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Cross-Section Analysis for TRADE Fuel

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The TRIGA core includes bounded hydrogen in Zirconium hydride in its fuel meat allowing for fast reactivity transients. The inherent safety mechanism is based on the immediate increase of neutron up-scattering by the hydrogen as a result of a fuel temperature increase. The temperature dependent resonance absorption is the second safety feature. The special fuel type together with the introduction of an external source within it for the TRADE project necessitates an accurate evaluation of the bounded hydrogen cross section generation technique as well as of the resonance treatment. By comparing deterministic tools and Monte Carlo solution methods the generated bounded isotopes cross sections are analysed. Further, the importance of the Doppler and the thermal up-scattering effects are quantified and the sensitivities to the solution method are discussed.

KEYWORDS: Bounded Hydrogen, TRIGA Fuel

1. Introduction

The TRADE [1] (**TR**IGA **A**ccelerator **D**riven **E**xperiment) project utilizes the TRIGA RC-1 reactor in ENEA-Casaccia Centre. This is a thermal power swimming pool type reactor, cooled by natural convection of water in the pool.
The project is aimed to demonstrate experimentally the feasibility of coupling an external source with multiplying medium at a power level with pronounced reactivity feedbacks. The fuel meat matrix in TRIGA contains zirconium hydride (ZrH). This hydrogen in the fuel ensures the highly inherent safety by shifting upwards the neutron energy spectrum in case of fuel heat up. The fission cross section of U235 decreases significantly with the growing neutron energy. Thus a considerable negative reactivity is introduced. An accurate assessment of the material cross-sections and of the hydrogen scattering kernel is needed to quantify safety parameters for such systems also in light of the additional external source within the TRADE project.

Bounded hydrogen in ZrH or in water exhibits different cross-sections and scattering kernels than the free hydrogen atom. Using unsuitable hydrogen data could lead in the TRIGA core to criticality differences of about 4%. Other bounded isotopes like zirconium in ZrH or carbon bounded in graphite have cross-sections, which also differ from their free atom values. The special bounded data of several isotopes and in particular of the bounded hydrogen appears separately on the ENDF [2] files and may be processed by the THERMR module of NJOY [3]. This data may be transferred to the stochastic code MCNP [4] by the NJOY module ACER which arranges the data in suitable probability tables. Contrarily, the data transfer to be used in deterministic codes is not straightforward within NJOY if thermal up-scattering is included. Auxiliary programs are needed to adopt the data for each specific multi-group cross

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section library structure. Such a procedure was prepared within KAPROS [5] (KArlsruhe PROgram System) to include new data for bounded atom cross sections.

The other important safety feature in TRIGA fuel is the Doppler-effect due to resonance broadening after an increase in the temperature. A detailed study was done to quantify its contribution at several temperatures.
In this paper results of Monte Carlo calculations with MCNP and of deterministic multi-group calculations are compared to validate the applied cross section procedure for the hydrogen and the available data for the other isotopes in particular U235 and U238.

2. Thermal cross sections of bounded Hydrogen

In the low thermal energy range the chemical binding effects are well pronounced. Thereafter bounded isotopes have their own evaluated data files and formalism in the basic ENDF libraries from which the scattering kernels and cross sections can be evaluated. The usual energy threshold for including binding effects is of few eV (maximal energy calculated in NJOY: 5 eV) above which the free atom cross section and scattering kernels are used. For the TRADE experiment the bounded hydrogen in zirconium is of high importance as it governs the large negative reactivity feedback in the TRIGA fuel. The processing of the special ENDF hydrogen file is done in the THERMR module in NJOY. Utilizing the ACER module, the so called $S(a,b)$ tables for the scattering kernels are transferred in a suited format for MCNP. The differences between the scattering kernels of hydrogen as free gas and hydrogen bounded in ZrH and water are plotted in figure 1 and 2 for 296 K and for 600 K. This plot is based on the tables from ACER. The two figures show the down-scattering probability below energies on the horizontal axis for incident 0.1 eV neutrons.

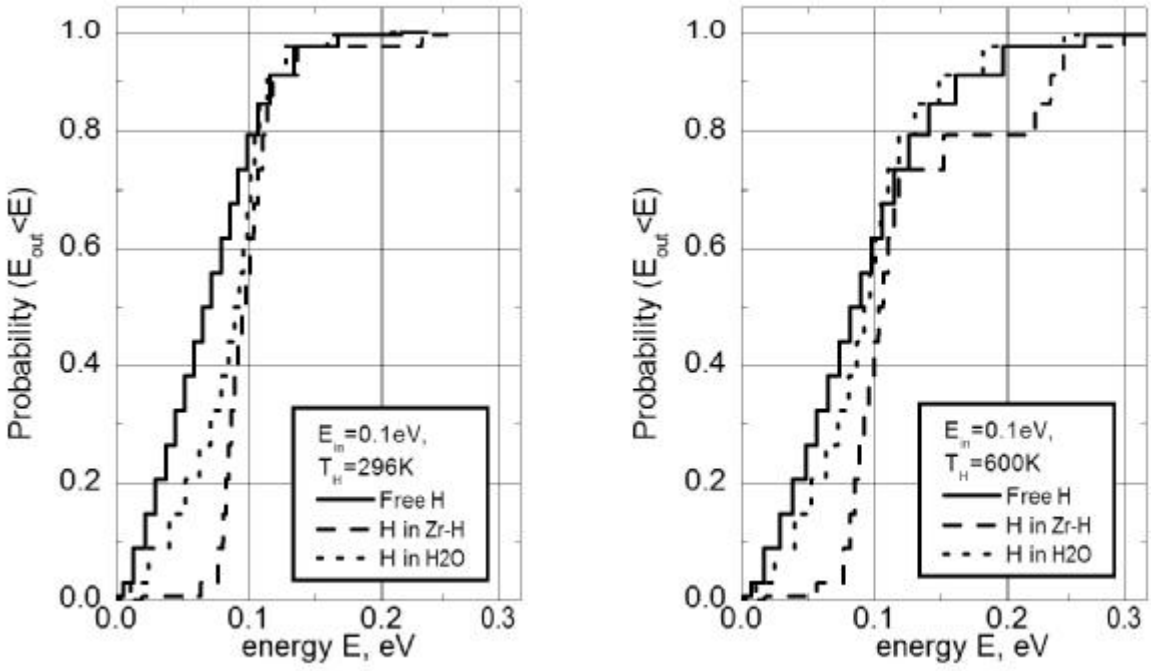

Fig. 1 & 2: Probability of neutrons to be scattered below specific energy E if the incident energy E_{in} is 0.1 eV at 296K (1-left) and 600 K (2-right) for 3 types of hydrogen binding.

In both figures it can be seen that the down-scattering probability is higher for the case where the hydrogen data is based on free gas treatment. At 600 K the enlarged up-scattering effect of H in ZrH is more pronounced comparing to the 296 K. The fission cross section of U235

decreases considerably at higher thermal energies and thus the inherent safety of the TRIGA core is improved.

In the current version of NJOY the Legendre moments for up-scattering are prepared in module THERMR and are processed to group data in GENDF format in module GROUPR. However, the module MATXSR only processes the slowing down data for storage on the commonly used MATXS format for group constants. The thermal up-scattering moments from GROUPR are not processed. In order to solve this problem the NSLINK [6] package was developed to transfer these moments to the well known code system SCALE [7]. It includes several options to read the output file in GENDF format of GROUPR and to process the modified data in its requested format. In order to transfer the GROUPR data to KAPROS library the MILER package of NSLINK was applied. The MILER code within NSLINK converts NJOY output (GENDF format) to AMPX [6] master format and includes the treatment of thermal scattering matrices at different temperatures. A new auxiliary code RAMPX was developed to produce the data structure needed for all materials including the "bounded" thermal up-scattered cross sections in normalized scattering-moments format. The data is then included in the master library of the KAPROS system in the so called GRUBA format. It can be seen that the data process for the deterministic code evolves several steps in which various approximation techniques are employed in particular for the thermal up-scattering. In order to analyse the cross section generation process a TRIGA fuel pin model was simulated by comparing two solution methods: a deterministic one, which uses the MILER/RAMPX procedure and the stochastic one, which utilizes the NJOY module: ACER.

3. MCNP and KAPROS comparative cell calculations.

Two types of cell were analysed to validate the cross sections generation technique:

-One dimensional unit cell with reflective axial boundaries and "white" (reflection with cosine distribution) radial boundary. The fuel type is a ternary alloy of uranium-zirconium-hydride where the uranium metal is 8.5% of the mixture by weight. The H to Zr ratio is 1.7 and the fuel has 20% enrichment of U235. The fuel matrix radius is 1.815 cm and it is enclosed by 0.05 cm thick cladding of stainless steel AISI 304 (7.8g/cm^3) and an additional 0.485 cm water ring.

-A two dimensional model which considers additionally an axial reflector and the aluminium grid plate on the top of the reflector.

The deterministic calculations were performed by utilizing the WIMS [8] 69 energy group structure data together with the TWODANT [9] Sn transport code. The upper quarter of the two dimensional fuel-assembly is plotted in figure 3. The calculation is performed with reflective boundary condition in the axial and radial direction. For this model a two step approach was applied. First the one dimensional fuel cell with the lower part (figure 3) containing fuel matrix, clad and water was homogenized in a unit cell calculation. In the second step the homogenized fuel data together with the graphite and the aluminium plate on top and bottom formed the two dimensional model. By means of the TWODANT code (using S_8 and P_3 for the scattering) the temperature dependent multiplicity values k_∞ were calculated.

The analysed characteristics are the two temperature feedback effects, the Doppler broadening and the thermal scattering kernel of the bounded hydrogen within the fuel.

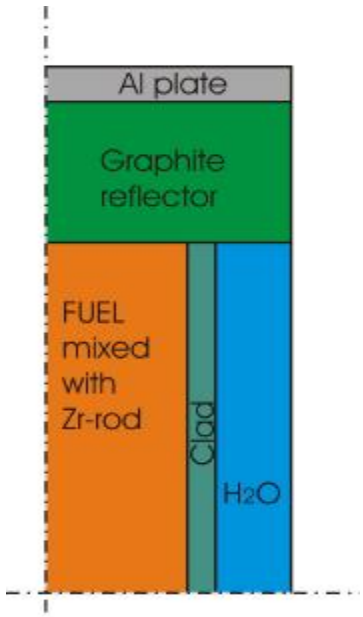

Fig. 3: Two-dimensional fuel pin geometrical scheme.

The temperature dependent k_∞ values are plotted in figure 4. For both cases the relative error between MCNP and KARBUS [5] –TWODANT is less than 1%. All MCNP calculations shown in the graphs have standard deviation of less than $7 \cdot 10^{-5}$. The derived effects for those results are all 10^{-3} and more.

The temperature feedback in terms of criticality change per degree at certain temperature is plotted in figure 5. The calculated data concerns only the effect of up-scattering through the hydrogen enhanced excitation. The data points were fitted by differentiation of an analytical formula for temperature dependent criticality values, suggested by the TRIGA manufacturer General Atomic (GA) [10] (equation 1):

$$K(T) = C_1 - C_2 \exp(-C_3 / T) \qquad (1)$$

The agreement in figure 5 between the TWODANT and MCNP using the same evaluated ENDF/B-VI data processed with NJOY is satisfactory. The curve shapes are qualitatively in accordance with the original one calculated by GA. Nevertheless, the existing deviations between MCNP and TWODANT in figure 5 were analysed extensively to understand better the roots of those discrepancies and in parallel to improve the reliability of the numerical tools. The thermal up-scattering and the Doppler effects were recalculated separately by changing virtually only the temperature of the heavy isotopes in the fuel and keeping the hydrogen temperature constant at 300 K for the Doppler and vice versa for the thermal up-scattering. It was found that the two effects are independent for both calculation methods: the sum of the separately calculated effects is practically equal to the result of the calculation with both effects together. The results of MCNP and KARBUS-TWODANT comparisons are shown in figure 6, 7 and 8. In figure 6 it can be seen that the Doppler-effect decreases as expected with increasing temperatures. In that sense, the first point of the MCNP data points is not physical as the temperature feedback for Doppler in lower temperature is less than the one at a higher temperature. Figure 7 shows the thermal up- scattering. Here again one point, namely the value at 450 K of the MCNP based results, seems to be incorrect. This point contributes to the differences in the peak value of KARBUS-TWODANT and MCNP as is seen in figure 4. The relative impact of the Doppler-effect is plotted in figure 7. Due to the unphysical data point of MCNP in figure 5 the Doppler-effect is suppressed at lower temperature in comparison with the deterministic solution. The Doppler makes about 35% of the total negative reactivity effect at 300 K and with the temperature growth its importance is reduced to less than 10% at temperature above 1000 K.

The inconsistent results of MCNP could be attributed to the use of ENDF/B-VI.2 data files, which were reported [11] to be inaccurate to some extent. Moreover the sampling method in the resonance region in MCNP is based partially on some approximations [4, chapter 2: sampling the target velocity] that might cause non-negligible deviations. The results of the deterministic methods seem to be consistent. Yet, the differences to the MCNP results could come to some extent from the treatment of the heterogeneity effects [5]. In particular, the several options of the Bell factor treatment [5] on criticality were examined. The influence using different treatments was about 1 pcm/degree, which is of the same order of magnitude of the discrepancies between the two calculation methods. Another source for the discrepancies is the effective absorption group cross section within the fuel for the main resonances of U238. The comparison between the methods was done by using the standard fuel pin model on KARBUS and also by dedicated codes like the special KARBUS module RESABK [5] and OZMA [12] for resonance reaction rates treatment where the cell is divided into several (10 in the current work) annular zones. Preliminary results show 3% to 10% differences in the group averaged $\Sigma_{A,eff}$ between MCNP and the deterministic methods. It should be mentioned that the MCNP data were based only on ENDF/B-VI.2 library. Similar evaluations with other ENDF versions are being processed.

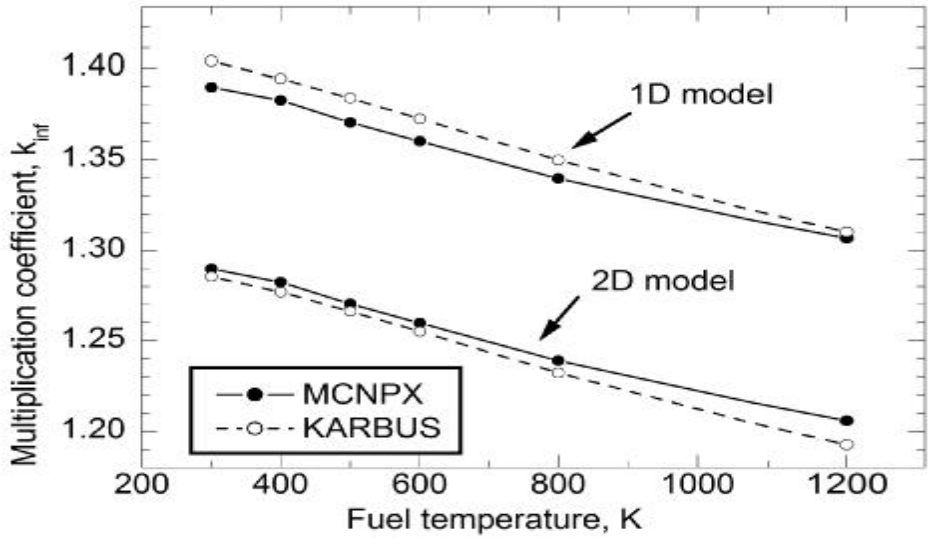

Fig. 4: Comparison of K_∞ values for 1D Model (unit cell) and 2D Model (Fuel Assembly) calculated with MCNPX and KARBUS-TWODANT

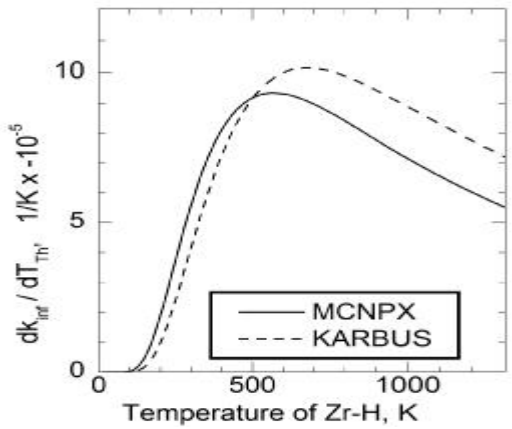

Fig 5: Thermal up-scattering fitting curve of MCNPX and KARBUS-TWODANT data points for 2D Model. The governing fitting formula is based on GA (U235 & U238 at 300 K)

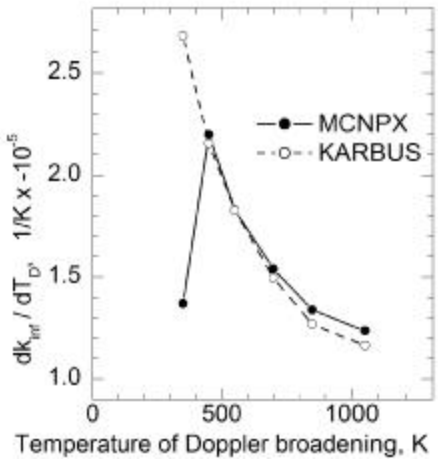

Fig 6: Comparison of the Doppler-effect between MCNPX and KARBUS-TWODANT for 2D Model (ZrH at 300 K)

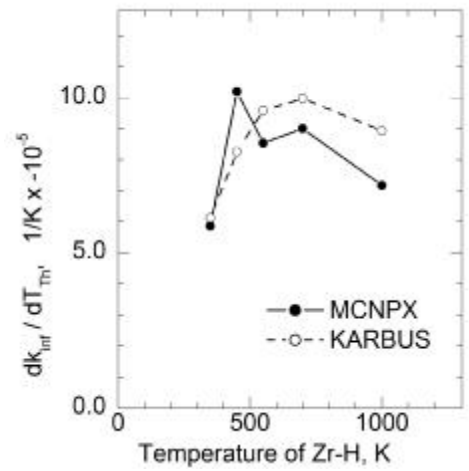

Fig 7: Comparison of the thermal up-scattering between MCNPX and KARBUS-TWODANT for 2D Model (U235 & U238 at 300 K)

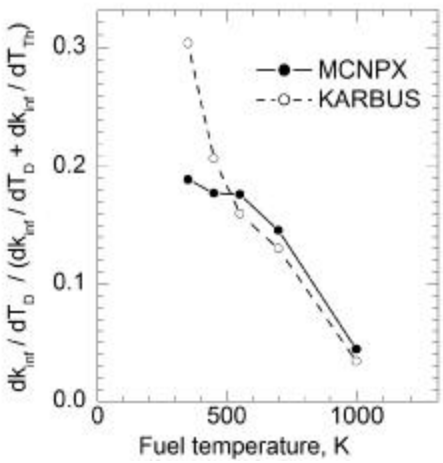

Fig 8: The ratio of the Doppler to total reactivity feedback effects for 2D Model

4 Conclusions

The analysis of a new procedure in the modular code system KAPROS for treatment of bounded atoms cross-sections was presented. There is an overall agreement between MCNP solution methods and deterministic calculation technique with KARBUS-TWODANT. Yet a more detailed examination reveals the deficiencies of the deterministic as well as the stochastic method. They come either from the basic cross section data or from the solution method. Concerning the MCNP cross sections, preliminary results with the ENDF/B-VI.5 show indeed an improvement and the unphysical solution at 300-500 K of the current use of ENDF/B-VI.2 vanishes. For the deterministic method more accurate analysis concerning the resonance treatment should be done to evaluate the uncertainties of the feedback reactivity.
The current study was performed with fresh fuel. The TRADE project will be probably carried out with burned up fuel. This will lead to more uncertainties regarding the Doppler and thermal up-scattering feedback parameters. On one side the content of the fuel is changed but more important may be the diffusion of hydrogen from the fuel. This leads obviously to changes in the reactivity feedback and further sensitivity analysis depending on the hydrogen and fuel concentration is necessary.

5. References

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