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High Energy Activation Data Library (HEAD-2009)

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A proton activation data library for 682 nuclides from ^{1}H to ^{210}Po in the energy range from 150 MeV up to 1 GeV was developed. To calculate proton activation data, the MCNPX 2.6.0 and CASCADE/INPE codes were chosen. Different intranuclear cascade, preequilibrium, and equilibrium nuclear reaction models and their combinations were used. The optimum calculation models have been chosen on the basis of statistical correlations for calculated and experimental proton data taken from the EXFOR library of experimental nuclear data. All the data are written in ENDF-6 format. The library is called HEPAD-2008 (High Energy Proton Activation Data). A revision of IEAF-2005 neutron activation data library has been performed. A set of nuclides for which the cross-section data can be (and were) updated using more modern and improved models is specified, and the corresponding calculations have been made in the present work. The new version of the library is called IEAF-2009. The HEPAD-2008 and IEAF-2009 are merged to the final HEAD-2009 library.

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I. INTRODUCTION

As a strategy for handling radioactive waste, the transmutation process is offered. For transmutation, the use of dedicated installations such as ADS is required. For the calculation of the integral characteristics of the ADS blanket, such as the effective neutron multiplication factor and the reactivity coefficients, nuclear data in the energy range up to 20 MeV appear to be sufficient in most cases. But for modelling of particle transport, accumulation of spallation products, heating, radiating damage of the structural materials and many other similar problems in which it is necessary to consider separate elements of the system, relevant evaluated nuclear data in a wider energy range are necessary, typically from several keV up to several GeV.

II. ACTIVATION DATA AND STRUCTURE OF THE HEAD-2009 LIBRARY

The collected experimental activation data are contained in the EXFOR library [1]. A typical experiment for material activation is an expensive and time consuming task. For this reason a wide application of nuclear data based computer codes for simulation of high energy nuclear reactions is required. Several data libraries and files containing activation cross-sections for a wide range of the nuclides and reactions were developed by different authors. The largest available proton and neutron activation data libraries are summarized in Tables 1 and 2, respectively. We can see a serious lack of activation data in the energy range above 200 MeV before our IEAF-2005 and HEPAD-2008 libraries were produced. The current HEAD-2009 library consists of proton and neutron sub-libraries. Each sub-library includes a set of separate files for 682 nuclides. The files contain the cross-section data of the proton and neutron reactions with target nuclides in the energy range from 150 MeV to 1 GeV.

III. NUCLEAR REACTION MODELS USED TO DEVELOP OUR HEPAD-2008 LIBRARY

Generally, several codes implementing the quantum molecular dynamic (QMD) and many different semi-classical models are used to simulate nuclear reactions in the energy range 150 MeV – 1 GeV. For semi-classical models, the application field is defined by the energy of the particle or nuclei involved in the interactions. For the description of high-energy interactions (above 150 MeV), different versions of the intranuclear cascade (INC) model have a wide application. In the energy range from several dozen of MeV up to 150 – 250 MeV, various preequilibrium exciton models are used. At

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Table 1. The largest available evaluated proton activation nuclear data libraries.

Library	Number of files / Nuclear charge number range	Primary proton energy range
The European Activation File, EAF-2007 [2]	816 / 1-100	up to 60 MeV
Proton Activation Data File, PADF-2007 [3]	2355/ 12-88	up to 150 MeV
JENDL High Energy File 2007, JENDL/HE-2007 [4]	106 / 1-95	up to 3 GeV
Joint Evaluated Fission and Fusion File, JEFF-3.1 [5]	26 / 20-83	up to 200 MeV
TALYS-based Evaluated Nuclear Data Library, TENDL-2009 [6]	2375 / 6-110	up to 200 MeV
High-Energy Proton Activation Data, HEPAD-2008	**682 / 1-84**	**up to 1 GeV**

Table 2. The largest available evaluated neutron activation nuclear data libraries.

Library	Number of files / Nuclear charge number range	Primary proton energy range
The European Activation File, EAF-2007	816 / 1-100	up to 60 MeV
JENDL High Energy File 2007, JENDL/HE-2007	106 / 1-95	up to 3 GeV
Joint Evaluated Fission and Fusion File, JEFF-3.1/A	774 / 1-100	up to 20 MeV
Medium Energy Nuclear Data Library, MENDL-2 [7]	505 / 13-84	up to 100 MeV
TALYS-based Evaluated Nuclear Data Library, TENDL-2009	2375 / 6-110	up to 200 MeV
The Intermediate Energy Activation File, IEAF-2005	**682 / 1-84**	**up to 1 GeV**

lower energies, the phenomenological evaporation model of Weisskopf [8] and the statistical model of Hauser and Feshbach [9] are usually applied. For heavy nuclei, along with evaporation, the fission process might take place. An important feature influencing the results of simulations, apart from the parameters of each model implemented in a complex code, is the transition criteria between models describing different stages of reactions.

For the calculation of the proton activation data files, the MCNPX 2.6.0 [10] and CASCADE/INPE [11] codes have been used. For the description of nucleon-nuclide interactions, there are several models included in the general purpose radiation transport code MCNPX 2.6.0: There is a possibility to use different combinations of models. A list of physical models implemented in the MCNPX 2.6.0 and CASCADE/INPE codes and used in our HEPAD-2008 calculations is presented in Table 3.

The INCL4 and JINR/Dubna-based intranuclear cascade models have some recent improvements in comparison with older models: The number of quantum effects taken into account by these models is higher and the results obtained using these codes are often in a better agreement with the experimental data. These models and the ISABEL INC model are still under development nowadays, while the development of the Bertini model used in MCNPX was stopped in 1970 – 1980. The possibility for cluster formation during the cascade stage is considered by INCL4 and is accounted via coalescence of nucleons emitted during the INC into complex particles up to ^{4}He by CEM03.01; this is a powerful feature of these models. The modified exciton model (MEM) of preequilibrium reactions developed at JINR, Dubna allows transitions that reduce the number of excitons, in contrast to the Los Alamos multistep preequilibrium model (MPM) that uses only the "never come back" approximation. For the calculation of the nuclear reaction cross-sections on light nuclides, only the MCNPX code was used. Moreover, the majority of the intranuclear cascade- preequilibrium- equilibrium models do not allow making reliable simulations for light nuclides with mass number A $<$ 5. The only model allowing calculations for light nuclides (A $<$ 5) within the MCNPX 2.6.0 is the Bertini INC; it was used in our calculations of the proton activation files for targets with A $<$ 5. Note that the ancient version of the Fermi Breakup model used by CEM03.01 is has some problems and requires further improvements, a problem solved in the latest versions of CEM (see details in Ref. 27).

1. Analysis of the EXFOR experimental data library

For cross-section calculations and the production of evaluated files, it is not enough to be guided only by analytical and expert estimations. Therefore, a detailed statistical analysis of correlations between the EXFOR experimental data and the results by MCNPX using eight different models listed in Table 3 (Bertini/Dresner, Bertini/ABLA, ISABEL/Dresner, ISABEL/ABLA, INCL4/Dresner, INCL4/ABLA, CEM03.01, and CASCADE) has been carried out. All the suitable experimental data from the EXFOR library were chosen in our analysis. In total, about 4000 proton experimental points (measurements) for more than 1000 reactions with nuclides ranging from Z = 6 to Z = 84 and for incident particle energies from 150 to1000 MeV have been analyzed.

2. Choice of the optimum models to calculate the HEPAD-2008 library files

We have used several statistical methods to determine the most appropriate models to use for the production of our library: a method of least squares, correlations, deviation factors, and regression analyses; but finally, the deviation factor analysis was chosen. For an estimation of correlations between the calculated and experimental data, the whole range of the experimental points

Table 3. Physical models of the MCNPX 2.6c and CASCADE/INPE codes used in our calculations.

Model	Code	Nuclear reaction models				
		INC	Preequilibrium	Equilibrium	Fission	Fragmentation
Bertini/Dresner	MCNPX 26C	Bertini [13,14]	MPM [19]	Dresner [21]	RAL [24]	Fermi Breakup Model [25]
Bertini/ABLA	MCNPX 26C			ABLA [22]		
ISABEL/Dresner	MCNPX 26C	ISABEL [15,16]		Dresner	RAL	
ISABEL/ABLA	MCNPX 26C			ABLA		
INCL4/Dresner	MCNPX 26C	INCL4 [17]		Dresner	RAL	
INCL4/ABLA	MCNPX 26C			ABLA		
CEM03.01 [12]	MCNPX 26C	JINR/ Dubna [18] (modified)	MEM [20]	GEM2 [23]		Fermi Breakup (modified) [26]
CASCADE	CASCADE/INPE	JINR/Dubna	-	JINR/ Dubna (Weisskopf model)	JINR/Dubna	not taken into account

Table 4. The models applied to calculate the HEPAD-2008 library files.

Nuclide set	Reference model
1-H-1 – 2-He-4	Bertini INC
3-Li-6 – 10-Ne-22	CEM03.01
11-Na-23 – 13-Al-27	INCL4/Dresner
12-Mg-28 – 27-Co-55	CASCADE
29-Cu-56 – 28-Ni-59	Bertini/Dresner
26-Fe-60 – 40-Zr-89	CASCADE
38-Sr-90 – 54-Xe-124	INCL4/ Dresner
50-Sn-125 – 75-Re-181	CASCADE
72-Hf-182 – 84-Po-210	CEM03.01

(measurements) was divided into approximately equal sets based on the mass number of the target nuclides. Every set included about 400 experimental points, for which the (p,x) reaction cross-sections were calculated using the eight models mentioned above and then the calculated cross-sections were compared with the experimental value. This procedure allowed us to apply the frequency description of the models and to compensate partially the absence of experimental data for certain nuclides. Within the deviation factor analysis, a product of the F- and H-factors was used as the estimated parameter [28]. Note that for the light nuclides from ^{1}H to ^{4}He, the deviation factor analysis was not performed, as the majority of models do not simulate reliably nuclear reactions on light nuclides (A $<$ 5).

For every set of mass numbers, an optimum model has been selected for further calculations. The selected models for all sets are presented in Table 4. These models have been used in our calculations of the HEPAD-2008 library files. The Bertini/Dresner model, which is the fastest among all INC models, has been chosen for the calculations in the target mass range A = 56 - 59. It produces results very similar to the INCL4 model, but is about ten times faster.

The proton activation data files are produced in the ENDF-6 format from the results in the MCNPX 2.6.0 and CASCADE/INPE output files. The relative error, R, was calculated as the ratio of the estimated variance to the average value of the residual cross-section obtained running N Monte-Carlo histories [29]. It has been chosen as a rejection criterion which defined the possibility for inclusion of the proton cross-section data in the library files. The cross-section data were compiled to form the library files if the relative error did not exceed 20%. Several examples of a good agreement between the experimental data and our HEPAD-2008 evaluated files are presented in Fig. 1.

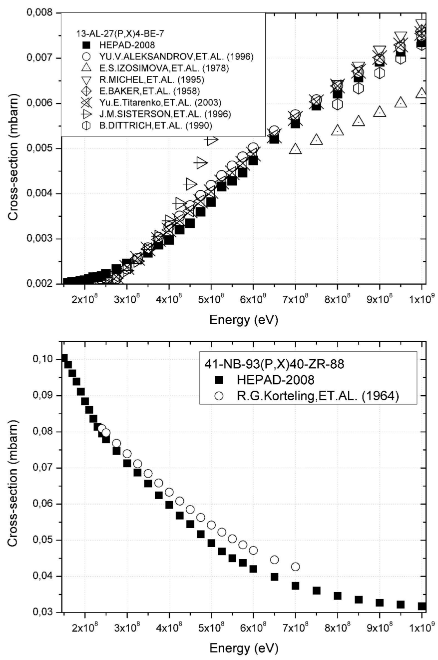

Fig. 1. Examples of excitation functions for several reactions comparing the available experimental data from EXFOR with our calculations from the HEPAD-2008 library.

IV. UPDATED VERSION OF THE IEAF-2005 NEUTRON ACTIVATION NUCLEAR DATA LIBRARY

The IAEF-2005 activation data library was prepared in 2005 as a part of the work on the high-energy activation data library development [30]. The library was developed using the MCNPX 2.5.d [31] and CASCADE/INPE codes and contains neutron-induced activation and transmutation cross sections for target nuclides with Z = 1 to Z = 84 and for neutron energies up to 1 GeV.

The IEAF-2005 and HEPAD-2008 libraries were created using several codes and models, taking advantage of the improvements in the nuclear reaction models over the last several years. Improved models have been applied to calculate the proton activation data. The MCNPX 2.5.d and CASCADE/INPE codes were used for the IEAF-2005 development and the MCNPX 2.6.0 and CASCADE/INPE codes were used for the HEPAD-2008. The CEM and INCL4 models within the MCNPX 2.6.0 code are the most extensively developed and tested nowadays; therefore, they are expected to be among the most reliable.

The files of the IEAF-2005 neutron activation library have been updated using the CEM03.01 model for the nuclides with mass numbers A = 5 - 22 (the Bertini INC is always used by MCNPX to calculate interactions with A < 5 nuclei) and for A = 206 - 209; for other target mass numbers, the IEAF-2005 library remains unchanged. On the whole, 23 files for light nuclei and 16 files for heavy nuclei have been updated in the present work.

V. CONCLUSIONS

The HEPAD-2008 proton activation data library was developed. The majority of the library files were calculated using the modified JINR/Dubna-based intranuclear cascade-exciton or cascade-evaporation models from the CEM03.01 or CASCADE/INPE codes. The remaining files were calculated using the MCNPX 2.6.0 radiation transport code: The INCL4 intranuclear cascade model was used in combination with the Dresner evaporation and RAL fission models. This choice of models has been dictated by the results of the comparison of the EXFOR experimental data with our model calculations. At the final stage, the HEPAD-2008 files have been corrected to the experimental data.

A revision of the IEAF-2005 neutron activation data library has been performed, a set of nuclides for which the cross-section data can be updated using available improved models were specified, and the corresponding calculations have been performed in this work. The files of the IEAF-2005 neutron activation library have been updated using the CEM03.01 model for the target mass numbers A = 5 - 22 and A = 206 - 209; the Bertini INC was used in MCNPX to calculate interactions with A < 5 nuclei. In total, 23 files for light nuclei and 16 files for heavy nuclei have been updated. The new version of the library is called IEAF-2009.

The HEPAD-2008 proton activation nuclear data library and the updated IEAF-2009 neutron activation nuclear data library are merged into the HEAD-2009 High Energy Activation Data Library. The HEAD-2009 Library files can be obtained upon request from the authors.

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