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Identification of Need for improved Nuclear Data
Summary Report

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SUMMARY

The calculations of important reactor reactivity parameters and fuel composition as a function of burn-up are biased due to uncertainties of the available nuclear data. The impact of the uncertainties in the basic data on the calculated quantities depends from type of fuel and from the moderation conditions. Therefore, for the HTR-N project by means of comparisons of calculated and experimental parameters of benchmarks and sensitivity analyses the quality of currently available nuclear data with reference on HTR specific systems was proven. Additionally, comparisons of calculated parameters for HTR systems performed by Monte Carlo calculations based on the evaluated nuclear data files JEF-2.2 (JEFF-3), ENDF/B-VI and JENDL-3.2 were performed, to investigate the influence of today's most actual nuclear data on criticality. The results of these comparisons showed sufficient good agreement for JEF-2.2 and JENDL-3.2 based calculations for a large variety of moderation ratios. ENDF/B-VI (release 5) based calculations for HTR wit UOX fuel showed a substantial under-estimation for low moderation ratios as it is the case for low moderated LWR systems with UOX fuel. Recently evaluated ENDF/B-VII (still preliminary) data for the main U isotopes show remarkable improvements and give much more reliable results for low enriched moderated systems.

Furthermore, sensitivity studies connected with uncertainty analysis were performed for the GTMHR with RG-Pu and WG-Pu fuel for zero and high burn-up. The variation of the capture and fission cross sections of Pu isotopes show the largest sensitivity coefficients with reference to reactivity corresponding to the number densities at zero and high burn-up. The influence of minor actinides is lower than 15 pcm/% for RG-Pu and about 5 pcm/% for WG Pu. Uncertainties due to the calculated sensitivities and covariance data for the regarded heavy nuclides are estimated to about 0.6 % for WG-Pu fuel (both for low and high burn-up). A need for actualised covariance data was found since there are rather few reliable processed data available for thermal systems.

The scattering law data and thermal neutron spectra in graphite were investigated based on newer publications since the present available data for thermal neutron scattering in graphite were not actualised for a considerable long time. Comparisons of a measured and calculated thermal neutron spectra in graphite were made for three different scattering law data sets derived from published frequency distributions. The main result of these comparisons confirmed the quality of the presently used ENDF/B and JEF scattering law data.

INTRODUCTION

The analysis of reactor reactivity behaviour and fuel composition as a function of burn-up depends largely on the quality of available nuclear data. Propagation of uncertainties in the basic data can lead to a substantial departure of calculated quantities from experimental one. Furthermore, also the calculation of criticality parameters of cores with fresh fuel depends on quality of nuclear data. Comparisons of calculated and experimental parameters of experimental configurations (benchmarks) as well as sensitivity and uncertainty analysis were done from CEA, NRG and IKE to prove the impact of today's available nuclear data on HTR and future VHTR specific nuclear analysis. The impact of the evaluated nuclear data files JEF-2.2 (JEFF-3), ENDF/B-VI and JENDL-3.2 on calculated criticality parameters was proven for HTR-systems. The results of comparisons showed comparable good agreement of JEF-2.2 and JENDL-3.2 based calculations for a large variety of moderation ratios. ENDF/B-VI (release 5) based calculations showed large under-estimation for low moderation ratios (high U based fuel load). This effect can be seen also for corresponding low moderated LWR systems. Recently there was a great effort to improve this situation; the (preliminjary) results are the new evaluations of the U isotopes U-235, U-236 and U-238 in ENDF/B-VII which is planned to release in near future.

Sensitivity studies and uncertainty calculations for GTMHR with RG-Pu and WG-Pu at low and high burn-up showed sensitivity coefficients for capture and fission for the main Pu isotopes and Am-241. From this results one can conclude that the capture and fission of Pu isotopes has the main influence on reactivity corresponding to the number densities at zero and high burn-up. The variation of the reactivity due to minor actinides is lower than 15 pcm/% for RG-Pu and even 5 pcm/% for WG Pu. Uncertainties derived from the sensitivity matrix and covariance data for the analysed heavy nuclides are about 0.6 % for WP-Pu fuel (for low and high burn-up). This means that the isotopes with high sensitivities have comparable small standard deviations, the less well-known isotopes, on contrary have a lower influence on reactivity. This situation changes, however, when hihg burnup is reached. Here also so called minor actinides can became important and the larger uncertainty (compared to the main actinides) cannot be accepted.

The results of the WP 2 studies are reported in following documents (Table 1). The idea was to compare existing data evaluations in respect to typical HTR fuel and performing simplified but typical burnup calculations for different irradiation histories representing reload strategies and specific fuel. From these calculations the impact of nuclides on safety related parameters due to its uncertainty can be derived.

Table 1: Documents for WP2

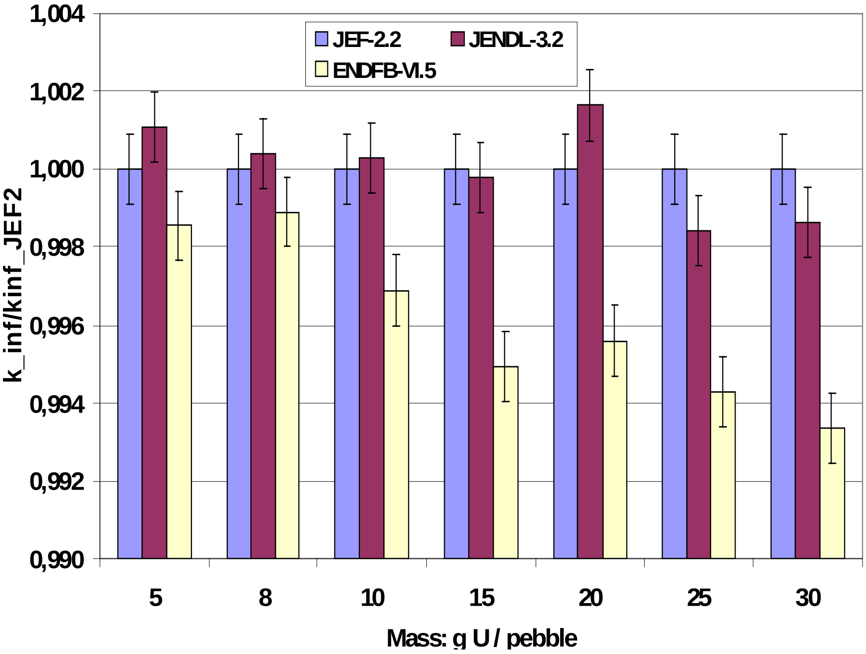
HTR-N-01/05-D-2.1.1	Specification of fuel cells composition and power histories relevant to WP1 and WP3	CO
HTR-N-01/05-D-2.1.3	Neutronics calculations for specified cells and power histories	CO
HTR-N-01/05-D-2.1.4	Sensitivity analysis and estimation of major impact of nuclear data uncertainties to reactivity & mass balance	CO
HTR-N-01/05-D-2.1.2 HTR-N-01/05-D-2.1.5 HTR-N-01/05-D-2.1.6	Generation of cross section sets based on newly released evaluations	CO
HTR-N-02/06-D-2.2.1	Quality Assurance Requirements on Nuclear Data	CO
HTR-N-04/07-D-2.2.2	Synthesis on Requirements for improvement of nuclear data	CO
Physor 2004, Chicago Ill, USA, Apr. 25-29, 2004	Scattering Law Data for Graphite in Gas cooled HTR	PU

VALIDATION

The Accuracy of neutronics calculation (e. g. criticality, power distribution and nuclide composition as a function of burn up) depend from quality of nuclear data and methods
The available modern data evaluations are compiled in JEF-2.2 , JEFF-3 (newest JEF data), ENDF/B-VI, revisions 0-8 and JENDL-3.2 (since 2002 also JENDL-3.3). Further data can be fount in CENDL (China) and BROND (Russia). These data are world-wide in use for all kind of power reactors and should also be used for HTR related studies.

The accuracy of nuclear data can be checked by re-calculation of well documented experiments (benchmarks) by best estimate methods (e. g. continuous Monte Carlo or multigroup transport methods). For HTR systems few simple and well documented benchmarks are available for checking the influence of nuclear data itself. For several HTR systems there exist experimental data from first criticality which are very valuable for validation of the methods for neutronics calculations but they are rather complicated and calculational results may be also influenced from uncertainties in geometrical or material descriptions and the methods and simplification used.

Comparisons of calculated multiplication factors for pebble bed cores based on different nuclear data evaluations showed a good agreement for low U load between for the three data evaluations JEF-2.2, ENDF/B-VI and JENDL-3.2. For high U load (strongly under-moderated systems) ENDF/B-VI (release 5) and JEFF-3t based calculations under-estimate multiplication factors significantly (Fig.1). As it is the case for systems with alternative moderators (e. g. H_2O). Generally, at least for fresh cores there is a good overall agreement for a large number of benchmarks for the three mainly available nuclear data evaluations (Fig.2).



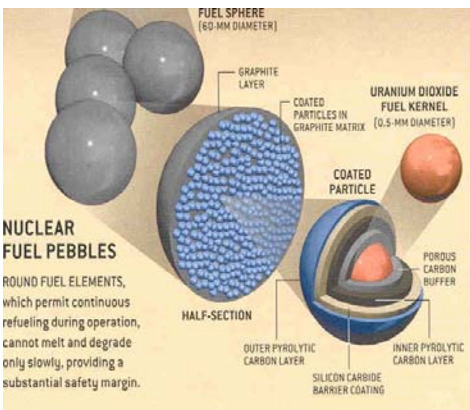


Fig. 1: Comparison of keff calculated for HTR-cells with UOX for different data evaluations as a function of U load per pebble

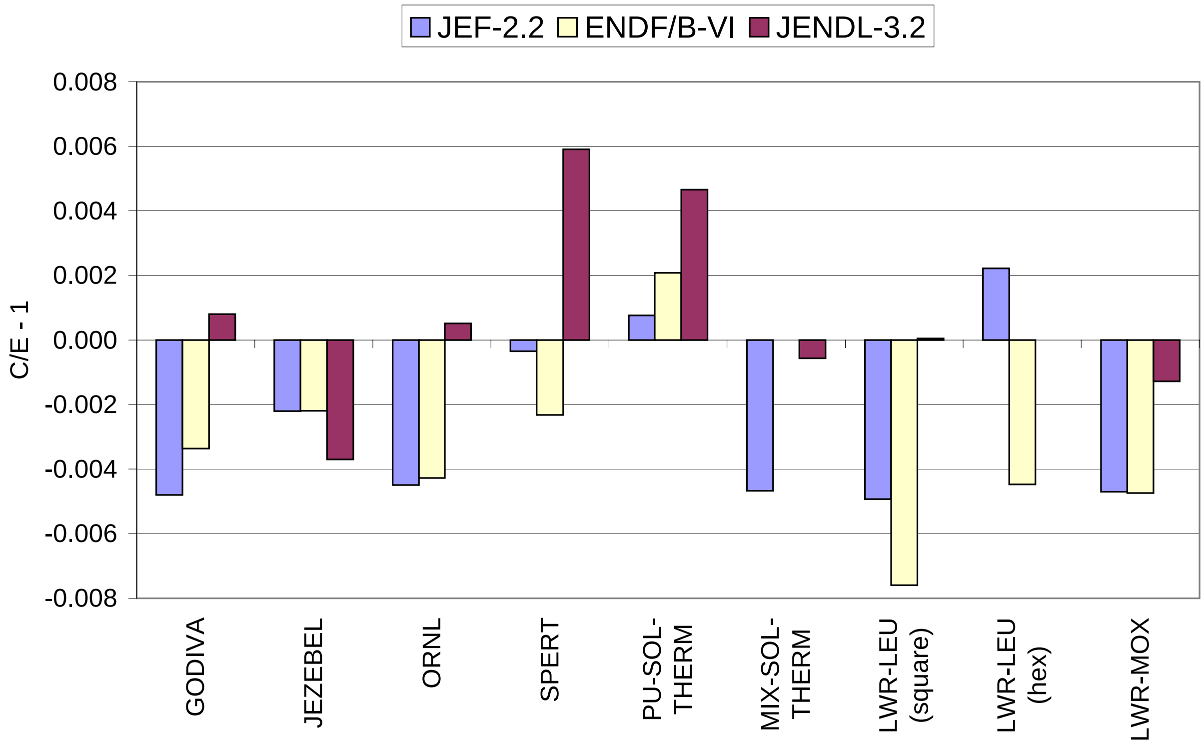


Fig. 2: Relative differences between MCNP calculations and measurements for different data evaluations and benchmark series.

The present working evaluation groups on nuclear data take into consideration many benchmarks for data evaluations. But at time, the HTR specific benchmarks are under-represented. Therefore, there is a need for co-working of HTR interested groups in corresponding working groups (e. g. in JEF data evaluation group).

The evaluation of design accuracy of power reactors can be performed also by means of sensitivity and uncertainty analysis using covariance data. By this method the importance of different calculational parameters and the identification of mayor sources of uncertainties can be found. Sensitivity analysis for HTGR design with WG Pu-fuel and RG Pu-fuel showed high k_{eff} sensitivities for Pu-239 (capture and fission) decreasing with burnup and for Pu-240 (capture) and Pu-241 (fission) increasing with burn up. Overall uncertainty of keff based on sensitivity analysis and covariance data for actinides are for WG Pu fuel about 0.6 %. Higher uncertainties in nuclear data for minor actinides are of less importance for k_{eff} but obviously they have an important influence for the calculation of nuclide composition of fuel with normal and especially with high burn up (see Fig. 3).
Sensitivity studies therefore should take into account also this aspect which is not only important for criticality but also for composition of waste in respect to burn up credit for storage, heat production, radiation sources and radiotoxicity. The nuclear data basis for the calculation of isotopic composition of irradiated fuel should be verified by experiments. At the PMM the need for re-calculation at least of some of the most important available experiments (e. g. spent fuel analysis for HTR fuel with distinct irradiation histories, performed at AVR) was identified.

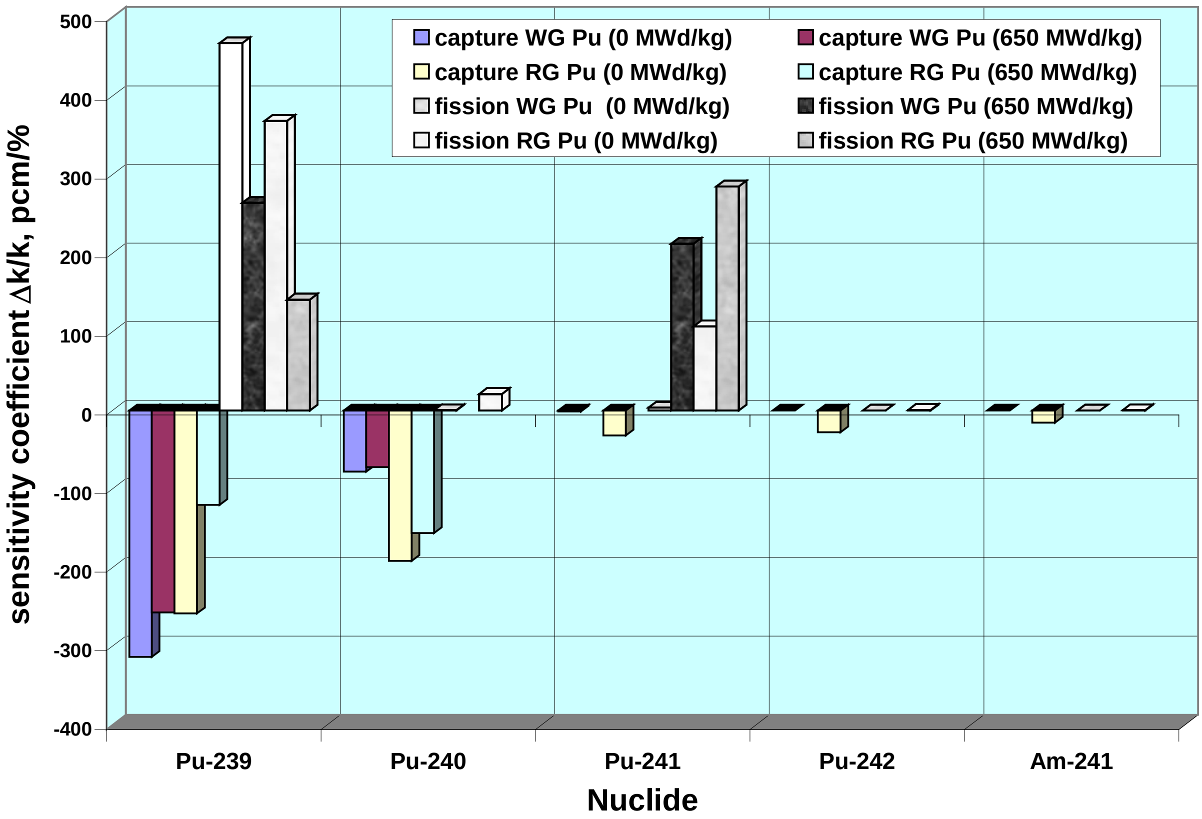


Fig. 3: Sensitivity coefficients k/k for capture and fission for Reactor Grade (RG)-Pu and Weapon Grade (WG)-Pu at 0 and 650 MWd/kg HM burn-up

The sensitivity analysis based on covariance data suffer on the quality of these data especially for applications for thermal systems. There are strong differences in covariance data of different data sources which lead to differences in uncertainty estimation:

- uranium fuel U-235 fission 0.21 % (JEF-2.2), 0.08 %(IRDF90)
- uranium fuel U-238 total 0.47% (JEF-2.2 incomplete), 0.26% (IRDF90)
- plutonium fuel: also strong differences between JEF-2.2 and IRDF90

The covariance data for uncertainty analysis are not complete in the different data evaluations; there are really few applications for thermal reactors. New releases of JENDL-3.3 are available now, but there are few applications. Covariance data for actinides are in IRDF90, JEF-2.2 (JEF-3.0) ENDF/B-VI.7 and CENDL-2.1. Also here, a co-operation with corresponding groups performing systematical uncertainty analysis of thermal reactors should be initiated to get synergy effects for HTR applications.
A further topic for WP2 was an analysis of present scattering law data for graphite. These data are established since ENDF/B-II, derived from Young Koppel phonon spectra. There are also new measurements from Nicklow, Wakabayashi and Smith and Hawari available. Difilippo et. al. analysed consequences of these newer frequency distributions to HTR systems (see Fig.4). He

reported that keff increases for well moderated systems and decreases slightly for undermoderated systems using scattering law data based on Nicklow et. al. Here, more comparisons of differeent models for thermal scattering on graphite should be made. Comparisons of measured and calculated thermal spectra are shown in Fig. 5. The importance of validation of graphit scattering data was emphasised of the HTRN partners. The present status of scattering law data for graphite, however seems to be adequate for HTR calculations.

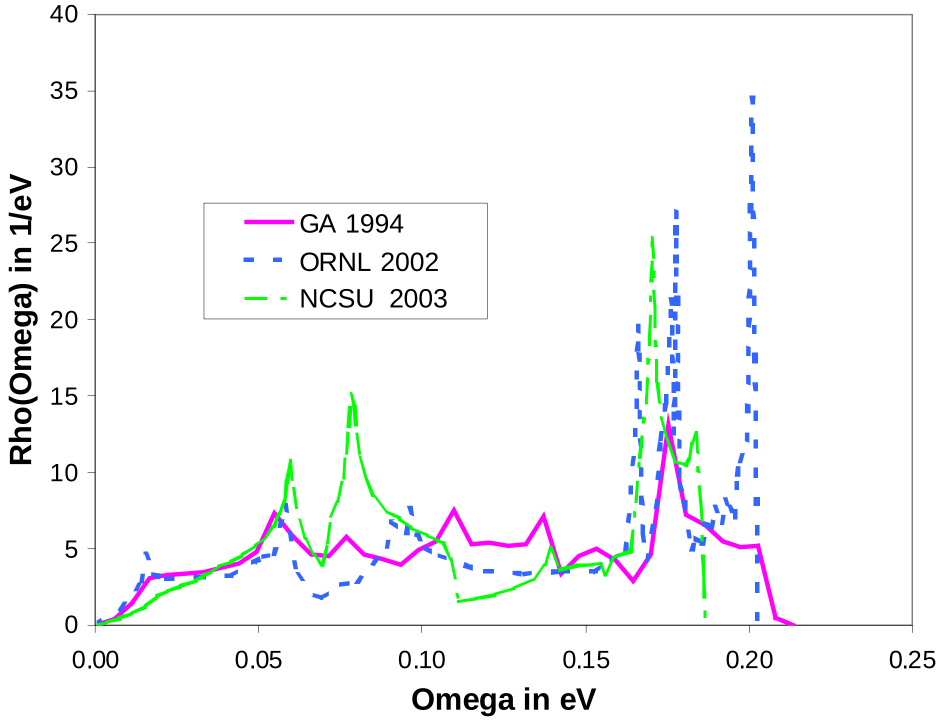


Fig. 4: Frequency distributions for polycristalline graphite

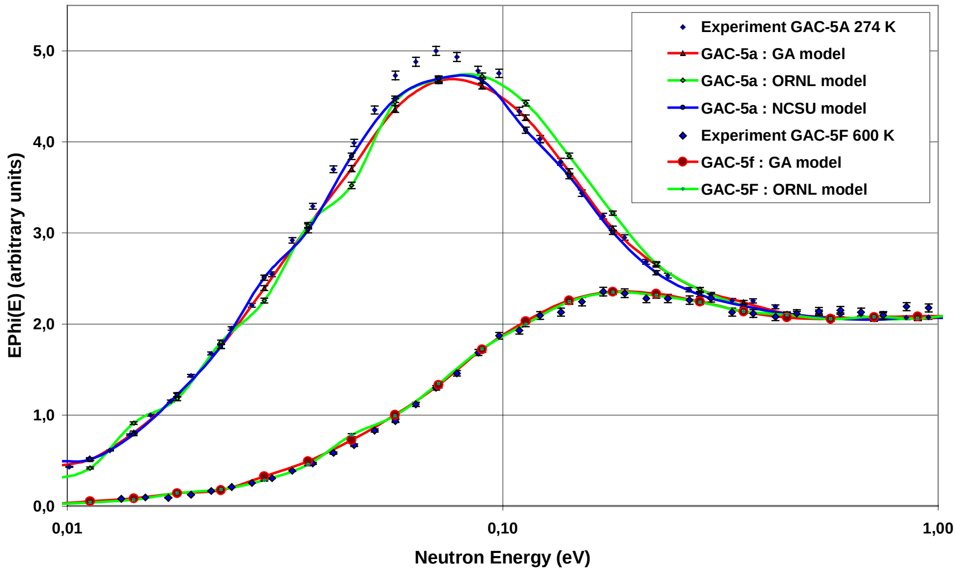


Fig. 5: Neutron spectra for the graphite Benchmark GAC-5A and GAC-5F

CONCLUSIONS

- The JEF-2.2 data evaluation which is the main basis for calculations in WP1 and WP3 is equivalent to other international data evaluation such as ENDF/B-VI and JENDL-3.2. JEF-2.2 based calculations show an overall good agreement
- For some nuclides there are new releases in JEFF-3, JENDL-3.3 and ENDF/B-VI which should be taken into account; the new U-235 release of ENDF/B-VI can lead to under-estimation of multiplication factor for harder spectra
- Sensitivity and uncertainty calculations for HTR fuel with WG Pu and RG Pu showed uncertainties of 0.6 % in k_{eff}
- The covariance data for uncertainty analysis are not complete in the different data evaluations; there are few applications for thermal reactors. New release of JENDL-3.3 is available now
- There are differences in cross sections for minor actinides between JEFF-2.2, JENDL-3.2 which lead to significant different nuclide compositions for irradiated fuel
- These differences and hence uncertainties have less impact to keff but direct impact to the number densities at high burnup. This aspect should be taken into account also in uncertainty calculations
- The neutronics calculations should be checked also against the composition of HTR fuel as a function of burnup; corresponding experimental composition analysis (e. g. for AVR) should be re-calculated
- Thermal scattering for graphite are of sufficient quality
- HTR aspects should also be regarded in nuclear data evaluation groups
- New evaluations or measurements seem to be necessary for Er isotopes, since there is a poor experimental data base see as an example Fig. 6

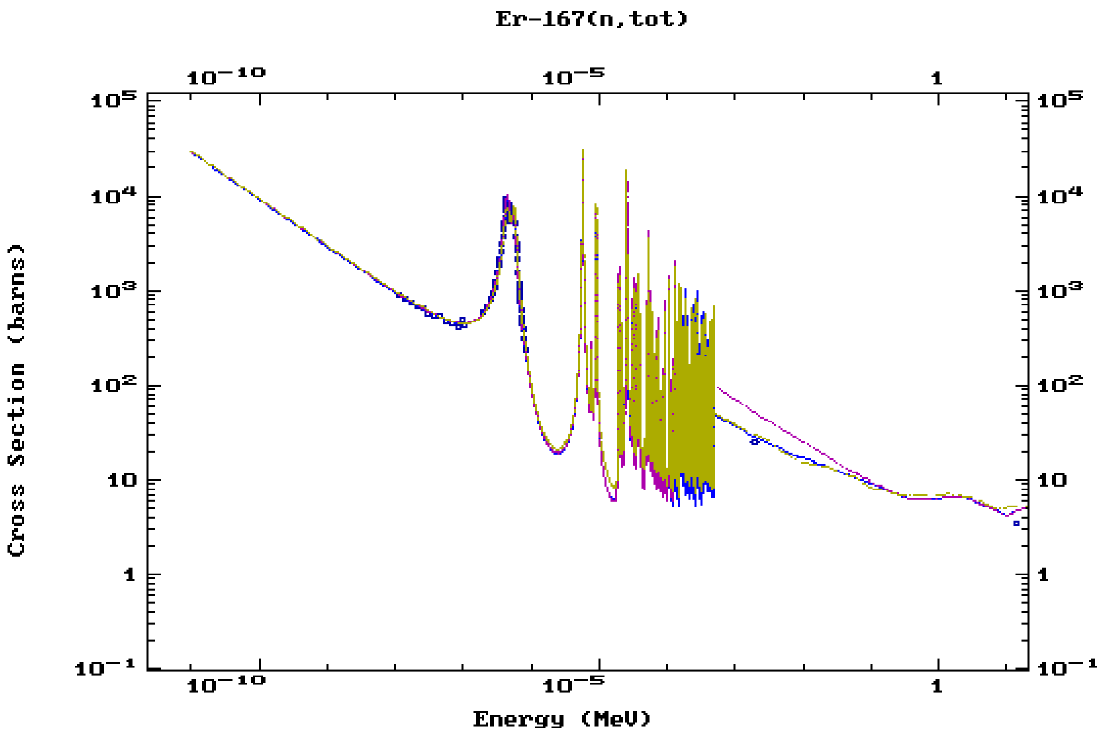


Fig. 6: Comparison of evaluated data for Er-167 (n,tot) with EXFOR measured data