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A COMPARATIVE STUDY OF TRITIUM BREEDING CALCULATIONS USING EFF-1 AND ENDF/B-V BASED NUCLEAR DATA LIBRARIES

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Abstract: A comparative neutronics study showed that there are large discrepancies in the breeding ratios calculated for lithium lead top-ranking fusion blankets with the EFF-1- and ENDF/B-V- based nuclear data libraries. Detailed analysis is still necessary and data testing integral experiments should be employed to identify the deficiencies in these nuclear data evaluations.

Introduction

The use of adequate nuclear data files is a main issue in the development of new nuclear technologies for D-T fusion power reactors. However, the generation of such files is a time- and money-consuming process and very often a multilaboratory, or international effort (see Howerton[1] and Pearlstein[2]). In the U.S. and Canada, the Evaluated Nuclear Data File (ENDF) is, in general, available for fusion applications. The most current version is ENDF/B-V, which was released in 1979. In the mean time ENDF/B-VI, including double-differential scattering cross sections, is under development. In Europe, the Joint Evaluated File (JEF) (see Rowlands[3]) is a computer-readable repository of (mainly) neutron and photon data in the energy range up to 20 MeV. This file was primarily designed for fission reactor analysis. Starting from JEF, the recently evaluated fusion file EFF (see Gruppelaar[4]) is rapidly becoming the standard data source for fusion and shielding calculations. The first version of this file, EFF-1, includes double-differential data for some nuclides relevant for fusion applications. At the present time EFF-2, an update of EFF-1, is under development.

International collaboration on the generation of evaluated data for nuclear systems applications has been established since 1982 among laboratories in Nuclear Energy Agency (NEA) Data Bank member countries including most western European countries and Japan (see Rowlands[3] and Campbell[5]). Furthermore, the International Atomic Energy Agency (IAEA) is formulating a detailed programme and time schedule for the development of the Fusion Evaluated Nuclear Data Library (FENDL) dedicated to the design of new fusion reactor concepts. FENDL will be based on five existing national files, namely ENDF/B-V and ENDF/B-VI, BROND (a library maintained by the USSR Nuclear Data Center at Obninsk), JENDL-2 and JENDL-3 (Japanese nuclear data libraries), EFF-1 and EFF-2, and ENDL-84 (a library maintained by the Livermore National Laboratory in the U.S.). The major purpose of these activities is to assure the availability of the most accurate nuclear data evaluations to the member countries, and to generate a suitable international fusion file available to any country.

In this framework it is important to perform suitable benchmark calculations against experiments to obtain information about the deficiencies of evaluated nuclear data and to identify actions to eliminate them.

Therefore we performed tritium breeding calculations for promising fusion blankets using nuclear data libraries processed from EFF-1 and ENDF/B-V files. We hope that by comparing the results of these calculations, deficiencies can be identified in both libraries. In this paper, a brief description of the benchmark fusion blanket employed in this comparison study is given. Furthermore the processing scheme for the generation of nuclear data libraries, and computational methods are explained. Finally, results and discussions are given together with the present recommendations on an international fusion nuclear data file.

Benchmark Fusion Blanket

The Benchmark fusion blankets employed in this comparative study are those top-ranking blankets identified in the recent Blanket Comparison and Selection Study (BCSS) (see Smith[6]). These include helium-cooled and self-cooled liquid lithium and lithium lead blankets, and a helium-cooled solid lithium-oxide blanket. The structural alloys are vanadium alloy (V15Cr5Ti) and ferritic steel (HT-9). Neutronic analyses were already performed for the liquid lithium and lithium-oxide blankets, resulting in a comparative study of tritium breeding calculations carried out with JEF-1 and ENDF/B-V based nuclear data libraries (see Cheng[7]). In this paper, only the results obtained for the lead blankets are reported. Table 1 includes the one-dimensional neutronics model showing blanket zoning and material compositions for this BCSS blanket. The simplified cylindrical model consists of a 49cm thick plasma zone, a 11cm vacuum scrape-off region, followed by a 3mm first wall of V15Cr5Ti, by a variably dimensioned tritium breeding zone containing the tritium breeder $Li_{17}Pb_{83}$ and structural material, a 30cm thick manifold consisting of V15Cr5Ti, the breeding material and manganese steel Fe1422, followed by a 2cm gap and a 30cm thick reflector shield of manganese steel and water. 30% and 90% enriched lithium are employed respectively in the breeding material. The plasma (zone 1) and first wall (zone 3) radii represent for this model the parameters of a typical tandem mirror reactor.

Methods of Nuclear Data Library Processing and Neutronics Calculations

Both EFF-1 and ENDF/B-V based nuclear data libraries were processed with the NJOY system (see MacFarlane[8]) from the basic data files. The processing of the EFF-1 based nuclear data library is described in detail in Vontobel[9].

First, pointwise EFF-1 cross sections were reconstructed and broadened with NJOY (Version 6/83) for almost all available isotopes (about 300) and temperatures up to 3000 K. Hereby the thermal region was treated according to the free

Zone No.	Outer Radius (cm)	Component	Materials Composition
1	49.0	Plasma	Void
2	60.0	Vacuum	Void
3	60.3	First Wall	V15Cr5Ti
4	80.3	T. Breeding	7.1% V15Cr5Ti + 73.7% $Li_{17}Pb_{83}$
5	120.3	Manifold	10% V15Cr5Ti + 20% $Li_{17}Pb_{83}$ + 70% Fe1422
6	122.3	Gap	Void
7	152.3	Shield	20% H_2O + 80% Fe1422

Table 1: Neutronics model for lithium-lead BCSS blanket (20 cm thick breeding blanket)

gas model and the available scattering laws (thermal $S(\alpha,\beta)$ matrices).

Second, pointwise data were converted with the NJOY module GROUPR into P_6 groupwise VITAMIN-J cross sections, using the VITAMIN-E input weighting spectrum. The VITAMIN-J structures are similar to VITAMIN-E with some additional energy boundaries (see Sartori[10]), and consist of coupled 175 neutron and 42 photon groups. The method of energy self-shielding of resonances used in this processing bases on the model of a single absorber in an infinite moderator. The narrow resonance approach (Bondarenko model) was employed for shielding the resonances of light structural isotopes. Data of heavier nuclides ($Z \geq 13$) were shielded on the basis of an accurate slowing down pointwise flux calculation in the resolved energy range of the absorber. The original EFF-1 lead file was written in ENDF/B-VI format and contains double-differential scattering data (MF=6 in the ENDF terminology). Since the 6/83 version of the GROUPR module is not able to process MF=6, double-differential cross sections were translated at ECN-Petten into uncoupled angular and energy dependent data (i.e. MF=4, 5 in the ENDF terminology). Therefore lead groupwise data which are referred to EFF-1 do not include in this study all features of the evaluated scattering laws.

Third, the groupwise cross sections were structured to form a MATXS library, using the NJOY module NMATXS. The MATXS file is a cross section library in a flexible format designed to generalize the existing standard CCCC files (see MacFarlane[11]). The new EFF-1 based MATXS file with VITAMIN-J structure is available for fusion and shielding neutronic calculations. It contains P_6 self-shielded temperature dependent neutron and photon data for about 80 nuclides, including all reaction cross sections available on the EFF-1 file, kerma factors and damage cross sections. This library can be coupled to most transport codes using the interface module TRANSX-CTR (see MacFarlane[11]).

The ENDF/B-V based library is a pointwise cross section library, named RMCCS prepared with the NJOY code system for the Monte Carlo Code MCNP (see Los Alamos Monte Carlo Group[12]), by the Los Alamos National Laboratory. Most of the materials in this library were processed with NJOY. The first step in this procedure is to prepare pointwise files as discussed above. The ACER module is then used to prepare an ACE-format (A Compact ENDF) for MCNP. As a first step, all the cross sections are put onto a single union energy grid selected for linear interpolation. Second, the angular distributions from the ENDF file are converted into 32 equally-probable cosine bins for each incident group. Next, secondary energy distributions for emitted neutrons are converted to cumulative probability distributions. Discrete photon yields are used directly, but continuum photon distributions are converted to cumulative distributions. Finally, a set of pointers to each type of data is constructed, and the ACE file is written to the specified output unit. Options for thinning the main energy grid and the incident energy for angle or energy distributions are sometimes used for large files.

This RMCCS nuclear data library and the MCNP code were used for the ENDF/B-V part of the neutronics calculations in this study. The ^{7}Li data were from revision 2 of the ENDF/B-V library (see Young[13]). Statistical uncertainty in the MCNP calculations is less than 1% in all cases.

The neutronics calculations with the EFF-1-based library were performed using the one-dimensional diffusion-accelerated neutral-particle transport code ONEDANT (see O'Dell[14]) and self-shielded transport corrected P_5 cross sections from TRANSX-CTR (Bell-Hansen-Sandmeier transport correction). S_{16} order of angular scattering was considered.

Previous work (see Pelloni[15]) comparing discrete-ordinates methods to MCNP indicates that the total discrepancy between reaction rates that is attribuable to statistics or transport code differences is about 1%. Thus, the primary source of discrepancy is differences in the data sets. For this reason, the statistical errors in MCNP can be omitted.

Results and Discussions

Tables 2-3 display the tritium breeding reaction rates calculated from the EFF-1 and ENDF/B-V based nuclear data libraries for the lithium-lead BCSS blanket with 30 and 90% ^{6}Li enrichment, respectively, for 0.2, 0.5 and 0.6m breeding zone thicknesses.

The maximum discrepancy in tritium production values between ENDF/B-V and EFF-1 is about 6% for ^{6}Li(n,α) in the 20cm thick blanket with 30% ^{6}Li in lithium. As the breeding zone becomes thicker, or the ^{6}Li enrichment increases, the still large discrepancy decreases down to 3%. This is because the system is well moderated and the breeding reaction is favored in such a way that all available neutrons are already absorbed by ^{6}Li, even if its concentration in the breeder is small. The ^{7}Li(n,n'α) rate agrees well in all calculations but is found to be almost irrelevant to the total tritium production, since in this BCSS blanket the neutron multiplier has been incorporated into the breeding material. Most differences between EFF-1 and ENDF/B-V results are found to come primarily from the different inelastic scattering, capture, and (n,2n) data of lead. The Pb(n,2n) rate from the ENDF/B-V calculations is higher by up to 7% in the case of thin BCSS blanket configurations and lower lithium enrichments. This results in enlarged tritium breeding ratio, and indicates significant differences in the (n,2n) lead cross sections up to the energy of the fusion peak (assumed at 14.1 MeV) between both evaluations. For thicker or higher enriched blankets, the multiplication and the breeding ratios tend to become more similar. This is due to saturation effects. The capture rate of lead shows similar trends, but it is smaller in magnitude. The discrepancies in breeding ratios and capture rates of lead are indicative for a different slowing down of fast neutrons mainly induced by the lead inelastic scattering cross sections.

Table 4 is aimed to confirm previous considerations. It includes the results pertaining to the lithium-lead BCSS blanket with 90% ^{6}Li in lithium and 60 cm thick breeding zone. In order to achieve a better comparison between lead cross sections in both evaluations, the energy of the fusion peak was assumed to vary between 14.1 MeV and 14.9 MeV.

Breeding Zone Thickness (m)	0.2	0.2	0.5	0.5	0.6	0.6
Library	EFF-1	ENDF/B-V	EFF-1	ENDF/B-V	EFF-1	ENDF/B-V
T6	0.718	0.769	1.122	1.169	1.225	1.282
T7	0.014	0.015	0.017	0.018	0.018	0.018
TBR	0.732	0.784	1.149	1.187	1.243	1.300
Pb(n,2n)	0.585	0.625	0.706	0.714	0.714	0.714
Pb(n,γ)	0.027	0.032	0.053	0.057	0.059	0.064

Table 2: Comparison of calculated reaction rates in lithium-lead BCSS blanket using EFF-1 and ENDF/B-V libraries (30% ^{6}Li in lithium)

Breeding Zone Thickness (m)	0.2	0.2	0.5	0.5	0.6	0.6
Library	EFF-1	ENDF/B-V	EFF-1	ENDF/B-V	EFF-1	ENDF/B-V
T6	1.085	1.138	1.448	1.495	1.520	1.560
T7	0.002	0.002	0.002	0.002	0.002	0.003
TBR	1.087	1.140	1.451	1.498	1.522	1.563
Pb(n,2n)	0.584	0.621	0.705	0.712	0.712	0.711
Pb(n,γ)	0.020	0.023	0.034	0.037	0.037	0.039

Table 3: Comparison of calculated reaction rates in lithium-lead BCSS blanket using EFF-1 and ENDF/B-V libraries (90% ^{6}Li in lithium)

Energy of Peak (MeV)	14.1	14.1	14.5	14.5	14.9	14.9
Library	EFF-1	ENDF/B-V	EFF-1	ENDF/B-V	EFF-1	ENDF/B-V
T6	1.520	1.560	1.532	1.562	1.542	1.589
T7	0.002	0.002	0.002	0.002	0.002	0.002
TBR	1.522	1.563	1.534	1.565	1.545	1.592
Pb(n,2n)	0.712	0.712	0.722	0.725	0.730	0.726
Pb(n,γ)	0.037	0.039	0.037	0.039	0.037	0.040

Table 4: Comparison of calculated reaction rates in lithium-lead BCSS blanket using EFF-1 and ENDF/B-V libraries, obtained different fusion sources

The tritium breeding reaction rates increase smootly of maximum 1.5% using both the EFF-1 and ENDF/B-V data libraries by shifting the fusion peak from 14.1 MeV up to 14.9 MeV. This is due to the corresponding increase of the Pb(n,2n) reaction rate. However, different trends can be recognized when comparing both libraries with respect to this reaction. Whereas the rate from the ENDF/B-V library increases of 2%, that from EFF-1 increases of 2.5%. If the fusion pick lies at 14.9 MeV the Pb(n,2n) rate predicted by EFF-1 becomes higher than that from ENDF/B-V. Thus the Pb(n,2n) cross sections in the highest energy range above 14 MeV must be larger in EFF-1 than in ENDF/B-V. As far as the capture rates of lead are concerned, these remain almost unchanged if the energy of the fusion peak is varied.

Conclusions

A comparative neutronics study showed that there are large discrepancies in the $^{6}Li(n,\alpha)$ reaction rates calculated for top-ranking fusion blanket concepts with lead as the neutron multiplier, when using EFF-1 and ENDF/B-V based nuclear data libraries. Detailed analysis is necessary to identify the deficiencies in the nuclear data evaluations. Particularly, future work should deal with the utilization of the new dutch module GROUPXS (see Gruppelaar[16]), which is able to process double-differential cross sections, especially important for lead based blankets.

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