VALIDATION OF TRIGA REACTIVITY COEFFICIENTS

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Abstract

The ECATS (Experiments Coupling Accelerator Target Sub-critical blanket) project within the EUROTRANS framework evolves the coupling of an external source with a TRIGA core. In order to simulate dynamical transients in source driven sub-critical systems the reactivity coefficients should be accurately determined. Experimental results of two TRIGA cores (Italian RC-1 in Casaccia, Slovenian MARK II in Ljubljana) showed however temperature dependent reactivity feedbacks which are different from the theoretical curve suggested by the TRIGA manufacturer General Atomics (GA).

In this study the effects of the scattering kernel of hydrogen bound in zirconium, which is mixed within the TRIGA fuel matrix, are further investigated. In particular the influence of the inter-molecular forces in form of the phonon distribution function is analyzed. Furthermore the sensitivity of the scattering kernel, known also as the S(α,β) tables, to the numerical treatment is considered. In particular the influences of the improvements in the beta version MCNPX 2.5f and of the optimization of the energy grid of the THERMR module of NJOY are discussed in view of the experimental results of the two TRIGA cores. It is shown that the experimental reactivity feedback curves can be better reproduced based on the above mentioned improvements.

KEYWORDS: reactivity coefficient, S(α,β) scattering tables, phonon distribution, hydrogen bound in zirconium.

INTRODUCTION

The suggested reactivity feedback curve provided by General Atomics (GA) [1] appears to be inadequate in comparison with new experimental data, in particular in the range of 100-150^{0}C. The reactivity measurements which were performed in RC-1 TRIGA Cassacia and Slovenian TRIGA Mark II core Ljubljana show a significant increase of the negative reactivity feedback in this range.

In previous work the influence of variation of the shape and of the standard number of energy points of the phonon spectrum of hydrogen bound in zirconium in the NJOY module THERMR were investigated [2,3]. It was shown that the 59 points energy grid used for years in the NJOY code is inadequate for hydrogen bound in ZrH_x. As a consequence, a new set of energy points was included in THERMR in the NJOY update 112 [4]. The new Gaussian shape of the phonon spectrum suggested in reference [3] showed to some extent different values of criticality, but could not explain the above mentioned differences in the reactivity feedback in the temperature range of 100-150 C.

In the current study the new energy grid of NJOY module THERMR is tested again for hydrogen bound in zirconium. In addition the impact of the numerical treatment of the S(α,β) tables in the beta version MCNPX 2.5.f is discussed. This version is very close to the current official MCNPX version 2.5.0 and eliminates numerical spikes in the flux due to the interpolation scheme of the Monte Carlo method. Preliminary results of this method on the criticality of TRIGA cores are presented.

The phonon states in metal hydrides appear to be affected by the hydrogen concentration [5]. Moreover the fine structure of the hydrogen admixture is associated with the optical peak [6]. The corollary of the above observation means that in the case of TRIGA fuel the phonon spectrum used could be not adequate. The hydrogen's stoichiometry is different from the one upon which the scattering data were generated and the structure of the fuel matrix might be to some extent deformed by the existence of the uranium. Thereafter it was decided to evaluate the influence of changes in the intermolecular structure and forces in the form of changes in the phonon distribution function. In

particular, the effect of shifting the optical part of the phonon spectrum on the temperature dependent reactivity feedback is investigated.

Experimental Results

Two independent reactivity measurements for TRIGA type cores are referred to in the current study. The TRIGA fuel elements are cylinders of ternary alloy uranium-zirconium-hydride with H-to-Zr atom ratio 1.7 and the total U of 8,5% of the mixture by weight for the Cassacia reactor and with H-to-Zr atom ratio 1.65 and the total U of 12% for the Slovenian reactor and the same enrichment (20% enriched ^{235}U). The fuel cladding consists of stainless steel AISI 304 of 0.05 cm thickness and 7.8 g/cm^3 density. There are two graphite cylinders of 38.11 cm length at the top and the bottom of the fuel rod.

The reactivity coefficient measurements performed within the TRADE project in the Cassacia RC-1 core [7] showed similar results to the experimental temperature dependent values measured at the Slovenian TRIGA core [8] although the fuel composition is different. The reactivity measurements in RC-1 were carried out with the existing core configuration, i.e. with burned-up fuel. The measurements at the TRIGA Mark II at Slovenia were performed with completely fresh uniform core. In both experiments only one or two temperature measurement points were performed from which an average temperature was evaluated. In Figure 1 the reactivity feedback per degree is plotted. The curves are subjected to uncertainties of about 3 degrees in temperature and about 5 pcm in the reactivity value [8]. All curves differ considerably from the GA curve between 110 – 150 ^{0}C. Two curves of the Slovenian core refer to the estimation of the total core averaged temperature based on measurements at point A located in the centre of the core (denoted in the figure with T_a). The radial form coefficient for T_a is C_a=1.26. The coefficient C_z is the axial form factor. The sensitivity to the form factor is investigated by looking at the evaluations of changing the axial form factor by about 10% from 1.25 to 1.12. The other two curves of the Slovenian core are based on two point measurements at the above centre point (T_a) and in the first ring of the core (T_b) for which the radial form coefficient is C_b=1.22. The sensitivity to the axial form factor is again demonstrated. As it is shown in figure 1 the differences between the curves emphasizes the necessity of an improved multi-point temperature measurement to evaluate more accurately the influence of the spatial flux distribution and the fuel content (fresh or burned up fuel) on the reactivity feedback. Nevertheless as can be seen in Figure1 all the measurements point out a phenomenon which is not shown in the GA recommendations, namely the increase of the absolute value of the reactivity coefficient above 100^{0}C. This emphasizes the necessity of a comprehensive survey of the numerical as well as the fundamental physical treatments of the bound hydrogen in zirconium scattering kernel and their possible impact on the criticality and temperature reactivity feedbacks of TRIGA cores, especially in view of the planned EUROTRANS experiments.

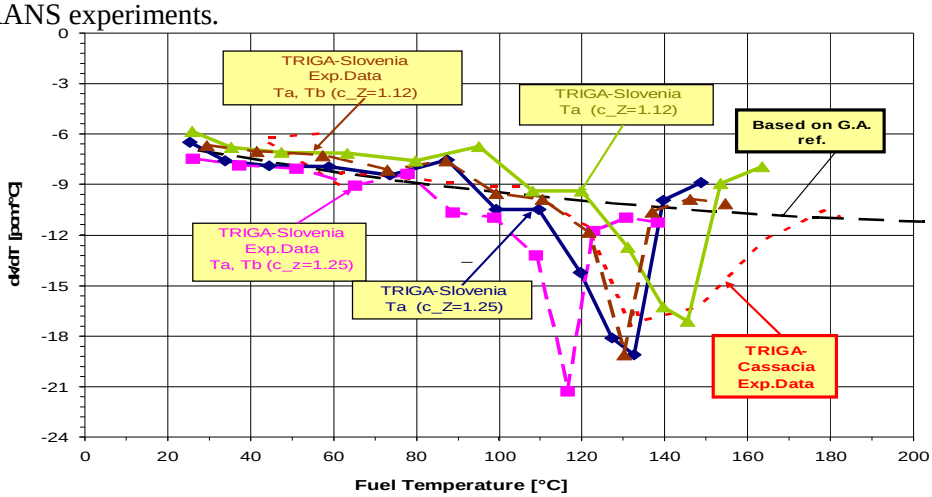

Fig. 1: Experimental temperature dependent reactivity feedbacks in RC-1 and Slovenian TRIGA cores

The influence of the numerical treatment

In previous studies [2] several numerical aspects with respect to the preparation of probability-S(α,β) tables for the secondary energy distribution concerning hydrogen bound in zirconium were analysed. The number of tables based on the standard 59 energy grid structure was shown to result in erroneous criticality values for TRIGA fuel. The increasing of the number of points in the energy grid (118) [4] based on the work of Mattes et al [3] differed by about 300 pcm in comparison with the standard grid as can be seen in figure 2. All the calculations in figure 2 and the following figures were performed with beta version 2.5.d of the MCNPX code with standard deviation of $7x10^{-5}$.

A new grid with 199 energy points was introduced in the current study taking into account all points from former studies dedicated to hydrogen bound in zirconium. These points were included in the NJOY updated grid definition [4]. The results deviate from the improved 118 points scheme by nearly 100 pcm (figure 2). A very fine, equal lethargy interval, energy grid with 2045 points, gave similar criticality values compared to the 199 points energy grid, (figure 2). This emphasizes the need to search further for an optimized grid for chemical binding of all isotopes of interest. The general grid for all bounded light isotopes as it is currently being done seems to be inadequate.

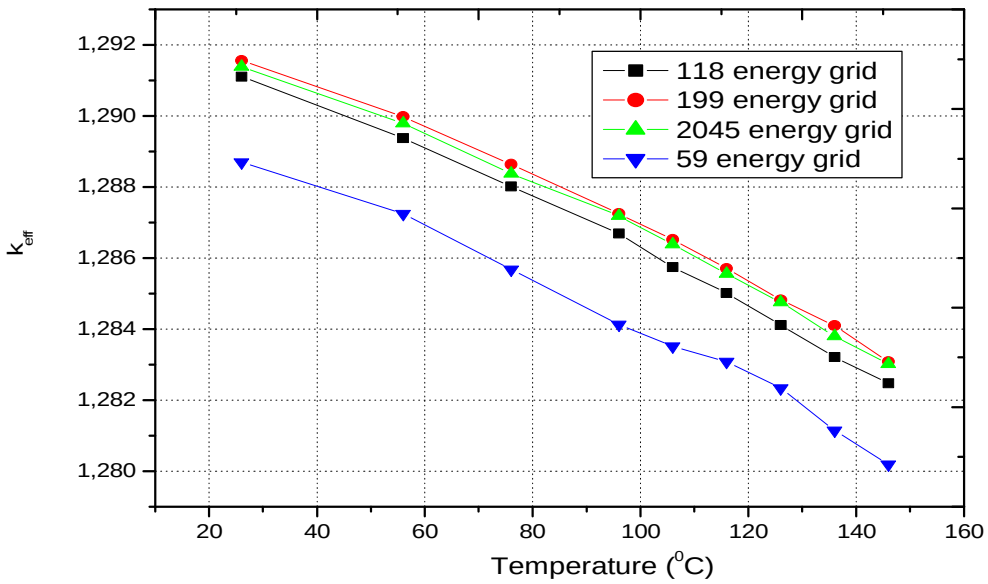

Fig. 2: Temperature dependent criticality values as a function of the energy grid points number.

Parallel to the modification of the energy grid the new method which removes the numerical spikes due to S(α,β) treatment in mcnp (mcnp4c3) and mcnpx (2.5d) was analysed. The spikes can be seen in figure 3 using the 2.5d version and are removed (figure 3) in version 2.5f. Two sets of calculations were performed, one with 118 points and the other with the new 199 energy grid. In both cases the numerical treatment was tested for its impact on the criticality values for several temperatures (figure 4). In the 2.5f version the NJOY updated grid still shows discrepancy of more than 100 pcm for both grids in comparison to the old version 2.5d. Taking into account the standard deviations it can be concluded that the numerical effects have only an impact on the criticality but not on the reactivity and thereafter can not explain the experimental results of figure 1 above 100^0C.

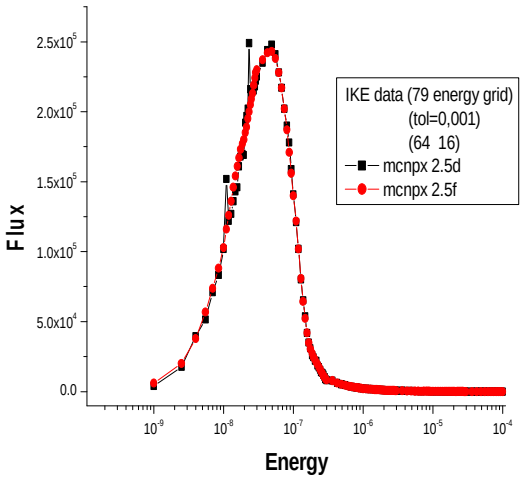

Fig. 3: Numerical spikes shown in MCNPX version 2.5.d against the corrected version 2.5.f

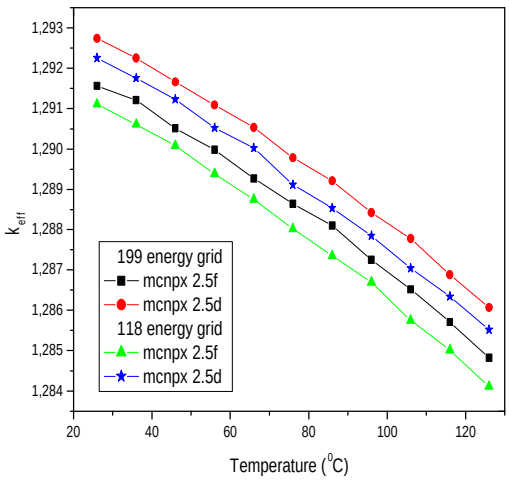

Fig. 4: Criticality values as a function of the numerical treatment for a TRIGA subassembly

The impact of a shifted phonon spectrum on the reactivity curve

The phonon spectrum of hydrogen bound in zirconium suggested by Slaggie [6] and commonly used by NJOY is given in figure 5. This spectrum is based on a central force model of ZrH_2. Using it one gets in the low temperature region (30-100^{0}C) good agreement in comparison to the reactivity measurements plotted in figure 1. However, at higher temperatures (100- 150^{0}C) the shape of the measured reactivity coefficient curve is not reproduced.

The work of Malik et al. [5] deals with the phonon spectrum of hydrogen bound in zirconium with an atomic ratio of 1.58 ($ZrH_{1.58}$). Malik describes in this work a phonon spectrum which is represented by three Gaussians with peaks at 0.132, 0.137 and 0.151 eV. He discusses the impact of the stoichiometry on the binding structure and the H-H interaction which could give a better insight also for the ZrH_2 model. Mattes [3] referred to experimental data from Evans [9] for ZrH_2. In figure 6 Evans's experimental optical mode curve and its equivalent spectrum suggested by Mattes with one Gaussian peak at 0.137 eV, are presented. This proposed spectrum agrees better with scattering measurements with atomic ratio 2, in comparison with Slaggie's model. The sensitivity of the above studies to different phonon spectrum shapes having several/single shifted peaks, and depending on the hydrogen concentration, leads obviously to different scattering phenomena, with possible impact on the reactivity coefficient.

In the current experiments of RC-1 and Slovenian cores the atomic ratio is 1.7 and 1.65 respectively for which the spectrum is only approximated from other stoichiometry as discussed before. The TRIGA experiments were performed for hydrogen bound in TRIGA fuel and not only in zirconium (for which the data is generated). As a corollary, the actual phonon spectrum in TRIGA cores might be slightly deformed or shifted.

The goal of this study is to analyse minor deviations of the phonon peak on the energy scale and in particular its potential impact on the criticality and the temperature dependent reactivity feedbacks.

In figure 7 various shifted optical spectra are plotted. The 161 energy points represent the original 0.137 eV phonon peak. The "121", "151" titles stand for a shifted peak by 0.04 and 0.01 eV respectively downwards where as the "171" introduce a phonon shifted 0.01 eV upwards. Decreasing the phonon spectrum energy tends in principle to enlarge the criticality which is in accordance with the results with the free gas model where the phonon peak location approaches 0. In order to retrace the experimental results one may assume that around 100 ^{0}C, due to currently unknown phenomena, the phonon spectrum is slightly shifted to higher energies by about 0.01 eV. and then the new spectrum

peak vibrates in this range of 0.137-147 eV. If this shift is taking place with a certain temperature dependency in the range 100- 150^{0}C, the corresponding reactivity values shown in figure 8 may explain the measurements of the reactivity coefficients depicted in figure 1. The calculated reactivity coefficients in figure 9 show that the temperature coefficients for constant phonon spectrum have only weak dependency on temperature. In any case, and in accordance with the conclusions of Malik [5] and the work of Slaggie [6] concerning the contribution of H-H forces to the vibration mode, it is evident that more experiments and verifications are mandatory in respect to feedback experiments within the temperature range 100-150 ^{0}C. Such investigations could contribute to an appropriate model for varying hydrogen content, bound in zirconium in a fuel matrix.

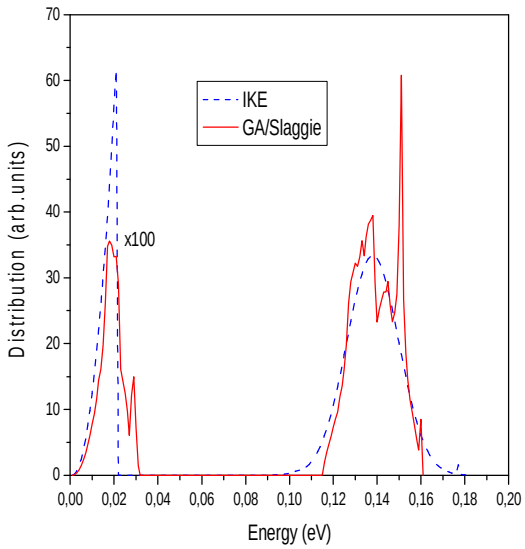

Fig. 5: Frequency distribution of H in zirconium (acoustic and optical part)

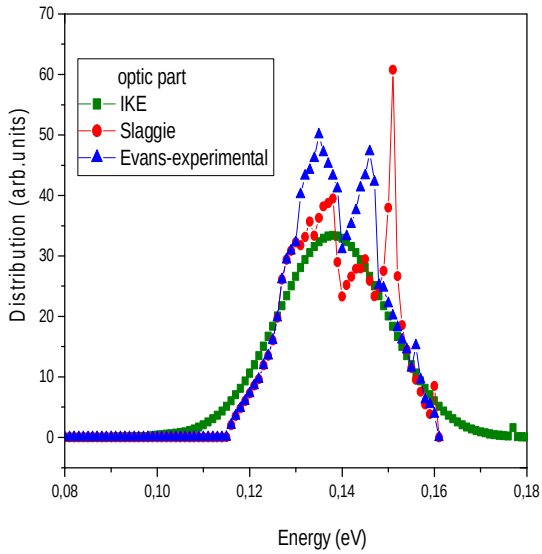

Fig.6: Frequency distribution theoretical and experimental (optical part)

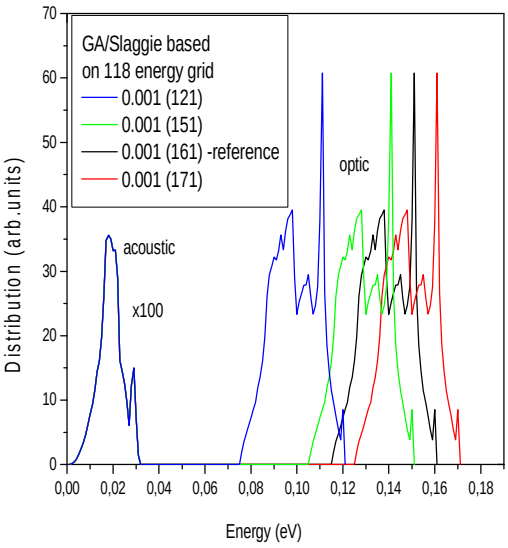

Fig.7: Shifted phonon spectrums around the original one (161 energy intervals)

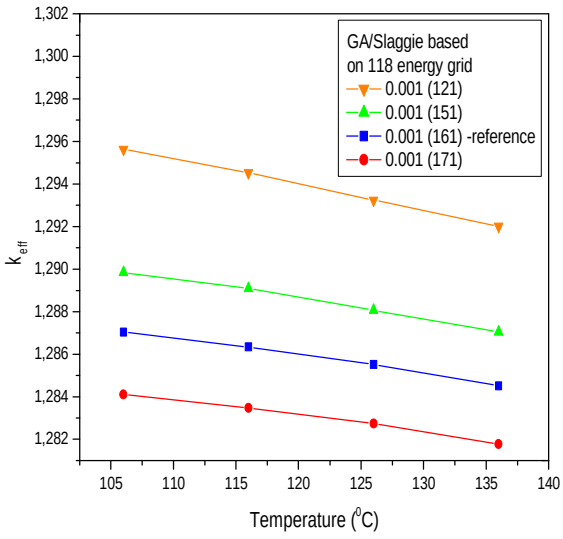

Fig. 8: Critical calculations with different spectrums for TRIGA fuel assembly

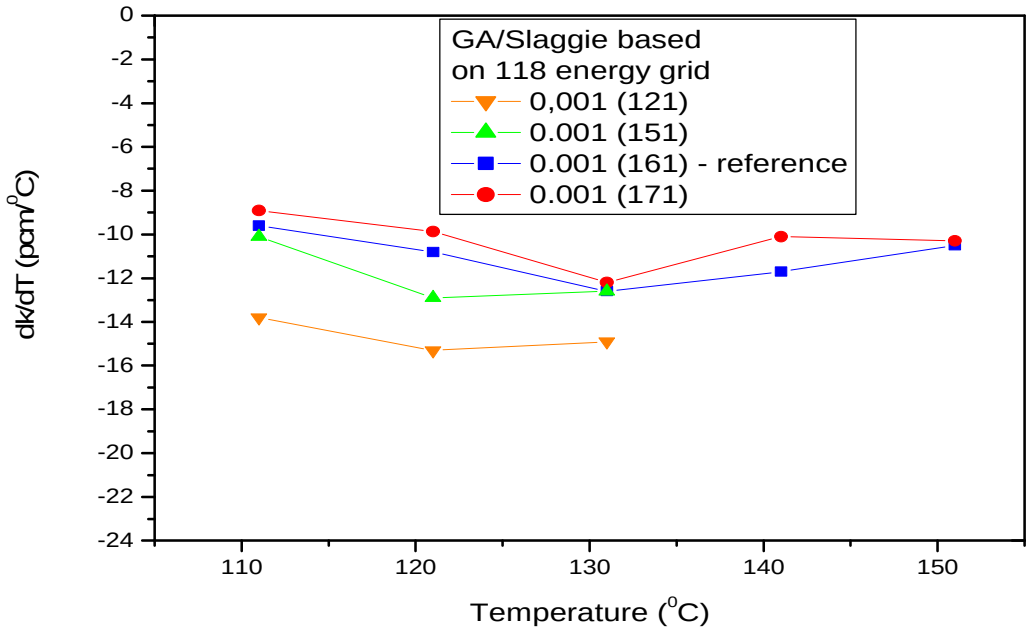

Fig. 9: The impact of different phonon spectrum (optical part) in the reactivity feedback

Conclusions

This study extends previous contributions concerning the numerical and physical treatment of scattering kernel models for criticality and reactivity coefficient calculations for TRIGA fuel. The improved energy grid scheme in the NJOY update 112 for module THERMR is not completely adequate and about 80 more points seem to be needed for hydrogen bound in zirconium. The modified S(α,β) treatment in newer MCNPX versions leads to removal of numerical spikes in flux distributions and causes also a non negligible criticality change in the simulation of TRIGA subassemblies.

The changes of the phonon spectrum itself in the temperature range 100-150 ^{0}C could explain to some extent the specific behaviour of the temperature dependant reactivity coefficient in the TRIGA subassembly. Theoretical results are presented, based on shifting the phonon spectrum. In any case, an experimental based physical confirmation is needed if feedbacks in the temperature range 100-150 ^{0}C are of interest, including also detailed measurements of hydrogen bound in an uranium matrix with zirconium, as all current data deal practically with hydrogen bound in zirconium ignoring the fact that the hydrogen is mixed within the fuel.

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