 14 MeV with, however, a tail extending to 50 MeV or more. For such projects like the Japanese ESNIT-project [13], there are important needs for neutron-induced cross section up to 50 MeV.

- For space exploration programs, intermediate-energy data are required to invesigate the radiation effects on astronauts and their equipment, and in order to minimize the uncertaincies concerning the shielding of spaceships.

- In fundamental nuclear science, intermediate-energy data files are required for the testing on reaction theories. A further possible application is the field of astrophysics. The relevant energies extend well beyond 100 MeV.

2 The importance of intermediate-energy data libraries for accelerator-based transmutation

Present day nuclear applications in the intermediate-energy region are almost invariably performed with high-energy transport codes, in particular HETC [5, 6] in its various incarnations. Such codes are based on classical models incorporating an *intra*nuclear cascade followed by evaporation. These high-energy transport codes have an integrated character in the sense that they internally generate the nuclear data which are subsequently supplied to the transport part of the code: the *inter*nuclear cascade. Hence, in the current nuclear data situation, an overall calculation of the transmutation process (from the $\sim$ 1.5 GeV incident proton beam down to the thermalized particles in the shielding) is restricted by the use of evaluated data files and their associated processing and transport codes for neutron-induced reactions below 20 MeV and the (integrated) high-energy transport codes for all other reactions and energies. This situation is unsatisfactory since it has been reported [14, 15] that the high-energy transport codes produce unreliable results for incident particle energies below about 100 MeV (a more systematic evaluation of this statement is currently under investigation in two NEA-Data Bank benchmark exercises [16, 17, 18]). In other words, it is not sufficient to describe the 20 to 100 MeV region with a single (intranuclear cascade + evaporation) model. Instead, a variety of nuclear models is required, whereby each model has its own appropriate purpose (e.g. optical model and coupled-channels calculations for elastic scattering and reactions to discrete states, pre-equilibrium and equilibrium models for reactions to the continuum, an adequate fission model for the intermediate-energy region, etc.). If the diversity of nuclear models needed to create a reliable data set becomes large, the best strategy is to create an evaluated data file for the relevant materials. Evidently, certain sections of the file have to be adjusted with up-to-date nuclear data from experiments, systematics and model codes. In this way, the closest possible connection between transport calculations and the available nuclear data is guaranteed. Therefore, as a complement to the high-energy transport codes, it is strongly recommended to subject the 20-100 MeV region to similar evaluation routines as the 0-20 MeV region.

2.1 Intermediate-energy nuclear reactions

To elucidate the indispensability of nuclear data files that go beyond 20 MeV, it is instructive to give an outline of the bulk properties of the total reaction chain in an incineration system. Above all, it is crucial to distinguish between a thin target (a single nucleon-nucleus interaction) and a thick target (internuclear or transport processes). Furthermore, since secondary neutrons represent the most occurring (and most important) outcomes of the reaction, we will mainly consider these particles in the following.

2.1.1 Thin target

After a non-elastic interaction of the incident hintermediate-energy proton with a nucleus, a large amount of secondary particles will be formed by a process called "spallation", see fig. 1. In this figure, the solid arrows represent the most probable processes in a single intermediate-energy nucleon-nucleus reaction (both for proton- and neutron-inducd reactions).

In the first stage of the reaction, which is an entirely direct process, the incident proton will cause the knock-out of a few intermediate-energy nucleons (this can be envisaged as a classical "billiard-ball" mechanism). Also other hadrons will be formed (such as π- and K-mesons). This intranuclear cascade stage has ended when a residual nucleus with an excitation energy of several tens of MeV to about 100 MeV is left. This excitation energy is still so high that a lot of energy may be accumulated on one or a few nucleons, implying the occurrence of direct-like processes. This time however, the emission of these nucleons can no longer be described by classical, direct mechanisms (because the wavelength of the fast nucleon is no longer much shorter than the size of the nucleus). Instead, the reaction process has now reached the stage where the equilibration of the excited nucleus starts to take place but where it is still possible for a fast nucleon to be emitted after a few collisions. This so-called precompound or pre-equilibrium emission can be described by the semi-classical exciton or hybrid models [19], or (preferentially) by quantum-mechanical multi-step reaction models [20]. Also intermediate-energy fission is possible in this stage. Finally, in the third stage, a compound nucleus is left that evaporates low-energy particles (mostly neutrons). This is called the compound or evaporation stage. In this stage also competition with fission occurs.

Note that this complex chain of reactions indicated with "spallation" includes a large number of processes which are difficult to distinguish or classify. One could consider to separate processes ending with fission from those ending by evaporation of particles or photons and speak about "spallation-induced fission" or "spallation-induced evaporation" if this is a useful distinction. Note that at lower energies first- and second-chance fission refer to inelastic scattering followed by fission and (n,2n) followed by fission, respectively. In fig. 1 most processes have been indicated. However, there are additional rare interactions, such as those leading to "fragmentation" of the target nucleus, as well.

For the actual transmutation process, the most important quantity is the yield of outgoing neutrons, together with their energy distribution. In fig. 2, we have sketched

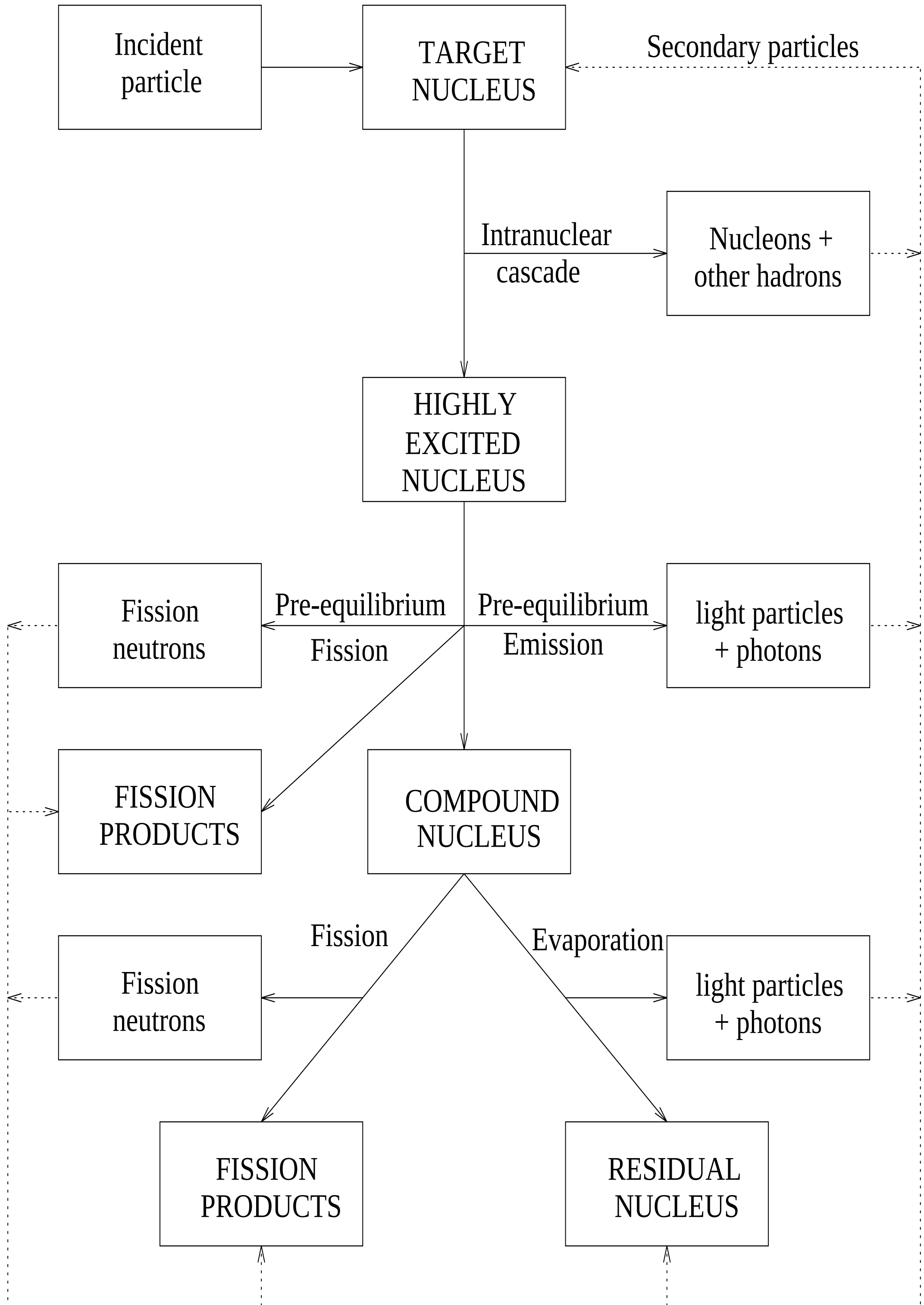

Figure 1: Intermediate-energy nuclear reaction. The solid arrows refer to an intranuclear cascade process (thin target; single proton-nucleus reaction), whereas the dotted arrows represent the internuclear cascade process (thick target).

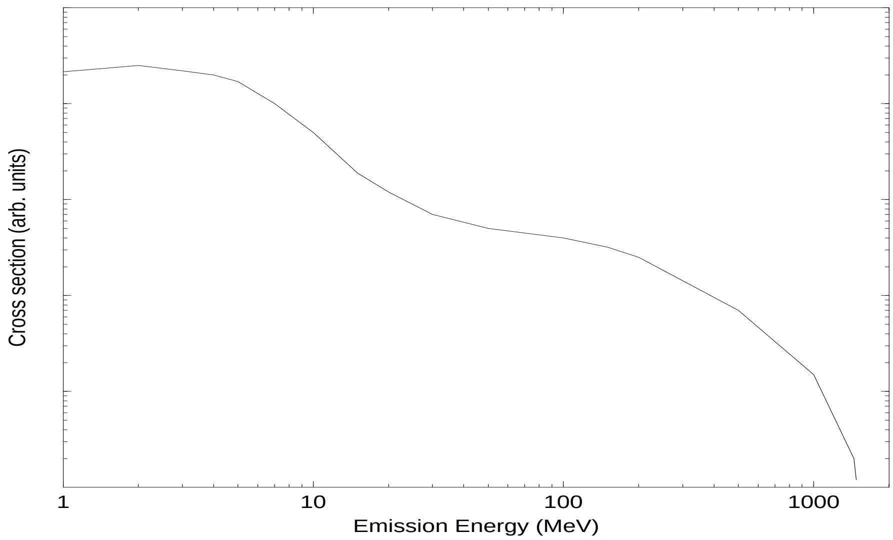

Figure 2: Typical neutron energy spectrum of a 1.5 GeV proton reaction on a heavy nucleus (thin target).

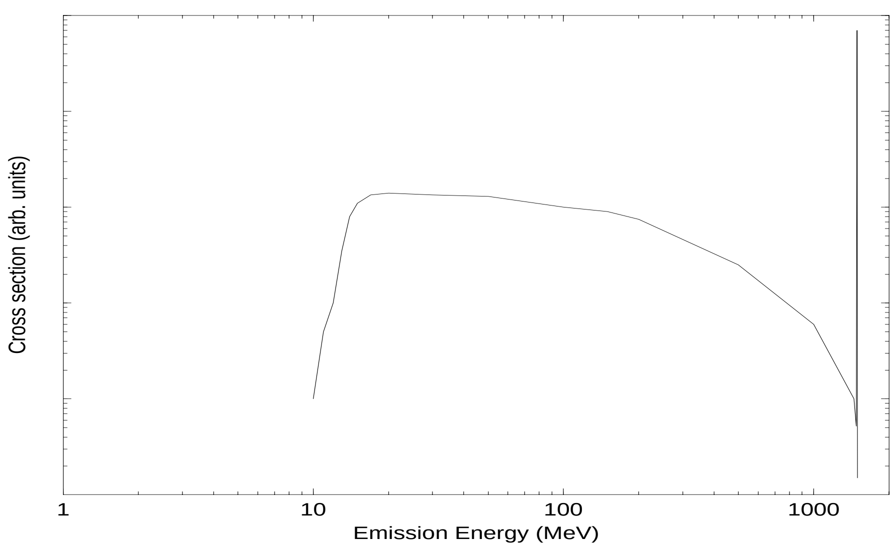

Figure 3: Typical proton energy spectrum of a 1.5 GeV proton reaction on a heavy nucleus (thin target).

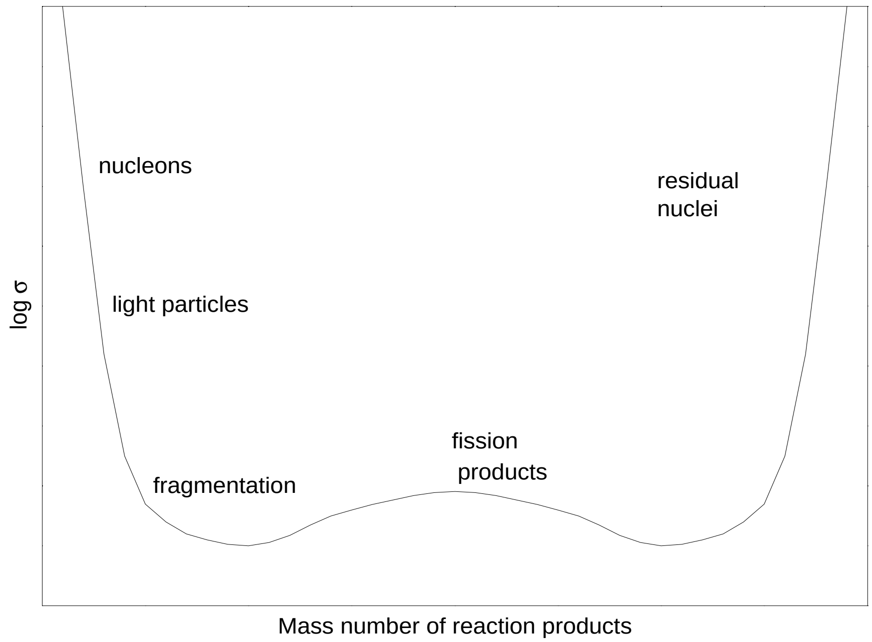

Figure 4: Schematic mass distribution of products in a intermediate-energy nuclear reaction.

the typical outgoing neutron spectrum resulting from a 1.5 GeV proton bombardment of a heavy nucleus. From this figure, it can be inferred that although the peak of the outgoing neutron spectrum will be found around a few MeV (resulting from the multiple evaporation processes), a substantial amount of secondary neutrons with energies higher than 20 MeV will be formed (these represent the intranuclear cascade and pre-equilibrium contributions). For a heavy nucleus like lead, about 20 to 30% of the total angle+outgoing energy integrated cross section for neutrons is located in the energy region between 20 MeV and the incident proton energy (see [21] for a more systematic study on this). The relative amount of secondary intermediate-energy protons (see fig. 3) is even higher than that of neutrons, because the Coulomb barrier, which is rather high for heavy targets, prohibits the evaporation of low-energy protons. In total, a considerable number of intermediate-energy secondary particles will be emitted from the (first) target nucleus. This will have a profound impact on the total (thick target) process, see below.

It is obvious that already after the first proton-nucleon interaction, the number of different outgoing channels is enormous. These include, besides all light particles, also particles with masses higher than that of alpha-particles (in which case the process is called fragmentation), with different emission energies. The mass distribution of product nucleons and nuclides resulting from a intermediate-energy nuclear reaction is depicted in fig. 4. Most of the spallation processes lead to light particles and residual nuclei with mass close to the target mass. However, in thick targets the fraction of fission products is more enhanced, see below.

2.1.2 Thick target

Turning to *thick* targets, the conclusions made with respect to the secondary particle spectra of a single nucleon-nucleus reaction imply that for a sizeable part of the secondary particles (namely the neutrons with energies below 20 MeV), we could use existing data files for the calculation of the *inter*nuclear process. However, the secondary particles with energies higher than 20 MeV will induce further (spallation) reactions producing tertiary particles, and so on.

The internuclear reactions are depicted in fig. 1 by the dotted arrows. The intermediate-energy secondary particles (intranuclear cascade emission from the first nucleus) that encounter a new target nucleus (which can also be a (fission) product from a reaction that has already taken place) will proceed through all stages again and will cause new particles (mainly nucleons) to be emitted from this nucleus. The low-energy secondary particles will skip the intranuclear cascade and pre-equilibrium stage and will at once form a compound nucleus with the new target nucleus, from which subsequent evaporation takes place.

At the end of the complete (thick target) reaction process, it will turn out that the secondary (tertiary, etc.) intermediate-energy particles have provided the main contribution to the total neutron yield. With these multiple collision mechanisms, the large difference in the average number of outgoing neutrons for an incident 1.5 GeV proton on a thin target (∼8-15) and a thick target (∼30-40) target can be explained. It is also evident that the number of fission products increases and that in general the mass distribution becomes more flat than in the case of thin target data.

These considerations concerning neutron production hold for the spallation target, the shielding of the accelerator (since they are both subject to the intermediate-energy proton bombardment) and to a lesser extent for the reactor part surrounding the target. In the case of shielding, the neutron production is less than for the spallation targets, because these shielding materials consist of lighter materials (and the neutron yield per proton is roughly proportional to $A^{\frac{2}{3}}$). In the reactor part, moderation or thermalization takes place.

2.2 Intermediate-energy data libraries

The discussion of the previous section indicates that, given a proton bombarding energy, nuclear data for (at least) incident protons and neutrons are required for incident energies *up to* the bombarding energy. We also stressed that the validity of the intranuclear cascade model may not extend to incident energies as low as 20 MeV, and should be replaced by more specialized nuclear models for incident energies below about 100 MeV. Given these conclusions, the central issue is to choose the best strategy for an adequate handling of nuclear data relevant to accelerator-based transmutation. At present, there seem to be two alternatives:

- a data library up to the energy where the high-energy transport codes are unreliable. For convenience, we have fixed this energy at 100 MeV throughout this report. The exact value (which will perhaps be indicated by the current NEA Data Bank benchmarks [16, 17, 18]) should be discussed.

- a data library for the full energy range, i.e. 0-1500 MeV.

We propose that at least the first type of library should be considered as an extension of the present general-purpose files which are limited to 20 MeV. The second type of library could initially be considered as a reference library, rather than as a standard library for calculations. For applications, both libraries should be combined with an extended activation library for high energies.

2.2.1 Transport data library to 100 MeV

For the reasons outlined in Section 2.1, we assign the highest priority to the construction of a neutron and proton intermediate-energy library to an energy of about 100 MeV (an example of an existing 100 MeV file can be found in Appendix B). These libraries can then be used in combination with a high-energy transport code that internally generates the data above 100 MeV. Note that the value of 100 MeV as maximum is also practical from the point of view that "spallation" is still not very important below 100 MeV. We recommend the construction of a starter library which contains ENDF-6 formatted data files for all relevant nuclides (these nuclides will be categorized in Section 4). For the construction of a 100 MeV data file, procedures different from those used in the low-energy files have to be employed since it is no longer possible to store each possible reaction in a separate MT-number. However, for accelerator-based transmutation calculations, detailed low-energy neutron data will probably be as important as they are in normal reactor calculations. Therefore, we recommend to retain the detailed representation of cross sections below 20 MeV, although some conventions for using the format could be adapted. For energies above 20 MeV, the detailed information concerning each individual excited state of the target nucleus is less important than for low-energy neutrons and a large number of data types should be lumped in MT5 (which comprises all non-elastic processes that are not explicitly considered in other MT numbers). The particle and product yields and the required energy-angle distributions should be stored in MF6. For incident protons, a more uniform approach can be followed (because there is no connection with existing low-energy files).

2.2.2 Reference data library to 1500 MeV

A possible further step is the construction of a data library to 1500 MeV (an example of an existing 1000 MeV file is given in Appendix A). In this way, the nuclear data part would be entirely decoupled from the transport part (just as for reactor calculations). Again, the main advantage of this decoupling is that specialized nuclear model codes and experimental data can be used for certain sections of a datafile. Furthermore, instead of performing comprehensive Monte Carlo calculations (with a code like HETC) repeatedly for a certain material, it could perhaps be more economical to read the data from an evaluated file. For files to 1500 MeV, the ENDF-6 format has to be extended if the creation of hadrons other than nucleons (such as K- and π-mesons) becomes significant. For this library, one may investigate the possibility to read ENDF-6 data directly into the high-energy transport codes, or perhaps even the possibility to extend existing low-energy transport codes to energies as high as 1500 MeV. Alternatively, a reference file could be made only for a few important reactions, serving as a reference for intercomparison with HETC calculations or as a standard for experimental measurements. In each case, the data should be stored as much as possible in MF6/MT5.

2.2.3 Activation data library to 100 MeV

The purpose of an activation library is the calculation of the activation/transmutation of the target and its use in the reactor part of the hybrid system. This library should contain a very large number of stable and unstable nuclides with only activation and transmutation cross sections and without energy-angle distributions. The purpose of this library is to follow activation and transmutation of all products formed during the spallation process, as shown in fig. 5. Therefore, it is practical to separate it from the aforementioned files. There are several low-energy activation files throughout the world. One version is the European Activation File EAF-3 [22], which contains 729 target nuclides ranging from ^{1}H to ^{248}Cm with 12899 reactions kinematically allowed below 20 MeV. This file makes use of a pseudo ENDF format and consists of pointwise given data in MF3 only. The prescribed ENDF-6 representation is MF10, and there is a code available that transforms EAF into MF10. Our provisional proposal is to extend such activation libraries up to 100 MeV. The proposed structure of the file will be outlined in Section 3.

2.3 Relation with processing and transport codes

In fig. 5, a typical scheme for hybrid system calculations is depicted. The present situation is obtained by setting E_{max}=20 MeV and the desired situation by setting E_{max}=100 MeV in this figure. Upon specification of the proton bombardment energy and the target geometry, the high-energy transport code performs the nuclear data and the transport calculations. The neutron source spectrum for $E < E_{max}$ can subsequently be handled by a transport code that makes use of processed (e.g. with NJOY) ENDF-6 formatted files. The calculated emerging neutron fluxes are then input for the reactor calculations and the activation/transmutation calculations for the target. Here, it is assumed that after the thick target reaction process virtually all neutrons have energies below E_{max}.

Figure 5 reveals another crucial aspect of a 100 MeV data library, namely the possible extension of processing and transport codes to higher energies. The incorporation of neutron- and proton-induced reactions up to 100 MeV in the processing code NJOY and the transport code MCNP is under investigation by the Los Alamos Group [11, 12]. The testing of the results is still in progress and preliminary calculations of MCNP with 100 MeV files have been compared with HETC-results [12]. Another potential possibility is to input a 1500 MeV intermediate-energy data file directly into a code like HETC or MCNP. In both cases adjustments in these codes are needed.

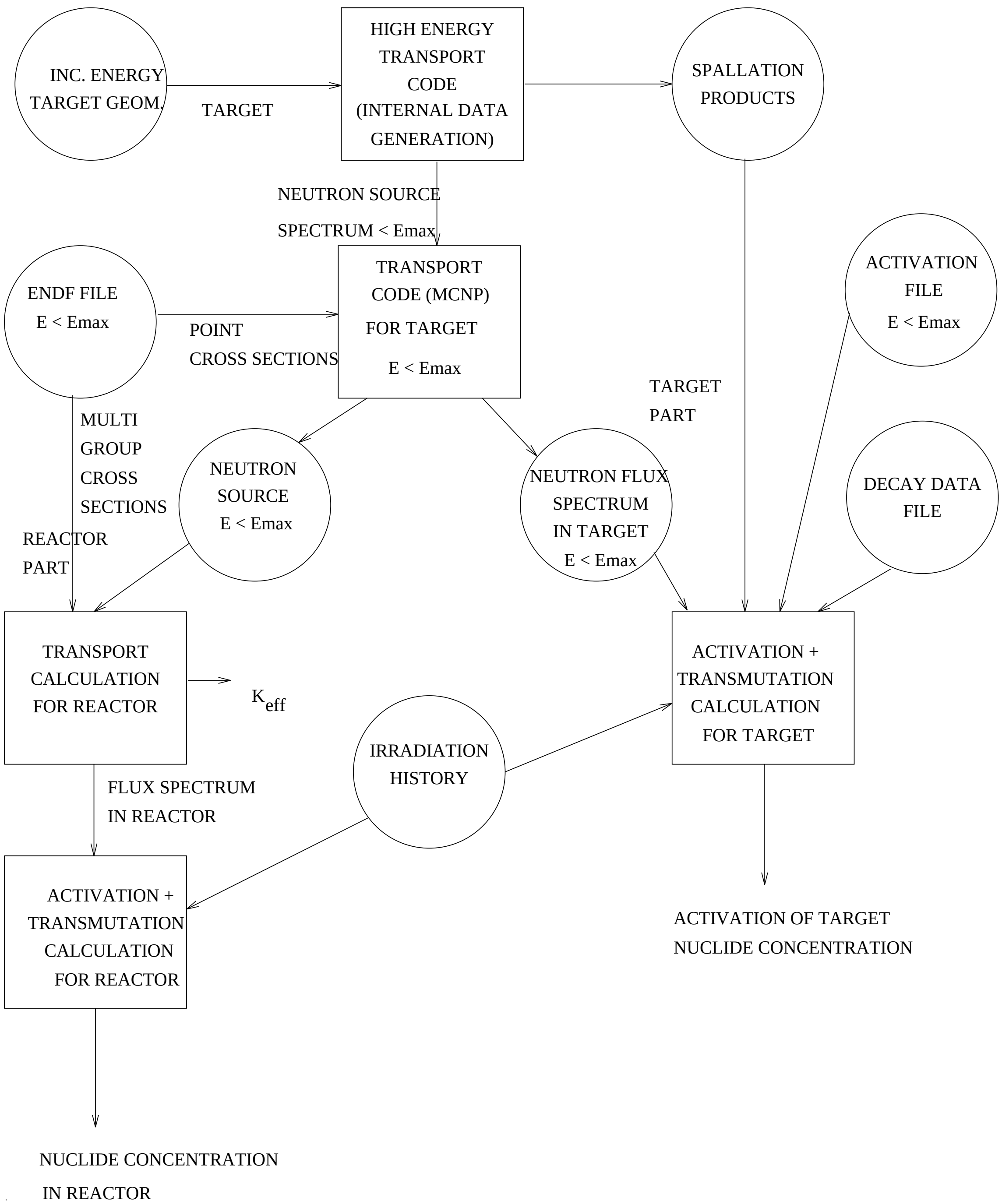

Figure 5: Global scheme for accelerator-driven reactor system calculations

3 Proposal for the structure of intermediate-energy data libraries

In this section, we will specify the global structure of the proposed intermediate-energy data files. In line with the indicated priorities, we will first discuss the set-up of a neutron and proton data library for incident energies up to 100 MeV. Next, we turn to the intermediate-energy transport libraries to 1.5 GeV. Finally, we describe the extension of activation libraries to intermediate-energy transmutation/activation libraries. First, however, we will outline several aspects of intermediate-energy data files that apply to each of these proposed libraries. With respect to the nomenclature, extensive use will be made of the conventions given in the ENDF-6 manual [23].

3.1 General

In the following description of intermediate-energy data files, it will become clear that we have, for the sake of simplicity and uniformity, made some slight changes of the ENDF-6 procedures. Consequently, a slight adjustement of processing codes will probably be necessary (which, however, mostly leads to more simple programming). An important technical aspect of the intermediate-energy data files is the increased use of MF6/MT5 for the storage of outgoing light particle yields and energy-angle distributions as well as the product yields. Furthermore, we have excluded MF4 and MF5 for elastic and inelastic scattering and included all distributions in MF6. Essentially, for non-fissionable isotopes, only MF1,2 (for low energy neutrons), 3 and 6 will be required. Since the storage of fission data is quite involved, we provisionally stick at the use (for incident neutrons only) of MF4 and MF5 for the secondary angle and energy distributions for outgoing fission neutrons.

In principle, we could alternatively store these quantities in MF6 and it is possible to transfer MF4 and MF5 to MF6 by using a tabular representation for the fission spectrum, rather than using the standard "laws" of MF4 and MF5. Furthermore, the prompt fission neutron data in MF6 could be stored under LIP=0 and the delayed fission neutron data under LIP=1, 2, ... for each precursor. Another general remark concerns the usage of the light-particle production cross sections of MT201-207 (as in Appendix A). Upon division of these cross sections by the reaction cross section of MT3/MF3, the resulting yields and energy-angle distributions can be stored in MT5/MF6, avoiding the redundant MT201-207 quantities. For a number of important materials also uncertainty and covariance information is required.

3.2 Neutron data file to 100 MeV

The purpose of this file is to use it in combination with a high-energy transport code (e.g. HETC) that provides the data above 100 MeV. The proposed directory of this file is given in table 1. It comprises the data up to 20 MeV which can be taken from existing evaluated files. The energy range above 1 MeV should be inspected and if necessary improved. Note that “spallation” is not entered explicitly. It is assumed that this process is not important below 100 MeV. However, fission should be described in detail, including first, second and higher-order components. This can be achieved with existing format rules. Most of the other non-elastic processes ending up with multiple evaporation can conveniently be stored in MF6.

3.2.1 File 1 (general information)

This file contains the usual descriptive data and information text. Formal agreements will have to be made on library identifiers and version numbers. The various fission quantities are stored in MT452, 455, 456 and 458.

3.2.2 File 2 (resonance parameters)

The resonance parameters can be taken from an existing low-energy neutron data file.

3.2.3 File 3 (cross sections)

In MT1 and MT2, the total and elastic cross sections can be given. Below 20 MeV, a sufficiently fine energy grid must be specified for a proper description of the cross section. Above 20 MeV, progressively larger steps in energy can be taken. Below 20 MeV, sections MT16-21,38,51-90,91,102 can be used to represent the data. For energies above 20 MeV, the cross sections in these MT numbers are zero. (Formally, this can be accomplished by setting the cross section equal to zero at the two energy points 20.00001 and 100 MeV). In MT5, the situation is reversed: all partial non-elastic cross sections, with the exclusion of fission, can be lumped in MT5 for energies above 20 MeV and the data are zero below 20 MeV (*i.e.* in practice, the cross sections are zero between 10^{-5} eV and 20 MeV and nonzero between 20.00001 and 100 MeV). In MT5, the breakup flag LR is set equal to 1, indicating that additional particles not specified by the MT number will be emitted.

Table 1: Directory of proposed neutron data file to 100 MeV.

MF	MT	Description	Remarks
1	451	General information	
1	452-458	Fission quantities	
2	151	Resonance parameters	Low energy file
3	1	Total cross section	0-100 MeV
3	2	Elastic cross section	0-100 MeV
3	5	(n,anything) cross section	20-100 MeV only
3	16	(n,2n) cross section	0-20 MeV only
3	17	(n,3n) cross section	0-20 MeV only
3	18	Total fission cross section	0-100 MeV
3	19-21,38	1st-4th chance fission cross section	0-100 MeV
3	51-90	(n,n') cross section for 1st-40th excited state	0-20 MeV only
3	91	(n,n') cross section for continuum	0-20 MeV only
3	102	(n,γ) cross section	0-20 MeV only
4	18	Total fission neutron angular distribution	0-100 MeV
4	19-21,38	1st-4th chance fission neutron angular distribution	0-100 MeV
5	18	Total fission neutron energy distribution	0-100 MeV
5	19-21,38	1st-4th chance fission neutron energy distribution	0-100 MeV
6	2	Elastic angular distribution	0-100 MeV
6	5	(n,anything) yields, energy-angle distribution	20-100 MeV only
6	16	(n,2n) energy-angle distribution	0-20 MeV only
6	17	(n,3n) energy-angle distribution	0-20 MeV only
6	51-90	(n,n') angular distribution for 1st-40th excited state	0-20 MeV only
6	91	(n,n') energy-angle distribution for continuum	0-20 MeV only
6	102	(n,γ) energy-angle distribution	0-20 MeV only
8	454	Independent fission-product yields	0-100 MeV
8	459	Cumulative fission-product yields	0-100 MeV

3.2.4 File 4 (fission neutron angular distribution)

In MT18-21,38, the angular distributions for possible fission neutrons can be specified. Following Ref. [23], it is recommended to give these angular distributions in the LAB system (LCT=1), but it seems better for intermediate-energy applications to use the CM system. Isotropic CM distributions use LCT=0, LTT=0, LVT=0, LI=1. Non-isotropic angular distributions should be given in the Legendre expansion (LCT=0, LTT=1, LVT=0, LI=0). In a later phase, MF6 may be more appropriate for the storage of these data (see subsection 3.1).

3.2.5 File 5 (fission neutron energy distributions)

In MT18-21,38, the energy distributions for possible fission neutrons can be specified. MF6 may also be appropriate for the storage of these data (see subsection 3.1).

3.2.6 File 6 (yields, energy-angle distributions)

Yields of important outgoing particles, photons and possible recoils should be stored here. The data should be represented in the CM system for secondary energy and angle (LCT=2). The elastic angular distributions can be given in MF6/MT2 by setting the yields equal to 1 for both the lowest and the highest incident energy. For the elastic CM angular distribution we advise LAW=2 (discrete two-body scattering) with option LANG=12 (tabulation with $p_i(\mu)$ linear in μ). For the excitation of "discrete" levels the CM angular distributions in MT51-90 should also be represented by LAW=2, LANG=12. Similar formats are available for storage of cross sections for other discrete level excitation. For formal reasons, an energy point at 100 MeV must always be added (e.g. with isotropic angular distribution). The same formal additions must be applied on MT16,17 and 91. For these energy-angle distributions, however, we recommend LAW=1 (continuum energy-angle distribution) with LANG=2 (Kalbach expansion) in the CM-system. These formal additions have no further impact if the corresponding cross sections of MF3 are set equal to zero. In MF6/MT5, the yields and energy-angle distributions of the light particles, photons *and* the product nuclides or recoils (excluding fission products) for energies above 20 MeV can be stored. First the yields and energy-angle distribution for photons, neutrons, protons, deuterons, tritons, He-3 and alphas can be given. We recommend LAW=1 with LANG=2 for these light particles. Discrete photons can be entered in MF6 format, but this option is not yet implemented in processing codes. Subsequently, MT5 can be filled with the yields of the product nuclides using LAW=0 (unknown distribution). For fission-product yields it is probably most easy to keep the special yield and decay library, of course with addition of intermediate-energy data points.

3.2.7 File 8 (fission yield data)

The fission product yield data can be stored here. The advantage is that the current contents of this file can easily be extended. At present this (separate) file typically contains yields at three energy "points": thermal, fission spectrum average and 14 MeV. A few more points should be added. Alternatively the fission yields can be stored in File 6.

3.3 Proton data file to 100 MeV

The purpose of the proton library to 100 MeV is threefold: calculation of the neutron production due to incident protons (for the actinide transmutation), proton transport calculations (future versions of MCNP) in addition to a high-energy transport code (HETC) and (for the low-energy part of the proton file) nuclear data for a basic technology accelerator (10 MeV) [1, 3] which is regarded as a first step towards the high-energy (1500 MeV) accelerator. For protons, there are no compatibility problems with low-energy evaluations (because these evaluations scarcely exist). Furthermore, the resonance parameters are, by ENDF-6 definition, not present. Moreover, for heavy materials the resonance range is suppressed by the Coulomb barrier. Anyway, the proton resonances should be represented pointwise with Doppler broadening at the required temperature. The proposed directory is given in table 2.

3.3.1 File 1 (general information)

This file contains the usual descriptive data and information text. Formal agreements will have to be made on library identifiers and version numbers.

3.3.2 File 3 (cross sections)

In ENDF-6, the total cross section of MT1 is undefined for protons. The elastic cross sections are given in MT2. Since resonance parameters are not allowed for protons, pointwise given cross sections with high resolution and at the required temperature(s) should be given in the low energy range. We recommend to include all non-elastic processes, possibly with the exclusion of fission, in MT5 for all energies. In MT5, the

Table 2: Directory of proposed proton data file to 100 MeV.

MF	MT	Description	Remarks
1	451	General information	
3	2	Elastic cross section	0-100 MeV
3	5	(p,anything) cross section	0-100 MeV
3	18	Total fission cross section	0-100 MeV
6	2	Elastic angular distribution	0-100 MeV
6	5	(p,anything) yields, energy-angle distribution	0-100 MeV
6	18	Total fission-neutron energy-angle distribution	0-100 MeV
8	454	Independent fission-product yields	0-100 MeV
8	459	Cumulative fission-product yields	0-100 MeV

breakup flag LR is set equal to 1. Note that only the total fission cross section (MT18) is given (the partial fission cross sections for protons are undefined in ENDF-6 format).

3.3.3 File 6 (yields and energy-angle distributions)

The data should be represented in the CM system for secondary energy and angle (LCT=2). The elastic angular distributions can be given in MT2 by setting the yields equal to 1 for both the lowest and the highest incident energy. The energy-angle distribution according to LAW=5 (charged-particle elastic scattering) can be used, with the data represented in the nuclear+interference expansion (LTP=12). In MT5, the yields and energy-angle distributions of the light particles *and* the product nuclides (excluding fission products) for energies above 20 MeV can be stored. First the yields and energy-angle distribution for photons, neutrons, protons, deuterons, tritons, He-3 and alphas can be given. We recommend LAW=1 (continuum energy-angle distribution) with LANG=2 (Kalbach expansion) in the CM-system for these light particles. Subsequently, MT5 can be filled with the yields of the product nuclides using LAW=0 (unknown distribution). In MT18, the fission neutron yields and energy-angle distributions should be stored. Probably only the sum of prompt and delayed neutrons is of interest.

3.3.4 File 8 (fission yield data)

The fission-product yield data can be stored here. However, in this case there is no existing data file with proton-induced fission yields at low energy. One could also store these data in MF6/MT18.

3.4 Proton and neutron data files from 20 to 1500 MeV

The purpose of these files is to compare the data with HETC calculations or the direct use of the data in high-energy transport codes. The directory for both neutrons and protons is given in table 3. Note that except for elastic scattering, no explicit cross sections are given. However, the relevant yields are given in MF6. Fission is not explicitly specified, because at intermediate energies it is difficult to distinguish between fission and spallation. It could be practical to separate fission including "spallation-induced fission" and "fragmentation" (i.e. all processes ending up in fission or fragmentation) and store that lumped quantity in MT18 (lumped fission cross section). In that case all other conventions for fission as discussed in Section 3.1 apply. The advantage would be that initially also an (updated) "fission-product yield" library MF8 could be used and that the main file contains less product yields (only those resulting from multiple scattering and evaporation). If in addition to the usual charged-particle reaction production cross sections also the production of π- and K-mesons is important, extension of the ENDF-6 format is required (MT871-999?). Perhaps it is even necessary to introduce separate libraries for *incident* hadrons (e.g. a pion library). If necessary, the part below 20 MeV could be added from existing libraries. For reference files also some restricted uncertainty/covariance information should be added.

3.4.1 File 1 (general information)

This file contains the usual descriptive data and information text. Formal agreements will have to be made on library identifiers and version numbers.

3.4.2 File 3 (cross section)

The total cross section is given in MT1 (neutrons only) and the elastic cross section in MT2. All non-elastic processes are lumped in MT5 with (LR=1). If this is wanted, one additional lumped fission cross section could be introduced under MT18, including "spallation-induced" fission and "fragmentation".

Table 3: Directory of proposed neutron or proton data file from 20 to 1500 MeV.

MF	MT	Description	Remarks
1	451	General information	
3	1	Total cross section	20-1500 MeV (neutrons)
3	2	Elastic cross section	20-1500 MeV
3	5	(z,anything) cross section	20-1500 MeV
3	18	Total fission, incl. spall. ind. fission	20-1500 MeV (optional)
6	2	Elastic angular distribution	20-1500 MeV
6	5	(z,anything) yields, energy-angle dist.	20-1500 MeV
6	18	Total fission yields + distr.	20-1500 MeV (optional)

3.4.3 File 6 (yields and energy-angle distributions)

The data should be represented in the CM system for secondary energy and angle (LCT=2). The elastic angular distributions can be given in MF6/MT2 by setting the yields equal to 1 for both the lowest and the highest incident energy. For neutrons, we advise the energy-angle distribution LAW=2 (discrete two-body scattering) with option LANG=12 (tabulation with $p_i(\mu)$ linear in μ). For protons, the energy-angle distribution according to LAW=5 (charged-particle elastic scattering) can be used, with the data represented in the nuclear+interference expansion (LTP=12). In MF6/MT5, the yields and energy-angle distributions of the light particles, photons *and* the product nuclides (excluding fission products) for energies above 20 MeV can be stored. First the yields and energy-angle distribution for photons, neutrons, protons, deuterons, tritons, He-3 and alphas can be given. We recommend LAW=1 (continuum energy-angle distribution) with LANG=2 (Kalbach expansion) in the CM-system for these light particles. It has to be checked whether the Kalbach expansion needs to be extended to higher energies. Subsequently, MT5 can be filled with the yields of the product nuclides using LAW=0 (unknown distribution). These product yields could be separated into "recoils" or "residual nuclides" and fission products and fragmentation products. Alternatively, the generalized quantity MT18 could be used to store the particle and photon yields and their energy-angle distributions and the fission-product yields could be stored in MF8.

3.5 Neutron and proton activation/transmutation file to 100 MeV

Basically, an activation file should contain the lumped cross sections for all possible reaction channels. In activation files below 20 MeV, this is accomplished (as in the European Activation File EAF-3 [22]) by using MF3 in combination with many MT-numbers (one for each combination of outgoing particles). In applications, the cross section of the reaction channels (MT-numbers) that lead to the same product nucleus are then lumped to obtain the activation cross section for that product nucleus. For an activation file to 100 MeV, this file structure cannot be adopted, since the number of possible different reaction channels becomes so large that a specification in terms of different MT-numbers is impracticable. Instead, it is more appealing to store the activation/transmutation cross sections themselves in the file. In this way, the information concerning the division of the activation cross sections in the various reaction components is lost, but this does not seem crucial from the applicational point of view. Therefore, for the extension to a intermediate-energy activation file, we propose to construct a file consisting of MF3/MT5 for the absolute values of the cross sections and MF6/MT5 for all possible product-nuclide yields, see table 4. The isomeric states can be specified in MF6 by means of the LIP-parameter.

As in the case of low-energy activation files, the intermediate-energy activation file must be constructed for all stable and unstable target nuclei with half-lives exceeding a certain time (about 1 day). The end products (to be included) could have much shorter half-lives (>1 sec). For proton-induced activation libraries, the library could initially be restricted to the low-energy range (0-20 MeV) and to important target nuclei only (in particular heavy masses).

Table 4: Directory of proposed neutron or proton activation/transmutation file to 100 MeV.

MF	MT	Description	Remarks
1	451	General information	
3	5	(z,anything) cross section	0-100 MeV
6	5	(z,anything) yields	0-100 MeV

4 Proposed contents of the data library

The data requirements for accelerator-based transmutation that have been specified so far, are of a rather global nature, see Refs. [1-3] and tables 1 and 2 of [7]. Given the required effort for the creation of a reliable (intermediate-energy) data file, it is obvious that further establishment of priority criteria within the total set of libraries, materials *and* reaction types is a necessity. Therefore, the following specification of the nuclear data needs in terms of the various proposed files must be regarded as a provisional set-up of intermediate-energy libraries for accelerator-based transmutation.

We have categorized the relevant materials as follows:

1. Target materials: Ta, W, Pb, Bi.
2. Actinides: ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{241}Am, ^{243}Am, ^{244}Cm, ^{245}Cm.
3. Structural, shielding, coolant and other materials (e.g. stainless steel, concrete, air): H, C, N, O, Na, Mg, Al, Ar, K, Ca, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr.

As mentioned, we shall not address to priority settings within a group of materials here. We can add, however, that the results of the current model code benchmarks [16, 17, 18], which involve lead and tungsten, may give an indication about the most promising target materials. This depends not only on the magnitude of the total neutron production, but also on the yields of unwanted (radioactive) product nuclides for these target materials.

In the following tables, we present a proposal for the translation of the data needs into the ENDF-6 formatted data files. For each group of materials and each type of library, the proposed directory of both the neutron and proton file is given, as well as a priority indication (A = highest priority) tentatively assigned by the author of this report. Also, in each table we indicate which data should at least be present in the files.

The assignment of a high priority depends on the design. In general high priority needs for intermediate energy data are assigned to target nuclides, which could be "inert" materials or actinides. In the blanket surrounding the target the flux spectrum might be quite moderated and therefore the need for intermediate-energy data is much less urgent, and it may be sufficient to extend existing data files up to a few tens of MeV, emphasizing the region above 1 MeV.

Proposed 0 - 100 MeV neutron data file for inert target materials

Materials : Ta, W, Pb, Bi (or restricted to one reference material)
Priority : A
Required data : (n,xn) (E,θ) (first priority)
(n,xγ) (E,θ) (first priority)
Neutron and photon yields (first priority)
Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
2	151	Resonance parameters	Low energy file
3	1	Total cross section	0-100 MeV
3	2	Elastic cross section	0-100 MeV
3	5	(n,anything) cross section	20-100 MeV only
3	16	(n,2n) cross section	0-20 MeV only
3	17	(n,3n) cross section	0-20 MeV only
3	51-90	(n,n') cross section 1st-40th excited state	0-20 MeV only
3	91	(n,n') cross section for continuum	0-20 MeV only
3	102	(n,γ) cross section	0-20 MeV only
6	2	Elastic angular distribution	0-100 MeV
6	5	(n,anything) yields, energy-angle distribution	20-100 MeV only
6	16	(n,2n) energy-angle distribution	0-20 MeV only
6	17	(n,3n) energy-angle distribution	0-20 MeV only
6	51-90	(n,n') angular distribution 1st-40th excited state	0-20 MeV only
6	91	(n,n') energy-angle distribution for continuum	0-20 MeV only
6	102	(n,γ) yields, energy-angle distribution	0-20 MeV only

Comment: MF6/MT5: give yields and energy-angle distributions at least for photons and neutrons according to LAW=1. Give product yields (residual nuclei) with LAW=0.

Proposed 0 - 100 MeV proton data file for inert target materials

Materials	:	Ta, W, Pb, Bi (or restricted to one reference material)
Priority	:	A
Required data	:	(p,xp) (E,θ)
		(p,xn) (E,θ) (first priority)
		(p,xγ) (E,θ)
		Neutron and photon yields (first priority)
		Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	2	Elastic cross section	0-100 MeV
3	5	(p,anything) cross section	0-100 MeV
6	2	Elastic angular distribution	0-100 MeV
6	5	(p,anything) yields, energy-angle distribution	0-100 MeV

Comment: MF6/MT5: give yields and energy-angle distributions at least for neutrons, protons and photons according to LAW=1. Give product yields (residual nuclei) with LAW=0.

Proposed 0 - 100 MeV neutron data file for actinides

Materials : ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{241}Am, ^{243}Am, ^{244}Cm, ^{245}Cm
Priority : A (B for hybrid accelerator-driven reactors)
Required data : (n,xn) (E,θ) (first priority)
(n,f) + neutron energy-angle distribution (first priority)
Neutron and photon yields (first priority)
Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
1	452-458	Fission quantities	
2	151	Resonance parameters	Low energy file
3	1	Total cross section	0-100 MeV
3	2	Elastic cross section	0-100 MeV
3	5	(n,anything) cross section	20-100 MeV only
3	16	(n,2n) cross section	0-20 MeV only
3	17	(n,3n) cross section	0-20 MeV only
3	18	Total fission cross section	0-100 MeV
3	19-21,38	1st-4th chance fission cross section	0-100 MeV
3	51-90	(n,n') cross section 1st-40th excited state	0-20 MeV only
3	91	(n,n') cross section for continuum	0-20 MeV only
3	102	(n,γ) cross section	0-20 MeV only
4	18	Total fission neutron angular distribution	0-100 MeV
4	19-21,38	1st-4th chance fission neutron angular distribution	0-100 MeV
5	18	Total fission neutron energy distribution	0-100 MeV
5	19-21,38	1st-4th chance fission neutron energy distribution	0-100 MeV
6	2	Elastic angular distribution	0-100 MeV
6	5	(n,anything) yields, energy-angle distribution	20-100 MeV only
6	16	(n,2n) energy-angle distribution	0-20 MeV only
6	17	(n,3n) energy-angle distribution	0-20 MeV only
6	51-90	(n,n') angular distribution 1st-40th excited state	0-20 MeV only
6	91	(n,n') energy-angle distribution for continuum	0-20 MeV only
6	102	(n,γ) yields, energy-angle distribution	0-20 MeV only
8	454	Independent fission product yields	0-100 MeV
8	459	Cumulative fission product yields	0-100 MeV

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 at least for neutrons and photons. Give product yields (excluding fission product yields) with LAW=0.

Proposed 0 - 100 MeV proton data file for actinides

Materials : ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{241}Am, ^{243}Am, ^{244}Cm, ^{245}Cm
Priority : A (C for hybrid accelerator-driven reactors)
Required data : (p,xp) (E,θ)
(p,xn) (E,θ) (first priority)
(p,f) + neutron energy-angle distribution
Neutron and photon yields (first priority)
Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	2	Elastic cross section	0-100 MeV
3	5	(p,anything) cross section	0-100 MeV
3	18	Total fission cross section	0-100 MeV
6	2	Elastic angular distribution	0-100 MeV
6	5	(p,anything) yields, energy-angle distribution	0-100 MeV
6	18	Total fission neutron yields, energy-angle distribution	0-100 MeV
8	454	Independent fission product yields	0-100 MeV
8	459	Cumulative fission product yields	0-100 MeV

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 at least for neutrons, protons and photons. Give product yields (excluding fission product yields) with LAW=0.

Proposed 0 - 100 MeV neutron data file for accelerator shielding and reactor

Materials : H, C, N, O, Na, Mg, Al, Ar, K, Ca, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr
Priority : A (B for reactor materials)
Required data : (n,xn) (E,θ) (first priority)
(n,xγ) (E,θ) (first priority)
Neutron and photon yields (first priority)
Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
2	151	Resonance parameters	Low energy file
3	1	Total cross section	0-100 MeV
3	2	Elastic cross section	0-100 MeV
3	5	(n,anything) cross section	20-100 MeV only
3	16	(n,2n) cross section	0-20 MeV only
3	17	(n,3n) cross section	0-20 MeV only
3	51-90	(n,n') cross section 1st-40th excited state	0-20 MeV only
3	91	(n,n') cross section for continuum	0-20 MeV only
3	102	(n,γ) cross section	0-20 MeV only
6	2	Elastic angular distribution	0-100 MeV
6	5	(n,anything) yields, energy-angle distribution	20-100 MeV only
6	16	(n,2n) energy-angle distribution	0-20 MeV only
6	17	(n,3n) energy-angle distribution	0-20 MeV only
6	51-90	(n,n') angular distribution 1st-40th excited state	0-20 MeV only
6	91	(n,n') energy-angle distribution for continuum	0-20 MeV only
6	102	(n,γ) yields, energy-angle distribution	0-20 MeV only

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 at least for neutrons and photons. Give product yields (residual nuclei) with LAW=0.

Proposed 0 - 100 MeV proton data file for accelerator shielding and reactor

Materials	:	H, C, N, O, Na, Mg, Al, Ar, K, Ca, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr
Priority	:	B (C for reactor materials)
Required data	:	(p,xp) (E,θ)
		(p,xn) (E,θ) (first priority)
		(p,xγ) (E,θ)
		Neutron and photon yields (first priority)
		Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	2	Elastic cross section	0-100 MeV
3	5	(p,anything) cross section	0-100 MeV
6	2	Elastic angular distribution	0-100 MeV
6	5	(p,anything) yields, energy-angle distribution	0-100 MeV

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 at least for neutrons, protons and photons. Give product yields (residual nuclei) with LAW=0.

Proposed 20-1500 MeV neutron data file for inert target materials

Materials	:	Ta, W, Pb, Bi (or restricted to one reference material)
Priority	:	B
Required data	:	(n,xn) (E,θ) (first priority)
		(n,xγ) (E,θ) (first priority)
		Neutron and photon yields (first priority)
		Product yields as a function of E (first priority)

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	1	Total cross section	20-1500 MeV
3	2	Elastic cross section	20-1500 MeV
3	5	(n,anything) cross section	20-1500 MeV
3	18	Total fission cross section (optional)	20-1500 MeV
6	2	Elastic angular distribution	20-1500 MeV
6	5	(n,anything) yields, energy-angle distribution	20-1500 MeV
6	18	Total fission neutron yields, energy-angle distribution (optional)	20-1500 MeV

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 at least for photons and photons. Give product yields (residual nuclei) with LAW=0.

Proposed 20-1500 MeV proton data file for inert target materials

Materials	:	Ta, W, Pb, Bi (or restricted to one reference material)
Priority	:	A
Required data	:	(p,xp) (E,θ) (first priority)
		(p,xn) (E,θ) (first priority)
		(p,xγ) (E,θ)
		Neutron, proton and photon yields (first priority)
		Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	2	Elastic cross section	20-1500 MeV
3	5	(p,anything) cross section	20-1500 MeV
3	18	Total fission cross section (optional)	20-1500 MeV
6	2	Elastic angular distribution	20-1500 MeV
6	5	(p,anything) yields, energy-angle dist.	20-1500 MeV
6	18	Total fission neutron yields, energy-angle distribution (optional)	20-1500 MeV

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 at least for neutrons, protons and photons. Give product yields (residual nuclei) with LAW=0.

Proposed 20-1500 MeV neutron data file for actinides

Materials	:	^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{241}Am, ^{243}Am, ^{244}Cm, ^{245}Cm (or restricted to a few reference materials)
Priority	:	B (C for hybrid accelerator-based systems)
Required data	:	(n,xn) (E,θ) (first priority) (n,f) + neutron energy-angle distribution (first priority) Neutron and photon yields (first priority) Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	1	Total cross section	20-1500 MeV
3	2	Elastic cross section	20-1500 MeV
3	5	(n,anything) cross section	20-1500 MeV
6	2	Elastic angular distribution	20-1500 MeV
6	5	(n,anything) yields, energy-angle dist.	20-1500 MeV

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 at least for neutrons and photons. Give product yields with LAW=0.

Proposed 20 - 1500 MeV proton data file for actinides

Materials	:	^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{241}Am, ^{243}Am, ^{244}Cm, ^{245}Cm
		(or restricted to a few reference materials)
Priority	:	C (less important for hybrid accelerator-based systems)
Required data	:	(p,xp) (E,θ)
		(p,xn) (E,θ)(first priority)
		(p,f) + neutron energy-angle distribution (first priority)
		Neutron and photon yields (first priority)
		Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	2	Elastic cross section	20-1500 MeV
3	5	(p,anything) cross section	20-1500 MeV
6	2	Elastic angular distribution	20-1500 MeV
6	5	(p,anything) energy-angle distribution	20-1500 MeV

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 at least for neutrons and protons. Give product yields with LAW=0.

Proposed 20-1500 MeV neutron data file for accelerator shielding and reactor

Materials	:	H, C, N, O, Na, Mg, Al, Ar, K, Ca, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr
Priority accelerator shielding materials	:	A or B
Priority reactor materials	:	C
Required data	:	(n,xn) (E,θ) (first priority) (n,xγ) (E,θ) (first priority) Neutron and photon yields (first priority) Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	1	Total cross section	20-1500 MeV
3	2	Elastic cross section	20-1500 MeV
3	5	(n,anything) cross section	20-1500 MeV
6	2	Elastic angular distribution	20-1500 MeV
6	5	(n,anything) energy-angle distribution	20-1500 MeV

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 at least for photons and neutrons. Give product yields (residual nuclei) with LAW=0.

Proposed 20-1500 MeV proton data file for accelerator shielding and reactor

Materials	:	H, C, N, O, Na, Mg, Al, Ar, K, Ca, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr
Priority accelerator shielding materials	:	A or B
Priority reactor materials	:	C
Required data	:	(p,xp) (E,θ) (p,xn) (E,θ) (first priority) Neutron, proton and photon yields (first priority) (p,xγ) (E,θ) Product yields as a function of E

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	2	Elastic cross section	20-1500 MeV
3	5	(p,anything) cross section	20-1500 MeV
6	2	Elastic angular distribution	20-1500 MeV
6	5	(p,anything) energy-angle distribution	20-1500 MeV

Comment: MF6/MT5: give yields and energy-angle distributions according to LAW=1 for neutrons, protons and photons. Give product yields (residual nuclei) with LAW=0.

Proposed 0 - 100 MeV neutron activation/transmutation file

Materials : ^{1}H,.....,^{248}Cm (half-life > 1 day)
Priority : B (in particular for target materials and contaminants)
Required data : Product yields as a function of E for stable and unstable nuclei with half-life > 1 day, including isomers

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	5	(n,anything) cross section	0-100 MeV
6	5	(n,anything) energy-angle distribution	0-100 MeV

Comment: MF6/MT5: Give product yields with LAW=0.

Proposed 0 - 100 MeV proton activation/transmutation file

Materials	:	Initially for selected target nuclei and for 0-20 MeV
Priority	:	C (in particular for target materials and contaminants)
Required data	:	Product yields as a function of E for stable and unstable nuclei with half-life > 1 day, including isomers

Directory:

MF	MT	Description	Remarks
1	451	General information	
3	5	(p,anything) cross section	0-100 MeV
6	5	(p,anything) energy-angle distribution	0-100 MeV

Comment: MF6/MT5: Give product yields with LAW=0.

5 Conclusions

This report is a working document, to be discussed by the Nuclear Science Comittee on June 7-9, 1993.

Following the analysis of the complete intermediate-energy reaction process in an incineration system, we have argued the importance of intermediate-energy nuclear data libraries for accelerator-based transmutation of radioactive waste. Therefore, the construction of three data libraries is proposed:

- a data library from 0 to about 100 MeV,
- a reference data library from 20 to 1500 MeV,
- an activation/transmutation library from 0 to about 100 MeV.

The highest priority is assigned to the data library up to 100 MeV, assuming a reasonable reliability of high-energy transport codes above this energy. The relation of intermediate-energy data files with processing and transport codes is briefly indicated (the extension of these codes to higher energies is under development). The global structure (in terms of ENDF-6 nomenclature) of each of the three libraries was presented. The most conspicuous change in the procedures is the idea to store the data as much as possible in MT5. In particular, in MF6/MT5, the yields and energy-angle distributions of the light particles and the yields of product nuclides can be specified. The present study indicates that the current ENDF-6 format is appropriate for intermediate-energy evaluation work, as long as hadrons other than nucleons are not involved. We have translated the current collection of specified data needs in terms of the proposed data libraries. Examples of existing intermediate-energy files are given in the appendices. Finally, it is noted that in this report only requests of intermediate-energy data for accelerator-based transmutation are discussed. There are, however, also important needs for intermediate-energy data in other nuclear applications in science, technology and in the medical field [10, 27].

As a result of this and the previous study [7] some recommendations could be made:

- The needs for intermediate-energy nuclear data should be further established and categorized. The present work gives some classification from the point of view of the evaluator, but more detailed information is necessary. The fact that the feasibility of accelerator-based transmutation is still under investigation means that initially a rather broad range of nuclear data is required. However, given the effort required to perform evaluation tasks, more detailed data needs (including target accuracies) and their priorities should be expressed, especially by the designers of accelerator-based transmutation systems.

- An international cooperation effort is needed for the set-up of intermediate-energy nuclear data files. The following tasks should be coordinated:

  1. Further compilation of experimental intermediate-energy data and an update of existing experimental cross section databases in numerical (EXFOR) and graphical representation [7].
  2. Evaluation of international code intercomparisons, such as [16, 17, 18] to determine to what extent theory can be used in evaluations. Further suggestions concerning comparisons of model codes and experimental data have been given in the conclusions of [7].
  3. The set-up of "starter files" for accelerator-based transmutation using available evaluations [7].
  4. Small adjustments in formats, and establishment of special procedures for intermediate-energy files (see the suggestions in the present report, e.g. the proposals related to fission quantities, in particular spallation-induced fission and the storage of fission product yields). In particular, storage of continuum emission data in MT5 with yields and energy-angle distributions in MF6 is recommended.
  5. Appropriate changes in processing codes (NJOY) and transport codes (HETC, MCNP, etc.)
  6. The definition of a detailed international programme for intermediate-energy nuclear data evaluation.

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References

[1] T. Nishida, H. Takada, I. Kanno, Y. Nakahara, M. Mizumoto, T. Mukaiyama and Y. Kikuchi, " Nuclear data needs concerning the OMEGA project", JAERI–memo.

[2] Y. Nakahara, " Nuclear and nucleon data needs for incineration of the radioactive waste from fission reactors with a proton accelerator", in *Nuclear Data for Science and Technology*, Jülich, 13–17 May 1991, 23.

[3] Y. Kikuchi, "Data needs in the 90's: Japanese position", internal report, presented at Working Party, Symposium on *Nuclear Data Evaluation Methodology*, Brookhaven National Laboratory, Upton, New York, Oct. 12–16 1992.

[4] S. Cierjacks, " Cross section measurements, integral validation experiments and nuclear model code developments of importance to accelerator–based transmutation", in *OECD/NEA Specialists' Meeting on Accelerator–Based Transmutation*, Würenlingen, Switzerland, 24–26 March, 1992, p. 556.

[5] H. Takahashi, " Survey of codes relevant to design, engineering and simulation of transmutation of actinide by spallation", OECD Nuclear Energy Agency (Paris) report 1991.

[6] F. Atchinson, in *OECD/NEA Specialists' Meeting on Accelerator–Based Transmutation*, 440, Würenlingen, Switzerland, 24–26 March, 1992.

[7] A.J. Koning, "Review of high-energy data and model codes for accelerator based transmutation", Nuclear Energy Agency (OECD) report NEA/NSC/DOC(92)12, 1992; report ECN-C-93-005 (1993).

[8] A.J. Koning, H. Gruppelaar and P. Nagel, "Nuclear Data Evaluation for Accelerator-Based Transmutation of Radioactive Waste", proceedings of the International Conference "GLOBAL '93 - Future Nuclear Systems: Emerging Fuel Cycles and Waste Disposal Options", Seattle, Washington, Sep. 12-17, 1993.

[9] T. Fukahori and S. Pearlstein, "Evaluation at the Medium Energy Region for Pb–208 and Bi–209", Brookhaven National Laboratory report.

[10] S. Pearlstein, Astrophys. J. **346**, 1049 (1989).

[11] P.G. Young, E.D. Arthur, M. Bozoian, T.R. England, G.M. Hale, R.J. LaBauve, R.C. Little, R.E. Macfarlane, D.G. Madland, R.T. Perry and W.B. Wilson, "Transport data libraries for incident proton and neutron energies to 100 MeV", Los Alamos National Laboratory, report LA–11753–MS (1989).

[12] E.D. Arthur, P.G. Young, R.T. Perry, D.G. Madland, R.E. Macfarlane, R.C. Little, M. Bozoian and R.J. LaBauve, in *Nuclear Data for Science and Technology*, Mito, May 30–June 3, 1988, p. 1185.

[13] M. Sugimoto, K. Noda, Y. Kato, H. Ohno and T. Kondo, "Overview of ESNIT and Nuclear Data", in Proceedings of the 1991 Symposium on Nuclear data, Nov. 28-29 1991, p. 58, JAERI-report M-92-027.

[14] K. Kwiatowski et al., Phys. Rev. Lett. **50**, 1648 (1983).

[15] K. Shin et al., Phys. Rev. **C29**, 1307 (1984).

[16] M. Blann and P. Nagel, "International Code and Model Intercomparison for Intermediate Energy Reactions: Phase 1", NEA Data Bank, in progress.

[17] P. Nagel, J. Rodens, M. Blann, H. Gruppelaar, H. Küsters D. Filges, "Intermediate energy nuclear reaction code intercomparison: Applications to transmutation of long lived reactor wastes", Meeting " GLOBAL '93 - Future Nuclear Systems: Emerging Fuel Cycles and Waste Disposal Options", Seattle Sep. 12-17, 1993.

[18] H. Küsters and D. Filges, "International Code and Model Intercomparison for Intermediate Energy Reactions: Phase 2", NEA Data Bank, in progress.

[19] H. Gruppelaar, P. Nagel and P.E. Hodgson, Riv. Nuov. Cim. **9**, no. 7, 1 (1986).

[20] E. Gadioli and P.E. Hodgson, *Pre–equilibrium nuclear reactions*, Oxford University Press 1992.

[21] S. Cierjacks, Y. Hino, F. Raupp, L. Buth, D. Filges, P. Cloth and T.W. Armstrong, Phys. Rev. **C36**, 1976 (1987).

[22] J. Kopecky, H.A.J. van der Kamp, H. Gruppelaar and D. Nierop, "The European Activation File EAF-3 with neutron activation and transmutation cross sections, ECN-C-92-058 (1992); also in J. Kopecky and D. Nierop, "Contents of EAF-3", ECN-report I–92-023 (1992).

[23] P.F. Rose and C.L. Dunford (eds.), "Data Formats and procedures for the evaluated nuclear data file ENDF-6", Brookhaven National Laboratory report BNL-NCS-44945, 1990.

[24] C.Y. Fu et al., Atomic Data and Nuclear Data Tables 16 (1975) 409.

[25] M. Blann, in *Intermediate energy nuclear data for applications*, Vienna, Austria, 9–12 Oct., 1990.

[26] S. Pearlstein, Nuc. Sci. Eng. **95**, 116 (1987).

[27] S. Pearlstein, "Data requirements for intermediate energy nuclear applications", in *Intermediate energy nuclear data for applications*, Vienna, Austria, 9–12 Oct., 1990.

Appendix A: Brookhaven evaluation

As an example of an existing evaluated intermediate-energy data file, we have investigated the structure of the ^{208}Pb-evaluation by Fukahori and Pearlstein [10] for the energy region 10^{-5} eV - 1000 MeV. We will discuss the neutron file in some detail and subsequently outline the differences with the proton file.

Intermediate-energy neutron file for ^{208}Pb

The directory for this file is displayed in table 5. For the low-energy part (below 20 MeV) the ENDF/B-VI data of Ref. [24] are used. At higher energies, the data are generated by ALICE-P [10, 25] and by systematics [9, 26]. For energies below 20 MeV, the adopted interpolation scheme for energies is linear-linear. At higher energies, progressively larger energy steps are taken and a log-log interpolation scheme is used. The energy grid above 20 MeV for MF3 is 5 MeV between 20 and 100 MeV, 20 MeV between 100 and 300 MeV, and 50 MeV between 300 and 1000 MeV. The elastic cross sections (MT2) are equal to the total (MT1) minus the nonelastic (MT3) cross sections. In MF3/MT5 the (n,anything) cross sections are stored. These comprise all non-elastic processes that are not explicitly considered in other MT numbers. Since the only further specification in MF3 is MT18, we have the sum rule MT5+MT18=MT3. The fission cross sections of MT18 were obtained from experiment-based systematics [9]. No partial (*i.e.* first-, second-, third- and fourth-chance) fission cross sections (MT19-21,38) are specified.

In MF3/MT201 the total neutron-production cross section (excluding elastic scattering) is given. It is defined as the cross section times the neutron yield summed over all reactions involving neutrons in the outgoing channel. In MF3/MT202-207 the total production cross sections for the other light particles are given.

In MF4/MT2 the elastic angular distributions are given in the center-of-mass system (LCT=2) using the normalized probability distribution $f(\mu, E)$ (LTT=2). Each angular distribution is specified by 101 values of μ (cosine of the angle).

In MF6, the used prescription for the energy-angle distribution is:

$$\sigma_i(\mu, E, E') = \sigma(E) y_i(E) f_i(\mu, E, E')/2\pi, \tag{1}$$

where i denotes one particular product, E is the incident laboratory energy, E' is the emission energy, μ the cosine of the emission angle, $\sigma(E)$ is the cross section as given in MF3, y_i is the product yield and f_i is the normalized distribution satisfying

$$\int \mathrm{d}E' \int \mathrm{d}\mu f_i(\mu, E, E') = 1. \tag{2}$$

Table 5: Directory of 0-1000 MeV neutron file for ^{208}Pb: Brookhaven evaluation.

MF	MT	Description
1	451	General information
2	151	Resonance parameters
3	1	Total cross section
3	2	Elastic cross section
3	3	Nonelastic cross section
3	5	(n,anything) cross section
3	18	Total fission cross section
3	201	Total neutron production cross section
3	202	Total photon production cross section
3	203	Total proton production cross section
3	204	Total deuteron production cross section
3	205	Total triton production cross section
3	206	Total He-3 production cross section
3	207	Total alpha production cross section
4	2	Elastic angular distribution
6	5	(n,anything) spallation product yields
6	201	Neutron energy-angle distribution
6	202	Gamma energy-angle distribution
6	203	Proton energy-angle distribution
6	204	Deuteron energy-angle distribution
6	205	Triton energy-angle distribution
6	206	He-3 energy-angle distribution
6	207	Alpha energy-angle distribution

In MF6/MT5 the yields of the product (residual) nuclides are specified (in increasing Z and A), with the outgoing energy in the LAB system (LCT=1) and unknown angular distribution (LAW=0). The yields for the product nuclides that are considered in this file are displayed in table 6. There are only "pure" spallation products: fission products have been neglected. In MF6/MT201, first the neutron yields are given (with emission energies in the LAB system). They have been set to 0 for E < 20 MeV and 1 (because they are already implicitly taken into account in MF3/MT201) for $20 < E < 1000$ MeV. The energy-angle distribution is given according to the laboratory angle-energy law (LAW=7). For incident energies greater than 20 MeV, the coefficients $f_i(\mu, E, E')$ are given at seven values of μ.

For the photon production as given in MF6/MT202, a continuum energy-angle distribution (LAW=1) is adopted. For incident energies above 20 MeV, the Legendre

Table 6: Product nuclides taken into account in intermediate-energy ^{208}Pb evaluation.

Z=76,	A=182-184
Z=77,	A=183-187
Z=78,	A=184-192
Z=79,	A=185-197
Z=80,	A=186-207
Z=81,	A=187-208
Z=82,	A=188-207

coefficients are expanded as follows (LANG=1)

$$f_i(\mu, E, E') = \sum_{l=0}^{NA} \frac{2l+1}{2} f_l(E, E') P_l(\mu) \tag{3}$$

In this file NA=0, giving an isotropic distribution. For MT203-207, the same procedure as for photons is followed.

Intermediate-energy proton file for ^{208}Pb

For protons, a completely new file was constructed, i.e. the part up to 20 MeV has not been taken from an existing evaluated file. The setup is analoguous to that of the neutron file. The directory for the proton file is displayed in table 7. The differences between the proton file and the neutron file are:

- No resonance file MF2 (undefined for charged particles).
- No MF3/MT1 (total cross section, undefined for charged particles).
- Instead of MF4/MT2, MF6/MT2 is used for proton elastic scattering. The secondary energies and angles are given in the CM system and LAW=5 (charged-particle elastic scattering) is used for the energy-angle distribution. The data are represented in the nuclear + interference expansion (LTP=12).

Table 7: Directory of 0-1000 MeV proton file for ^{208}Pb: Brookhaven evaluation.

MF	MT	Description
1	451	General information
3	2	Elastic cross section
3	3	Nonelastic cross section
3	5	(p,anything) cross section
3	18	Total fission cross section
3	201	Total neutron production cross section
3	202	Total photon production cross section
3	203	Total proton production cross section
3	204	Total deuteron production cross section
3	205	Total triton production cross section
3	206	Total He-3 production cross section
3	207	Total alpha production cross section
6	2	Elastic energy-angle distribution
6	5	(p,anything) spallation product yields
6	201	Neutron energy-angle distribution
6	202	Gamma energy-angle distribution
6	203	Proton energy-angle distribution
6	204	Deuteron energy-angle distribution
6	205	Triton energy-angle distribution
6	206	He-3 energy-angle distribution
6	207	Alpha energy-angle distribution

Appendix B: Los Alamos evaluation

As a sample case of the approach by the Los Alamos group [11, 12], we discuss the evaluation of ^{238}U for the energy region $10^{-11} - 100$ MeV.

Intermediate-energy neutron file for ^{238}U

The directory for this file is displayed in table 8. Although this directory is more comprehensive than that of the previously discussed ^{208}Pb evaluation, only a part of the original low-energy evaluation is extended to higher energies. In MF3/MT1, the total cross sections for energies between 20 and 100 MeV are added. The same is done for the elastic cross section of MF3/MT2. Between 20 and 40 MeV, energy steps of 1 MeV are taken and between 40 and 100 MeV energy steps of 2.5 MeV. The intermediate-energy interpolation scheme is linear-linear. For energies below 20 MeV, the partial reaction cross sections are completely specified by MF3/MT4, 16-21, 38, 51-77, 91 and 102. Therefore, in MT5 the cross sections are zero for energies between 0 and 20 MeV. For energies between 20 and 100 MeV, the situation is reversed: all partial cross sections are lumped in MT5 and the cross sections in the aforementioned sequence of MT numbers are zero. The elastic angular distributions of MF4/MT2 are also extended to energies between 20 and 100 MeV. Sections MF4/MT16-21, 38 are not extended to higher energies (these angular distributions are taken as isotropic in the LAB system) and in MF4/MT51-77 the single energy point 100 MeV is added for formal reasons (with an isotropic angular distribution). In all the sections of MF5, data at 100 MeV are added with the same value as those at 20 MeV. In MF6/MT5, the yields and energy-angle distributions for energies between 20 and 100 MeV are given for outgoing neutrons and photons. The secondary energies and angles are given in the CM system (LCT=2) and the energy-angle distributions are given according to LAW=1 (continuum energy-angle distribution). For neutrons LANG=2 (Kalbach representation) is used. For photons, legendre coefficients are expanded as in Eq. (3), with NA=0 (isotropy). The remaining files MF8 and MF14 retain their original form while for all sections in MF12, 13 and 15 the energy point 100 MeV is added with the same data as those at 20 MeV.

In sum, the non-trivial extensions to energies between 20 and 100 MeV are performed in MF3/MT1, 2 and 5, MF4/MT2 and MF6/MT5.

Table 8: Directory of 0-100 MeV neutron file for ^{238}U: Los Alamos evaluation.

MF	MT	Description
1	451	General information
1	452-458	Fission quantities
2	151	Resonance parameters
3	1	Total cross section
3	2	Elastic cross section
3	4	(n,n') cross section
3	5	(n,anything) cross section
3	16	(n,2n) cross section
3	17	(n,3n) cross section
3	18	Total fission cross section
3	19-21,38	1st-4th chance fission cross section
3	51-77	(n,n') cross section for 1st-27th excited state
3	91	(n,n') cross section for continuum
4	2	Elastic angular distribution
4	16	(n,2n) angular distribution
4	17	(n,3n) angular distribution
4	18	Total fission angular distribution
4	19-21,38	1st-4th chance fission angular distribution
4	51-77	(n,n') angular distribution for 1st-27th excited state
4	91	(n,n') angular distribution for continuum
5	16	(n,2n) energy distribution
5	17	(n,3n) energy distribution
5	18	Total fission energy distribution
5	19-21,38	1st-4th chance fission energy distribution
5	91	(n,n') energy distribution for continuum
5	455	Delayed neutron energy distribution
6	5	(n,anything) neutron, photon yields and energy-angle distribution
8	454-459	Fission product yields quantities
12	18	Photon production multiplicity for fission
12	102	Photon production multiplicity for radiative capture
13	3	Non-elastic photon production cross section
14	3	Non-elastic photon angular distribution
14	18	Photon angular distribution for fission
14	102	Photon angular distribution for radiative capture
15	3	Non-elastic photon energy distribution
15	18	Photon energy distribution for fission
15	102	Photon energy distribution for radiative capture

Table 9: Directory of 0-100 MeV proton file for ^{238}U: Los Alamos evaluation.

MF	MT	Description
1	451	General information
3	2	Elastic cross section
3	5	(p,anything) cross section
6	2	Elastic angular distribution
6	5	(p,anything) neutron, proton, photon yields, energy-angle distribution

Intermediate-energy proton file for ^{238}U

For protons, the situation is somewhat simpler (see table 9) since the intermediate-energy proton file is not an extension of an existing low-energy file. Proton elastic angular distributions are given in MF6/MT2 instead of MF4/MT2. Furthermore, MF3/MT1 does not exist. In contrast with the detailed specification as used in the neutron file, the non-elastic cross sections are now lumped in MT5 for *all* energies. A further difference with the neutron evaluation is that in MF6/MT5, besides the neutron and photon yields, also the proton yields are given.