

# APPLICATION OF JADE V&V CAPABILITIES TO THE NEW FENDL V3.2 BETA RELEASE

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## 1. INTRODUCTION

The production chain of nuclear data libraries, that starts from experiments and models and goes up to evaluated nuclear cross sections ready to be used in the transport codes, is quite complex [1][2]. For this reason, nuclear data libraries must undergo extensive quality assessment procedures and Verification & Validation (V&V) process. This is true also for FENDL libraries, the fusion-dedicated libraries developed and maintained by the IAEA Nuclear Data Section. A recent IAEA-FENDL consultant meeting [3] underlined the need for a standardized, automated and exhaustive V&V procedure that would help to speed up the process for new FENDL releases and to help in improve their quality. This input, a collaborative effort started between NIER, Fusion For Energy (F4E) and the University of Bologna (UNIBO) focused on the development of JADE [4], a new Python 3 based tool, that is able to automatically run and post-process a suite of both experimental (for libraries validation) and computational benchmarks (for libraries comparison and verification). The transport code on which JADE run its simulations is MCNP v6.2 [5].

A new FENDL nuclear data library (v3.2) is currently being beta-tested before its official release using the Sphere Leakage computational benchmark contained in the JADE tests suite.

## 2. METHODOLOGY

The geometry of the Sphere Leakage benchmark is reported in Figure 2.1. It consists of a 1 m diameter sphere composed by a single isotope hosting a central 14 MeV neutron point source. Several outputs are tallied including neutron and secondary photons leak flux (both in fine and coarse energy binning), tritium and helium production, nuclear heating and DPA values.

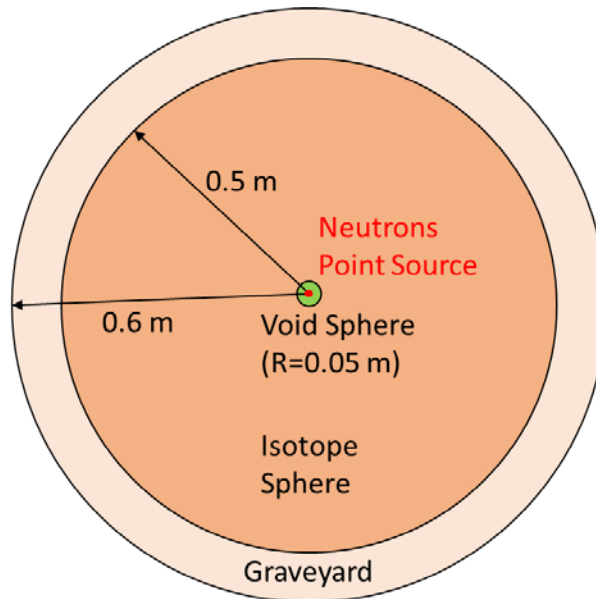


Figure 2.1 – Sphere Leakage benchmark geometry

JADE automatically creates a different MCNP input for each isotope available in the library under assessment plus a number of typical ITER materials. After that, the automated post-process is launched both for the single library and for the comparison among libraries. FENDL v3.2 was assessed and compared against the FENDL v3.1, FENDL v3.0 and ENDF-VII.1.

### 3. RESULTS

For brevity, only the more significant results from JADE's output are reported using the as abbreviations:

- FENDL v3.2: 32c;
- FENDL v3.1: 31c;
- FENDL v3.0: 30c;
- ENDF-VII.1: 70c.

As far as the sanity checks on the FENDL v.3.2 are concerned, no anomalies have been spotted. That is, all the values of neutron and photon leakage flux (in all energy bins), DPA production, tritium production and helium production are positive or zero for all the isotopes contained in the library. Additionally, no significant differences are spotted for the nuclear heating computation (both of neutrons and photons) using the F4+FM or F6 MCNP tallies.

An extract of the JADE comparison xls sheet of FENDL v3.1 Vs FENDL v3.2 is shown in Figure 3.1. As it can be observed, the sheet contains the comparison of the results obtained using the two libraries for each isotope and each tally of the Sphere Leakage benchmark. Each of these comparisons constitutes an individual comparison cell as highlighted in the figure. From this extract it can be seen how the two libraries under assessment performed significantly different for the Potassium-40 (K-40) and Potassium-41 (K-41). In particular, a substantial difference is recorded in the low energy neutron leakage flux (<0.1 MeV) that reasonably influenced also the secondary photons leakage flux and, consequently, the photon heating in the sphere and tritium production.

In order to have a global perspective of the comparison between FENDL 3.2 and FENDL 3.1, it is recommended to examine Table 3.1, which summarize, for each tally, what is the percentage of individual comparison cells (i.e. the number of isotopes) that presented a difference in the ranges [0 , 5%], [5%,10%], [10%,20%] or more than 20%. It can be observed that the major differences between the libraries appear to be in the lower energy bins of the photons leakage flux (t22) and in the neutron heating. The reason causing the first result is still under investigation while the second one can be easily explained.

GLOBAL QUICK RESULT: % of cells per range of comparison differences																		
Range	1e-06 [MeV] [t12]	0.1 [MeV] [t12]	1.0 [MeV] [t12]	10.0 [MeV] [t12]	20.0 [MeV] [t12]	Total [t12]	0.01 [MeV] [t22]	0.1 [MeV] [t22]	1.0 [MeV] [t22]	5.0 [MeV] [t22]	20.0 [MeV] [t22]	Total [t22]	T production	He ppm production	DPA production	Neutron heating F6	Gamma heating F6	Tot
0 < % of cells < 5.0	84%	98%	99%	99%	100%	99%	15%	69%	96%	98%	89%	98%	97%	96%	98%	82%	99%	89%
5.0 < % of cells < 10.0	9%	0%	1%	1%	0%	1%	8%	16%	2%	0%	5%	0%	0%	0%	1%	0%	0%	2%
10.0 < % of cells < 20.0	4%	1%	0%	1%	0%	1%	19%	9%	1%	1%	2%	1%	1%	0%	1%	2%	0%	2%
% of cells > 20.0	3%	1%	0%	0%	0%	0%	58%	6%	1%	1%	4%	1%	2%	4%	0%	16%	1%	6%

Table 3.1 - JADE comparison recap table, FENDL v3.2 Vs FENDL v3.1

Individual comparison cell

LIBRARY:		31c_Vs_32c																
SPHERE LEAKAGE COMPARISON RECAP																		
ZAID		TALLIES																
		Neutron Flux (Coarse energy bins) Tally n. 12						Gamma Flux (Coarse energy bins) Tally n. 22						T production	He ppm production	DPA production	Neutron heating F6	Gamma heating F6
		1e-06 [MeV] [t12]	0.1 [MeV] [t12]	1.0 [MeV] [t12]	10.0 [MeV] [t12]	20.0 [MeV] [t12]	Total [t12]	0.01 [MeV] [t22]	0.1 [MeV] [t22]	1.0 [MeV] [t22]	5.0 [MeV] [t22]	20.0 [MeV] [t22]	Total [t22]					
18036	Ar-36	0.00%	0.00%	Identical	Identical	0.00%	Identical							0.00%	Identical	0.00%	0.00%	
18038	Ar-38	0.00%	0.00%	Identical	Identical	0.00%	Identical							0.00%	0.00%	0.00%	0.00%	
18040	Ar-40	Identical	0.00%	0.00%	0.00%	0.00%	Identical							0.00%	Identical	Identical	Identical	0.00%
19039	K-39	0.00%	0.00%	2.33%	Identical	0.67%	Identical	-0.16%	-0.04%	0.00%	0.00%	-0.02%	0.00%	0.01%	0.61%	0.00%	-0.01%	
19040	K-40	36.25%	-0.81%	2.74%	0.06%	-5.71%	25.85%	21.14%	27.05%	25.20%	34.12%	25.13%	-16.80%	-29.21%	11.81%	-2.77%	30.20%	
19041	K-41	398.34%	51.55%	-3.83%	0.34%	-0.92%	-11.71%	64.53%	27.81%	21.37%	15.12%	39.95%	20.68%	46.74%	-2.75%	8.96%	17.74%	25.21%

Potassium comparison Results

Figure 3.1 – Extract from the JADE comparison excel sheet between FENDL v3.1 and FENDL v3.2

The reason lies in the errors contained in the KERMA tables of many FENDL v3.1 isotopes that cause a negative heating value as already discussed in [6] and re-spotted by JADE consistency checks. Since this anomaly was fixed in FENDL v3.2, a difference is registered between the two libraries heating values.

The differences highlighted by the xls comparison regarding the neutron leakage flux of K-40 and K-41 can be better visualized in the plots contained in the JADE produced atlas. Such plots are reported in Figure 3.2 where not only the flux resulting from FENDL v3.1 and v3.2 are reported, but also from v3.0 and ENDF-VII.1.

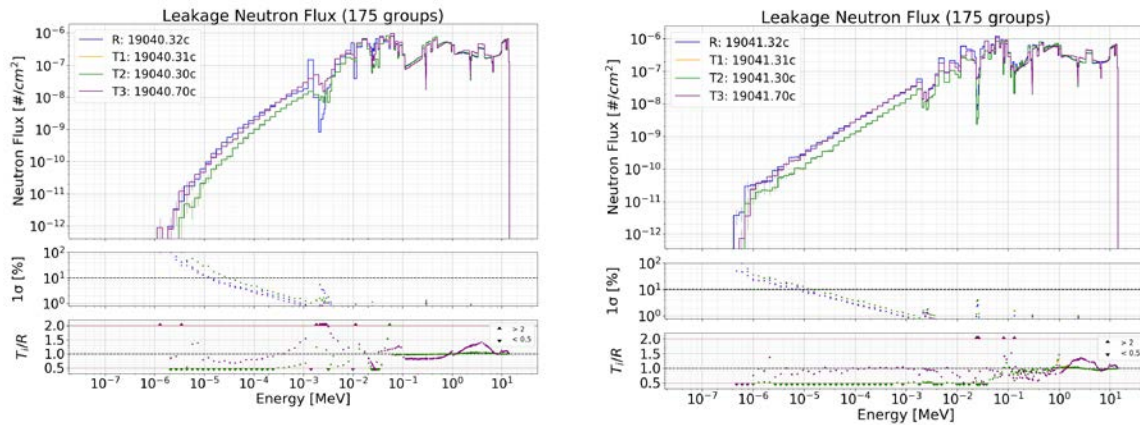


Figure 3.2 – Neutron leakage flux comparison between FENDL v3.2, FENDL v3.1, FENDL v3.0 and ENDF-VII.1 for the Potassium-40 (left) and Potassium-41 (right)

As it can be observed, the flux of FENDL v3.2 is substantially higher than the one of v3.1 (same as v3.0), being more similar to the one obtained using ENDF-VII.1 instead.

To conclude, minor differences are also spotted in Fe56 evaluation, production of He ppm in W isotopes and Mn-55 and need to be further examined.

#### 4. CONCLUSIONS

A new FENDL nuclear data library, v3.2, is being tested before being officially released supporting IAEA FENDL mission. A new and under development V&V tool, JADE, has been used to provide additional testing implementing the Sphere Leakage benchmark for each isotope contained in the library. As a result, the consistency checks on the FENDL v3.2 have all been passed and the library appears to perform in a very similar way to its predecessor, the FENDL v3.1. The main exception appears to be the behaviour of Potassium-40 and Potassium-41 isotopes which, instead, present significant differences in the neutron leakage flux obtained using the two libraries.

#### 5. ACKNOWLEDGEMENTS

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