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FUSION NEUTRONICS CALCULATIONAL BENCHMARKS FOR BASIC NUCLEAR DATA
AND TRANSPORT CODES INTERCOMPARISON*

by

M. Youssef

J. Jung

M. Sawan

MASTER

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FUSION NEUTRONICS CALCULATIONAL BENCHMARKS FOR BASIC NUCLEAR
DATA AND TRANSPORT CODES INTERCOMPARISON

M. YOUSSEF, School of Engineering and Applied Science, Uni-
versity of California at Los Angeles, Los Angeles, CA 90024

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J. JUNG, Argonne National Laboratory, 9700 South Cass Avenue,
Argonne, IL 60439

M. SAWAN, Nuclear Engineering Department, University of
Wisconsin, 1600 Johnson Drive, Madison, WI 53705

Abstract Four calculational benchmarks have been selected to
compare various nuclear data libraries based on both ENDF/B-
IV and V, and to compare results from various transport
codes. Discrepancies up to 20% in tritium production from

${}^7\text{Li}$ were found and have been attributed mainly to differences
in current ENDF/B-IV and V evaluations while ~4% is attri-
buted to differences in the group structure of the libraries
used. Results from MCNP and VIP Monte Carlo codes are in
good agreement but MORSE calculations show good agreement
only for high threshold reactions.

INTRODUCTION

The range of the uncertainty in predicting reaction rates of
importance in fusion blanket design has been identified by select-
ing four benchmarks for basic data and codes intercomparison.
Items that have been investigated are: (a) results for different
order of Legendre expansion in the neutron scattering cross-sec-
tion; (b) impact of using various multigroup neutron cross section
libraries on results; (c) results of calculations based on ENDF/B-
IV and V; (d) differences in results between various Monte Carlo
and discrete ordinates codes. The cross section libraries used
are the LANL 80-group library MATXS6 (ENDF/B-V), the LANL 30-group
library MATXS5 (ENDF/B-V), the LANL 30-group library MATXS1
(ENDF/B-IV), the ANL 46-group library ANL46 (ENDF/B-IV), and the
continuous energy library of the MCNP Monte Carlo code, RMCCS13/23
(ENDF/B-V) and RMCCS3 (ENDF/B-IV). The codes used in the analysis
are ONEDANT (1-D), DOT 4.3 (2-D discrete ordinates), MCNP, VIM,
and MORSE (3-D Monte Carlo).

The first benchmark is a closed Li_2O spherical geometry surrounding a fusion point source. The second benchmark is a series of infinite slab geometry consisting of natural lithium, SUS316 stainless steel, Be, ^{16}O , Pb, and C, considered individually. A point source incident on a pseudo-cylindrical Li_2O assembly located in a vacuum was considered in the third and fourth benchmarks. In the latter, a 4 cm-thick SUS316 first wall was included. Both a 14.1 MeV source and a moderated source (spectrum #1 and spectrum #2) were independently considered in the analysis. Details of the atomic densities, mesh dimensions and various spectrum used in the intercomparison can be found in reference (1).

Results were compared at selected locations for the reactions $^6\text{Li}(n,t)$ [T_6], $^7\text{Li}(n,\alpha)t$ [T_7], $\text{Al}(n,\alpha)$, $\text{Au}(n,\gamma)$, $\text{Ni}(n,2n)$ and the fission rate in ^{235}U , ^{238}U , ^{232}Th , and ^{237}Nb . The angular neutron spectra at the outer boundary of the series of slabs in benchmark #2 were compared for the materials considered.

RESULTS OF ANALYSIS

Several discrepancies have been identified in the analysis. The P_3S_{16} calculation for tritium production rate gives lower results than only 0.5 % in benchmark #1 than the P_5S_{16} calculation. However, this discrepancy is larger (4-6% for the 14.1 MeV source, 3-5% for spectrum #1) in benchmarks #3 and #4 for all the reactions considered. The small difference obtained in benchmark #1 is due to the fact that an appreciable portion of neutrons incident on the first wall in benchmark #1 includes low energy neutrons that are collided and reflected from the other side of the closed geometry considered. Hence, considering higher order scattering in closed geometries does not improve the results much.

The impact of the neutron group structure on results is that with spectrum #2, the MATXS5 library yields 1-3% larger T_6 and 1-2% lower T_7 in benchmark #1 as compared to results with the MATXS6 library. The discrepancy is slightly lower (0.5-2.5% larger T_6 , 0.5-1.5% lower T_7 with MATXS5) in the case where the 14.1 MeV source is considered. The same trend was found in benchmarks #3 and #4. However, the discrepancy is 4-9% larger T_6 and 1-3% lower T_7 with spectrum #1 and similar differences were found with the 14.1 MeV source. Thus, using fewer groups tends to increase T_6 and to decrease T_7 . For the threshold reactions $^{238}\text{U}(n,f)$ and $^{232}\text{Th}(n,f)$, the agreement between the two libraries is excellent (less than 1%) in all benchmarks and for all different sources. The $^{235}\text{U}(n,f)$ reaction rate has relatively larger discrepancies. With the MATXS5, the values are larger as follows: benchmark #1: up to 11% with spectrum #2, and 12% with the 14.1 MeV source; benchmark #3 and #4: up to 3-7% with spectrum #1, and 2-6% with the 14.1 MeV source. The $\text{Ni}(n,2n)$ reaction rate in

benchmarks #3 and #4 shows discrepancy of the order of 1-3% between the two libraries. The largest discrepancy found is for the Au(n, γ) reaction rate. The difference at all locations considered reaches a value of ~26% larger with the MATXS5 for both the 14.1 MeV and spectrum #1 cases. The cause for this discrepancy has not been identified yet and it may be due to error in data processing since both libraries are based on ENDF/B-V. Table (I) displays one case for this discrepancy.

TABLE I The Au(n, α) Reaction Rate in Benchmark #4 With MATXS5 (30-Group) and MATXS6 (80-Group) Libraries. A 14.1 MeV Source Was Used in a P₅S₁₆ Approximation

P ₅ S ₁₆			
Position r = 0 cm	MATXS5	MATXS6	% Difference
Z = 2 cm	4.8976-29	3.9511-29	23.6
6	6.7425-29	5.3389-29	26.3
10	6.5739-29	5.2020-29	26.4
20	5.3154-29	4.2634-29	24.7
30	3.6569-29	3.0328-29	20.6
40	2.2034-29	1.9003-29	15.9
50	1.1082-29	9.0722-30	22.2

Comparison between results based on both ENDF/B-IV and V have also been performed. The MATXS1 library gives 1-5% larger T₆ and 13-15% larger T₇ as compared to the MATXS5 in benchmark #1 and this range is the same with the 14.1 MeV source. The ANL46 library (ENDF/B-IV) yields 2-12% larger T₆ and 4-20% larger T₇ as compared to results with the MATXS6 library in benchmark #3. Including a first wall in benchmark #4 makes the discrepancy for T₇ get larger (5-22%). Discrepancies among fission rates in ²³⁵U, ²³⁸U, ²³²Th, and ²³⁷Np in benchmark #1 (spectrum #1) are 0.3-4%, 2-5%, 1-6%, and 0.5-3%, respectively. In benchmarks #3 and #4, the discrepancies are as follows: ²³⁵U(n,f): 0.5-7% in benchmark #3, 0.5-6% in benchmark #4; ²³⁸U(n,f): 1.5-8% in benchmark #3, 2-7% in benchmark #4; Al(n, γ): 0.5-12% in benchmark #3, 2-11% in benchmark #4; Ni(n,2n): 7-27% in benchmark #3, and 8-25% in benchmark #4. For the last reaction, the ENDF/B-V gives the larger values.

The calculations for benchmark #2 were performed using P₅S₃₂ approximation with the MATXS1 and MATXS5 libraries. The angular flux at the back of the slab was evaluated for the angles 9.7° and 42.9°. Deviations up to ~20% were observed when ENDF/B-IV and V

data were compared. The least deviation occurs for oxygen case while the largest deviation occurs for the lead and beryllium cases. ENDF/B-V data yields harder spectrum in the lead case and a softer spectrum in the beryllium case.

The results for the MCNP, VIM, and MORSE calculations for benchmarks #3 and #4 have shown excellent agreement between MCNP and VIP (continuous energy and angle) particularly in the first 30-40 cm and the error is less than few percent. However, good agreement between MCNP and MORSE is only obtained for high-threshold reaction, e.g., $^{238}\text{U}(n,f)$ and $^7\text{Li}(n,\alpha)t$. The large deviation of MORSE from MCNP for non-threshold reactions, e.g., $^{235}\text{U}(n,f)$ and $^6\text{Li}(n,\alpha)t$ may be due to the current technique for the variance reduction in MORSE which is characteristic to multigroup methods since the same variance reduction method, e.g., Russian Roulette, was used for all the three codes. The agreement between the MCNP and DOT results is reasonable as shown in Table (II).

TABLE II Comparison Between MCNP and DOT 4.3 Results in Benchmark #3

Position r = 0 cm (cm)	T_6			T_7		
	DOT ^a	MCNP	% ^b	DOT ^a	MCNP	% ^b
Z= 0- 4	2.21-7	2.09-7(3.0%)	5.7	2.65-6	2.46-6(1.4%)	7.7
= 4- 8	2.88-7	2.81-7(3.2%)	2.5	1.79-6	1.65-6(1.7%)	8.5
= 8-12	2.99-7	2.69-7(3.5%)	11.2	1.18-6	1.09-6(2.2%)	8.3
=12-15		2.55-7(3.6%)			7.56-7(2.7%)	
=15-25	2.46-7	2.14-7(2.9%)	14.9	4.34-7	4.31-7(3.0%)	0.7
=25-35	1.65-7	1.58-7(6.1%)	4.4	1.67-7	1.75-7(4.6%)	-4.6
=35-45	9.81-8	9.33-8(5.3%)	5.1	6.52-8	6.91-8(7.4%)	-5.6
=45-55	4.92-8	4.54-8(7.5%)	8.3	2.55-8	2.43-8(11.0%)	-9.9

^aCalculation performed with MATXS6 library (80-Group), P₅S₁₆, with spectrum #1.

^b $\frac{\text{DOT} - \text{MCNP}}{\text{MCNP}} \times 100$

REFERENCES

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