MCNP and MATXS Cross Section Libraries Based on JENDL-3.3

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The continuous energy cross section library for the Monte Carlo transport code MCNP-4C, FSXLIB-J33, has been generated from the latest version of JENDL-3.3. The multigroup cross section library with the MATXS format, MATXS-J33, has been generated also from JENDL-3.3. Both libraries contain all nuclides in JENDL-3.3 and are processed at 300 K by the nuclear data processing system NJOY99.

1. Introduction

The MCNP-4C code [1] is a recent three-dimensional Monte Carlo code which has been widely used over the world. The cross section data in evaluated nuclear data file are reproduced as precisely as possible in a continuous energy library of MCNP without any averaging of cross sections. The discrete ordinary codes have been used as convenient tool in the field of nuclear design and shielding. Their codes use the multigroup cross section library which needs the average and approximation.

As past continuous energy neutron cross section libraries for MCNP in Japan, FSXLIB-J3 [2] was produced from the Japanese Evaluated Nuclear Data Library Version 3 Revision 1 (JENDL-3.1) [3] in 1991. FSXLIB-J3R2 [4] was produced from JENDL-3.2 [5] in 1994. These libraries have been provided for public use.

JENDL-3 was re-evaluated to yield JENDL-3 Revision 3 (JENDL-3.3) [6], and JENDL-3.3 was released at May 2002. Therefore, the continuous energy cross section libraries for MCNP, FSXLIB-J33, has been produced based on it. The multigroup cross section library with the MATXS format [7], MATXS-J33, has been produced also. A MATXS library is converted to a macroscopic cross section of ANISN multigroup library by the TRANSX-2.15 code [8].

2. Modification of NJOY

The NJOY code [7] is a nuclear data processing system used as a standard code throughout the world. NJOY is a unique code to produce a continuous energy library for MCNP and a multigroup library with MATXS format.

The modified version of latest NJOY99.67 was used for processing of JEDNL-3.3. The major modifications are as follows (square brackets represent the name of corresponding module in NJOY).

(1) The nuclides with discontinuous MT in gamma-ray production data are Nb-93 (MT=51), Hg-199 (MT=57) and Pb-207 (MT=53). The energy levels of discontinuous MT were added within code. [HEATR, ACER, GROUPR]

(2) The energy distribution data (MF=5) has the unit base interpolation (linear-linear of INT=22). The unit base interpolation was allowed in only GROUPR module. [GROUPR]

(3) The incomplete treatment of input/output part for MF=32 (covariance of resonance parameters) was modified. [MODER]

(4) Minimum energy for processing unresolved resonance parameters was modified 10 eV to 1 eV, for Pm-148m. [RECONR, UNRESR, PURR]

(5) The KERMA factors of some nuclides that aren't kept the energy balance in evaluation are negative or large values. The KERMA factors of their nuclides aren't calculated with the energy balance method and then they are done with the kinematics method. [HEATR]

(6) If probability at an incident energy in LAW=7 angle-energy distribution is zero, the temporary normalization factor is 1 for avoiding division by zero. [ACER]

There is an incomplete modification for the 'rkal' and 'akal' variables in subroutine acelcp (ACER). These variables are rarely undefined variables in the heating calculation of charged particle on MF=6/LAW=1/LANG≠2. In this case these are initialized to zero as a tentative measure.

3. Production of FSXLIB-J33 and MATXS-J33

First, JENDL-3.3 was processed by the modified NJOY99.67 to produce ACE type cross section data [7] for each nuclide. The ACE type data were compiled into the FSXLIB-J33 library by an exclusive program. FSXLIB-J33 is a library for MCNP-4C as follows: 1) contains a probability distribution table (ptable) as cross section data in unresolved resonance energy region, 2) uses a new format of cumulative angular distribution table (MF=6 /LAW=1/LANG=1) by 'newfor=1' input option in NJOY.

The processing parameters for NJOY to process FSXLIB-J33 are shown in Table 1. The precision of 0.1 % was adopted for the numerical processing by expansion of calculation resource. The temperature considered in Doppler broadening is 300 K. The nuclides used kinematics method for KERMA factor are S-33, 34, 36, Ca-42, 46, 48, Ti-47, Mo-92, 94, 95,

96, 97, 98, 100, Eu-151, 153, Hf-174, 176, 177, 178, 179, 180, Ta-181, W-182, 183, 184, 186, Pb-206, 207, 208, Bi-209. The number of resonance ladders is 1000 and the background cross sections for ptable are 10^{10}, 10^{4}, 10^{3}, 300, 100, 30, 10, 1, 0.1, 10^{-5}. It contains all 337 nuclides in JENDL-3.3. The evaluation identifications in ZAID used to identify nuclide are 42 for elements and isotopes in the ground state and 43 for isotopes in the isomeric states. The data size is about 965 Mbytes in the MCNP type-1 format.

Second, JENDL-3.3 was processed by that to produce MATXS-J33 cross section data for each nuclide. The self-shielding factor is calculated by the PURR module. The photon interaction cross section file for photon transport calculation was the EPDL97 [9]. The processing parameters for NJOY are shown in Table 2. The energy group structure was adopted typical of VITAMIN-J. The basic processing condition is same as FSXLIB-J33. The name of MATXS-J33 data file for each nuclide is “symbol of element”, “3 digits of mass number” and “.m” (for example, fe056.m). The total data size of 337 nuclides is about 592 Mbytes in text format. It is note that MATXS-J33 is inadequate for a critical calculation.

4. Plan of Verification

It is inevitable to verify the consistency of FSXLIB-J33 with the original JENDL-3.3 data. Verification of FSXLIB-J33 has been planed by using the MACROS code [4] with both direct comparison of numerical data between JENDL-3.3 and FSXLIB-J33 and visual checking of cross section data plots.

In order to demonstrate reliability of FSXLIB-J33 and MATXS-J33, benchmark calculations are going to carry out for several integral experiments. A test calculation of FXLIB-J33 for MCNP-4C was made of aluminum sphere with radius 50 cm having point source of 15 MeV neutron at center. Figure 1 is comparison of leakage neutron spectra from sphere. FSXLIB-J33 and FSXLIB-J3R2 finely agree.

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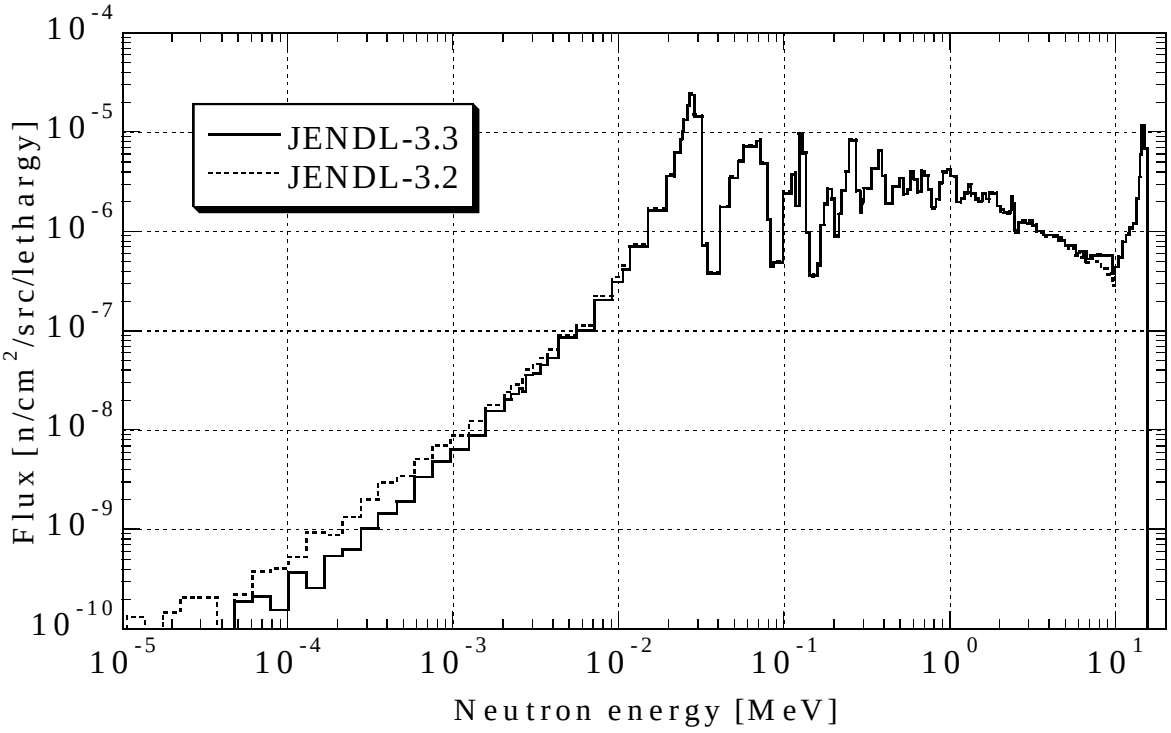

Fig.1 Leakage neutron spectra from Aluminium sphere
(radius 50 cm; 15 MeV neutron source at center)

Table 1 Processing parameters for NJOY99.67 to produce FSXLIB-J33.

Processing Parameter	Adopted Data
precision of point-wise cross sections	0.1 %
temperature of cross sections	300 K (2.53×10^{-8} MeV)
upper-limit energy of thermal energy region	4.6 eV
inelastic option of thermal energy region	free gas model
type of gamma-ray production data	detail form
number of equal-probability angular cosine bins	32
probability table of unresolved resonance	with ptable (length=20)
newfor option	1 (LAW61 format)
calculational method of KERMA	energy balance method
evaluation identification in ZAID	42 for ground state isotopes 43 for isomeric state isotopes

Table 2 Processing parameters for NJOY99.67 to produce MATXS-J33.

Processing Parameter	Adopted Data
precision of point-wise cross sections	0.1 %
group structure	VITAMIN-J (neutron 175g, photon 42g)
order of Legendre coefficients	P-6
temperature of cross sections	300 K (2.53×10^{-8} MeV)
upper-limit energy of thermal energy region	4.6 eV
inelastic option of thermal energy region	free gas model
background cross sections of self-shielding factors	$\sigma_0 = 10^{10}$, 10^4, 10^3, 300, 100, 30, 10, 1, 0.1, 10^{-5}
calculation method of KERMA	energy balance method
storage data	damage (MT=444), μ (251), χ (252), γ (253), 1/v (259)