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BENCHMARKING OF THE SCALE CODE PACKAGE AND MULTI-GROUP CROSS SECTION LIBRARIES FOR ANALYSIS OF LEAD-COOLED FAST REACTOR

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ABSTRACT

The Generation IV [1] International forum identified six advanced reactor concepts and related fuel cycles along with the R&D programs necessary to achieve the four key goals: (1) sustainability, (2) safety and reliability, (3) economics, (4) proliferation resistance and physical protection. Among these six promising reactor concepts, the lead-cooled fast reactor (LFR) has been selected for development by EURATOM, which in 2006 decided to finance the European Lead Cooled System (ELSY) project. The aim of the project is to demonstrate the possibility to design a safe and competitive lead-cooled fast power reactor using simple engineering solutions. This paper demonstrates the use of the code package SCALE5.1 and its NEWT/TRITON modules [3] for preliminary neutronic core analysis of a LFR within Generation IV Nuclear Energy systems program. More specifically, the analysis of the reference design of the ELSY-600 open square fuel assembly is presented. In particular, the use of ENDF/B-V and ENDF/B-VI.7 and multigroup energy structure was investigated. The homogenized cross sections calculated for the ELSY fuel assembly 2D model have been evaluated and compared to the results obtained with calculations performed with the deterministic code ERANOS/ECCO using JEFF2.2 cross section library. A good agreement has been observed in the energy range of interests, and generally for energy above 1eV.

Key Words: Lead-cooled fast reactor (LFR), European Lead Cooled System (ELSY), SCALE code package, Benchmarking of data libraries

1. INTRODUCTION

The R&D program on ELSY was started in 2006 and is aimed to the demonstration of the possibility to design a safe and sustainable lead cooled fast reactor in order to cope with the four key goals of Generation IV. Among the activities included in the ELSY R&D program the neutronics design plays a very important role. Any diffusion or transport theory model of the

[1] The presented work was performed during the first author's research visit to Georgia Institute of Technology.

core for the evaluation of the most important reactor physics parameters (such as neutron fluxes, fission rates and neutron spectrum) needs reliable values of the group constants. This work is focused on the demonstration of the use of the coupled NEWT/TRITON [2, 3] code sequence of the SCALE5.1 code package for lead cooled fast reactor core analysis. In particular, the use of ENDF/B-V and ENDF/B-VI.7 and multigroup energy structure was investigated. NEWT solves the time-independent two dimensional neutron transport equation in multi-group energy approximation by using the extended step characteristic approach. The functional module TRITON provides the ability to create a weighted master-format broad-group cross section library collapsed from the original fine-group library used in the NEWT calculation. The nuclear libraries available in SCALE5.1 were developed and tested primarily for light water reactors, thus a benchmark analysis has been carried out by using MCNP[5] Monte Carlo code and the deterministic code ERANOS. The benchmark calculations are the pin cell and the fuel assembly with a fuel composition corresponding to the average composition of the whole core of the tentative design of ELSY-600.

2. DEVELOPMENT OF THE MODEL

The model implemented in NEWT is a two-dimensional representation of the ELSY fuel assembly. As the first step, calculations of the ELSY pin cell using the 238 group cross section library available in SCALE5.1, have been performed in order to generate broad group libraries to be used in the final fuel assembly calculation. The energy structure of the collapsed libraries is based on the 33 group energy structure used in sodium fast reactor calculations with ERANOS/ECCO code[7]. While not optimized for a lead fast reactor, it is believed to be a reasonable starting point. Generating broad group cross section libraries becomes necessary to enable effective analysis of the whole reactor core. In fact in this case the computational burden can become an issue if a fine group structure is used in transport or diffusion calculations. The following subsections describe the nuclear dataset and model implemented in NEWT/TRITON.

2.1 Nuclear Data

The nuclear data used for the analysis are based on ENDF/B-V and B-VI.7. These data are available in SCALE5.1 as multi-group cross section libraries, 238groupndf5 (ENDF/B-V) and v6-238(ENDF/B-VI). The multi-group libraries were collapsed in a 33 group energy structure whose boundary values are shown in Table I.

2.2 Geometry and Assumptions of the Fuel Assembly Model

Two options for fuel assembly configurations are currently under investigation: the square and the hexagonal lattice geometry. In this work the square lattice option is considered. The fuel assembly presents an array of 21x21 fuel pins. In the center of the assembly a stainless steel channel is located for the finger absorber insertion. The fuel is mixed oxide (MOX) UO_2/PuO_2 fuel. Its porosity has been assumed to be 0.95 of theoretical density for the purpose of this computational benchmark. The fissile content in plutonium corresponds to the average fissile content of the whole core of ELSY which in the tentative design includes three radial regions with different compositions, the plutonium content increasing from the centre of the core to the

periphery in order to flatten the neutron flux profile. Figure 1 shows the layout of the fuel assembly[2]. The geometrical parameters are listed in Table II.

Table I. Energy Structure of the 33 group library

group	Upper En (eV)	group	Upper En (eV)	group	Upper En (eV)	group	Upper En (eV)
1	2.00E+07	**11**	1.28E+05	**21**	9.50E+02	**31**	7.15E+00
2	1.73E+07	**12**	8.50E+04	**22**	6.70E+02	**32**	3.73E+00
3	1.57E+07	**13**	5.20E+04	**23**	2.85E+02	**33**	4.50E-01
4	8.19E+06	**14**	2.50E+04	**24**	2.40E+02	**Cut off**	1.00E-05
5	2.48E+06	**15**	1.30E+04	**25**	1.19E+02		
6	1.50E+06	**16**	9.50E+03	**26**	8.20E+01		
7	1.25E+06	**17**	6.00E+03	**27**	6.50E+01		
8	7.50E+05	**18**	3.74E+03	**28**	3.91E+01		
9	4.40E+05	**19**	2.58E+03	**29**	2.10E+01		
10	2.00E+05	**20**	1.55E+03	**30**	1.19E+01		

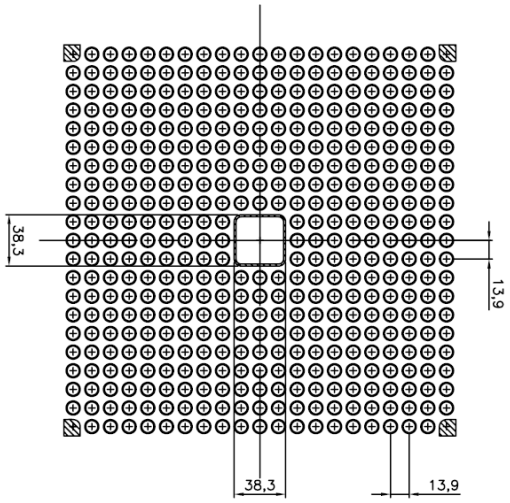


Figure 1. Fuel Assembly Design

The cladding material is ferritic martensitic steel T91 which is characterized by high radiation resistance. The ongoing R&D activities are demonstrating the possibility to improve the protection against the corrosion using particular coating techniques like GESA treatment or superficial aluminization. The objective is to reach an operation period of 5 years or longer. The current analysis doesn't take into account this possibility.

The model implemented in SCALE is based on the following assumptions:

1) Material densities (Table III) are calculated for the nominal operating conditions and temperatures i.e. 1200K for the fuel, 750K for the cladding and 700K for the coolant. These

2 designed by Ansaldo

temperatures are based on a preliminary thermo-hydraulics analysis [4] of the core. The temperature of the coolant at the core inlet is around 400 °C and should not be higher than 480°C at the core out-let because of the corrosive effect of the lead on the structure material.

2) The neutron cross sections of the material composition are corrected for the operating temperatures.

Table II. Fuel Assembly Design Parameters

Fuel rod pitch	13.9	[mm]
Fuel rod diameter	10.5	[mm]
box structure inner	32.3	[mm]
box structure outer	38.3	[mm]
box thickness	3	[mm]
FA pitch	291.9	[mm]
Linear ext fuel in/FA	288.5	[mm]
Linear extension SS	291.9	[mm]
Fuel Pellet Diameter	8.98	[mm]
Clad Inner Diameter	9.3	[mm]
Clad Outer Diameter	10.5	[mm]
Pu Enrichment	15.24%	Pu/(Pu+U)

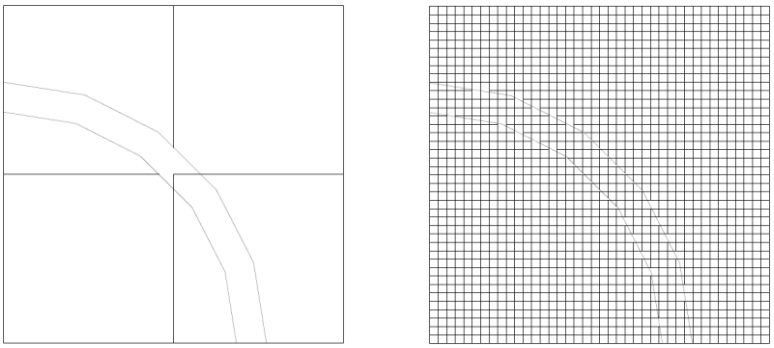
Table III Material densities

Material	**Density @ 293 K (g/cm3)**	**Density @ working Temperatures (g/cm3)**
UO_2+PuO_2	PuO_2 - 11.32 UO_2- 10.91	10.137 (mixture)
Stainless Steel	7.73	7.59
Lead	11.02	10.515

3. ANALYSIS AND RESULTS

3.1 Pin Cell Calculation

The results of the pin-cell calculation are “fuel pin-cell” cross sections. These cross sections are used in the second step, which embodies the full-assembly calculation. Thus the spectra obtained from the pin cell calculations have been used to collapse the neutron cross sections from 238 to 33 energy groups. In order to choose an adequate spatial mesh, its influence on the multiplication factor was studied. In Fig. 2 are shown the two of the four mesh structures considered in the sensitivity analysis.



(a) (b)

Figure 2. Pin Cell Mesh Structures considered in the sensitivity analysis. (1) Coarse Mesh – 8 cells; (2) Fine mesh – 1659 cells.

The results of the criticality calculation are shown in Fig.3 where the behavior of the k as a function of the mesh size, more precisely as a function of the number of the computational cells is plotted. The results show that the k-effective is weakly dependent on the mesh size; the k varies from a maximum of 1.18005, which corresponds to the a number of cells equal to 8, to a minimum value of 1.17987 which means a difference smaller than 20pcm (per cent mille); in this case the number of cells is greater than 1600.

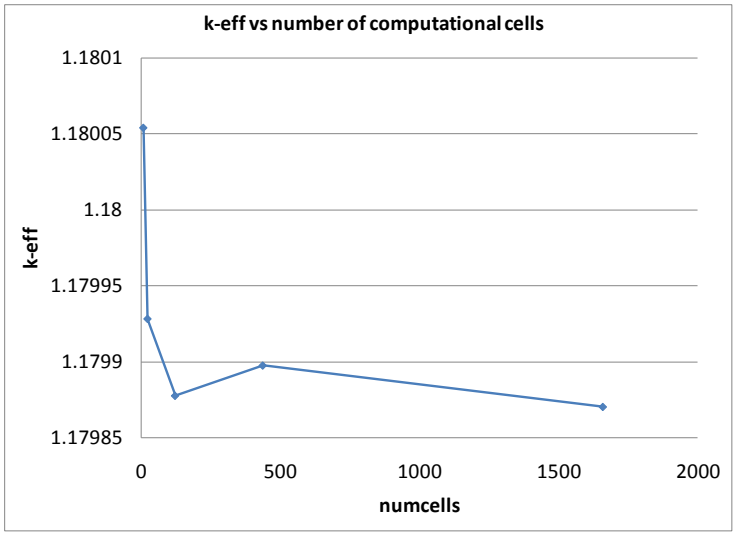


Figure 3. Effective k as a function of mesh size

Given the relatively small impact on k of the mesh structure, the coarsest mesh structure was used in fuel assembly calculations.

Table III summarizes the results obtained from the pin cell criticality calculations with the two available nuclear data, libraries, 238groupndf5 and v6-238 libraries. The effective multiplication factor values differ by approximately 1%. Nevertheless, as the Fig. 4 shows, the two different sets of nuclear data give different results for energies below 10^{-5}MeV. The energy behavior of the normalized flux per unit of energy is shown. In the low energy range, the spectrum calculated

with ENDF/B-V is higher and the difference increases as the energy decreases, reaching several orders of magnitude. Although the neutrons at those energies do not have as much "importance" as to modify the integral result represented by the k effective; this discrepancy has not been fully understood and further investigations are needed to find its source.

Table III Pin cell multiplication factors

Multi-group Library	k-eff
ENDFB-V 238 groups	1.17990
ENDFB-VI 238 groups	1.18382

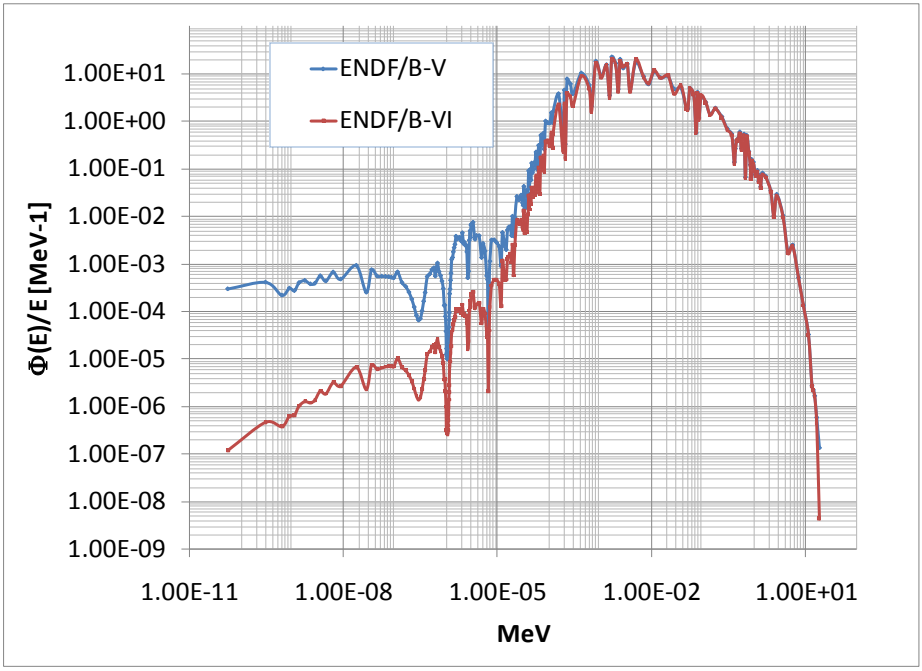


Figure 4. Neutron Flux Energy spectrum

In order to verify the correctness of the previous results, a Monte Carlo calculation of the pin cell has been performed using nuclear data of the same origin (ENDF/B-V). The energy binning of the MCNP flux tally is based on the energy structure of the 33g collapsed library rather than the 238-g structure of NEWT. The energy spectrum obtained with MCNP using the ENDF/B-V nuclear data set is compared to the spectrum calculated with NEWT in Fig. 5.

The MCNP calculated value of k-effective is 1.17007 with an estimated standard deviation of 0.00059, obtained with a total of 400,000 histories. For energies below 10 eV the statistics in the MCNP calculation makes it difficult to produce reliable results. It should be noted that while the comparison at lower energies may be interesting to understand various features of different libraries, it does not impact the neutronics of ELSY, which is driven by higher energies.

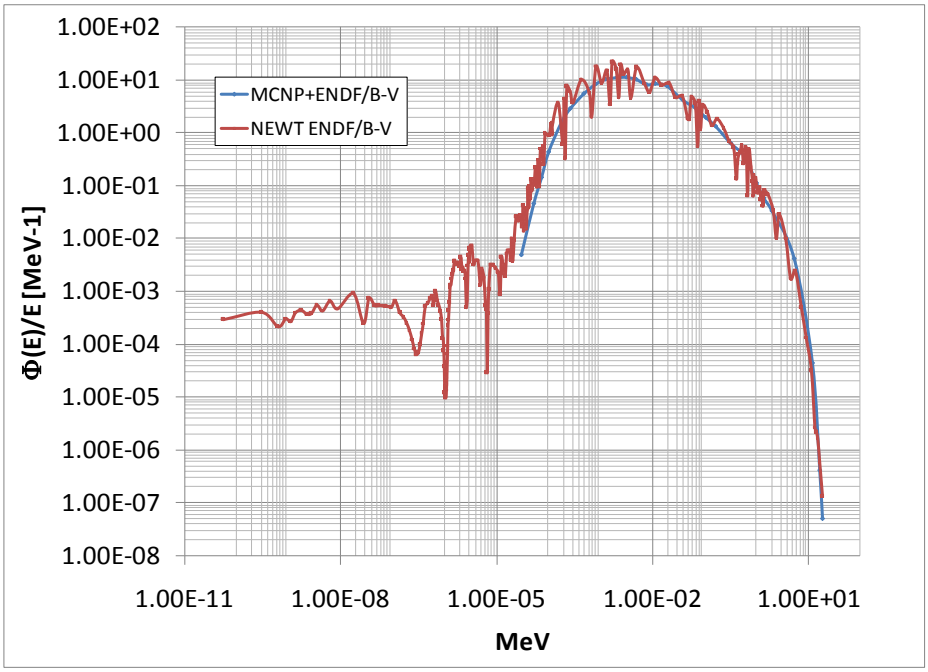


Fig. 5. MCNP, NEWT calculated neutron energy spectra

3.2 Fuel Assembly Calculation

The neutronic analysis of ELSY fuel assembly (Fig. 6) has been carried out using the 33 group collapsed library obtained from the pin cell model. The fine group library has been used to obtain a reference solution in order to assess if the energy structure of the collapsed library is suitable to adequately describe the ELSY fast neutron spectrum. Table IV lists the results of the fuel assembly criticality calculations.

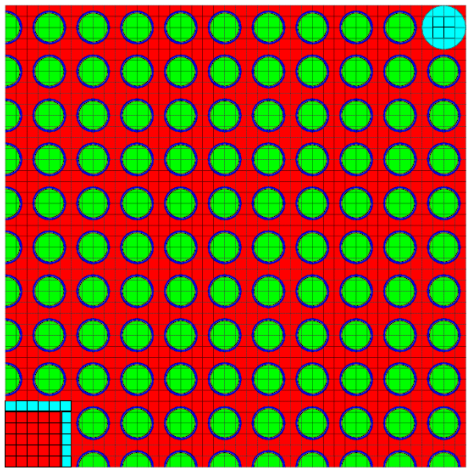


Fig. 6. Fuel Assembly NEWT model

Table IV Comparison of multiplication factor for fine and coarse energy structure

	238 groups	33 groups collapsed using the pin cell spectrum
ENDF/B-V	1.16023	1.15960
ENDF/B-VI.7	1.17031	1.17632

The reason why the difference between the broad and the fine group library based on ENDF/B-VI is higher than in ENDF/B-V is still not clear and is being further analyzed. Nevertheless, the difference between the k-effective values is less than 1 % which can be considered acceptable for a preliminary design of the reactor core.

NEWT also provides the ability to produce macroscopic weighted cross sections homogenized over one or more mixtures. The flux weighted collapsed cross sections are combined with number densities and added such that reaction rates in homogenized materials are conserved. This procedure has been applied to the ELSY fuel assembly in an attempt to better understand the differences between the nuclear data sets. The macroscopic cross sections have been calculated with NEWT using the two collapsed libraries showing small difference at low energies (Figs. 7 and 8). In particular in Fig. 8 the $\nu\Sigma_f$ macroscopic cross section is shown for both investigated libraries. At high energies the behavior is practically indistinguishable.

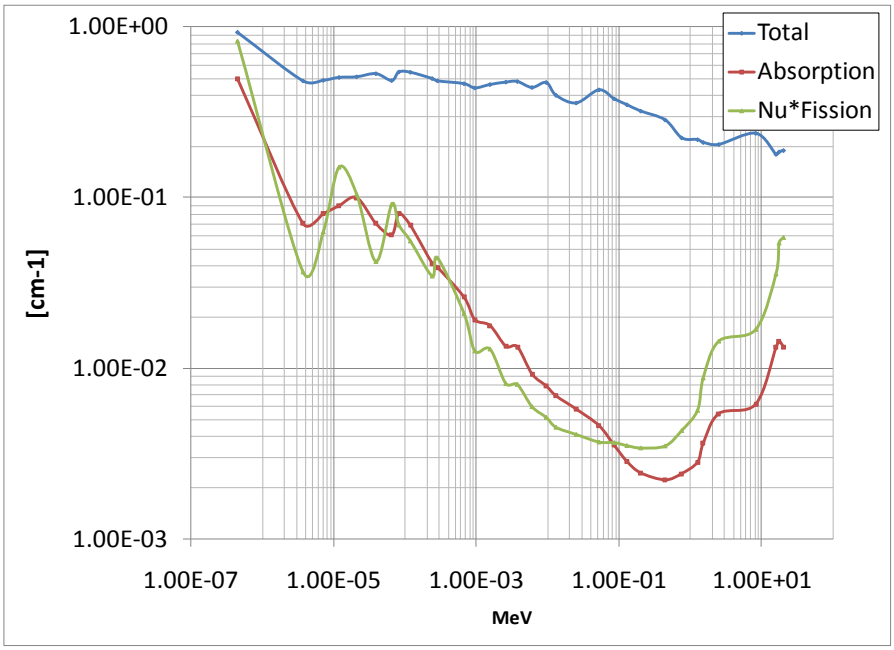


Fig. 7 Homogenized macroscopic cross sections with ENDF/B-V

The same calculation on the fuel assembly has been performed by ENEA with ERANOS with JEFF2.2 library [4]. The comparison of the $\nu\Sigma_f$ macroscopic cross section calculated with NEWT/TRITON (ENDF/B-V) and ERANOS (JEFF2.2) shows significant discrepancies at low energies (<10 eV) and a good agreement at higher energies (Fig. 9). This difference is being

further investigated. The same comment as before is in place: the agreement is relatively good in the energy range of interest.

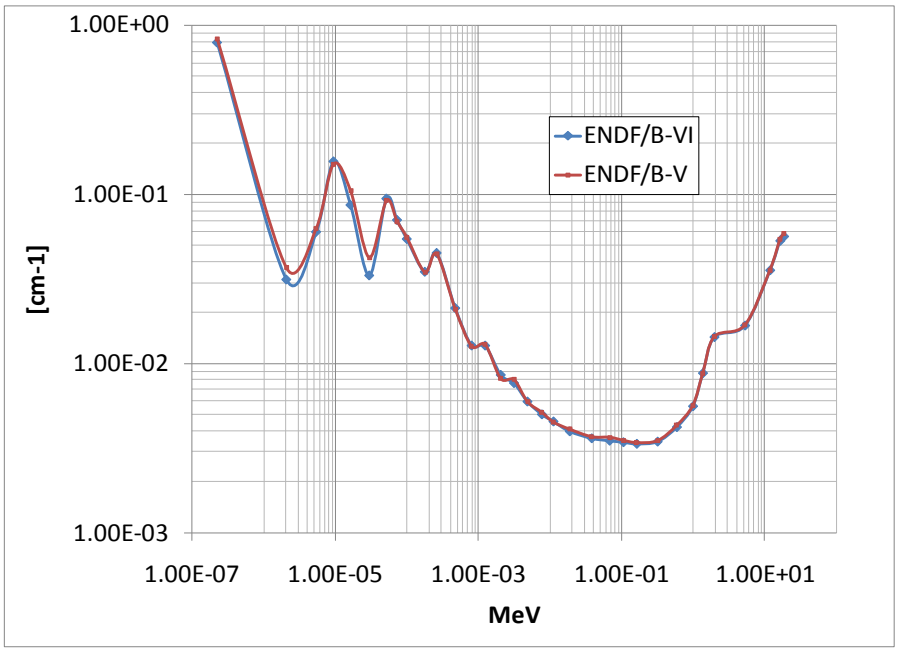


Fig. 8 NEWT $\nu\Sigma_f$ homogenized macroscopic cross sections calculated with ENDF/B-V,VI

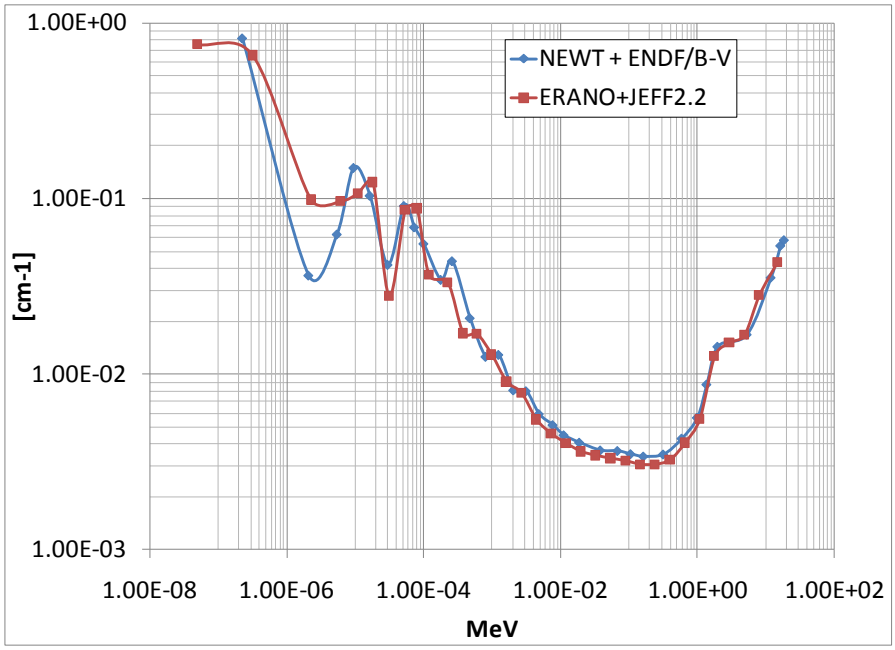


Fig. 9 NEWT-to-ERANOS $\nu\Sigma_f$ homogenized macroscopic cross sections comparison

4. CONCLUSIONS

This work has demonstrated the adequacy of the SCALE 5.1 code system and in particular its component NEWT/TRITON for a preliminary neutronic analysis of a lead cooled fast reactor core, using a collapsed 33-group library. The benchmark calculations have been performed for the pin cell and the square fuel assembly of the ELSY reactor. The fuel assembly analysis has been performed using the 238 group libraries and the 33 group cross section libraries obtained by weighting the 238 group data with the spectrum of the ELSY pin cell. The results have shown that the broad multi group cross sections give reasonable results in terms of the flux spectrum and multi group constants. Results obtained using ENDF/B-V and B-VI.7 libraries present several orders of magnitude discrepancies in the neutron flux spectrum for energies below 10 eV. However this difference has only a small impact on the calculation of integral parameter k-eff, which, in the pin cell model, varies by less than 1% as a function of the nuclear data library. Homogenized cross sections have been evaluated and compared to the homogenized cross sections calculated with ERANOS/JEFF2.2. The agreement is evident for energy above 1eV. Below this energy the $\nu\Sigma_f$ macroscopic cross section shows a different behavior. Further benchmark calculations are needed to establish the accuracy of the results obtained with the 33 broad group library which will be optimized in the future work.

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