Comparative Analysis of the Reference GCFR-PROTEUS MOX Lattice with MCNPX-2.5e and ERANOS-2.0 in Conjunction with Modern Nuclear Data Libraries

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Abstract

During the 1970s, a wide range experimental program (GCFR-PROTEUS) was carried out at PSI's critical facility PROTEUS to study the physics characteristics of gas-cooled fast reactors. This paper presents the results of a series of new calculations based on the analysis of the reference test lattice in these experiments, viz. a regular hexagonal array of steel-clad, 15%-total-Pu PuO_2/UO_2 rods in air. The current study has been carried out using the deterministic fast-reactor code system ERANOS-2.0, largely employing the cell code ECCO and the Monte Carlo code MCNPX-2.5e, in conjunction with different modern nuclear data libraries.

Globally, good agreement is obtained between the different calculations for most of the important reaction rates which were measured at the center of the test lattice (relative to the fission of ^{239}Pu). For these reaction rate ratios, ERANOS-2.0 results obtained in conjunction with adjusted JEF-2.2 data (adjustments primarily made from the analysis of sodium-cooled fast-spectrum systems) have been found to be in good agreement (i.e. within ~1σ), with both MCNPX-2.5e using the (unadjusted) JEF-2.2 data library and, even more important, with the experimental results. This provides useful indication that existing computational tools show an adequate level of accuracy for design studies of advanced gas-cooled fast reactors using conventional fuel pins.

KEYWORDS: integral experiments, gas-cooled fast reactors, PROTEUS facility, ERANOS, MCNPX, modern nuclear data libraries

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1. Introduction

The current study has been carried out in the framework of PSI's FAST project, the goals of which include the establishment of a unique analytical code capability for the core and safety analysis of gas-cooled fast reactors (GCFRs) [1]. Existing GCFR experimental data [2] has been reanalyzed with modern computational tools, including the deterministic fast-reactor code system ERANOS-2.0 (largely employing the cell code ECCO) [3,4,5] and the Monte Carlo code MCNPX-2.5e [6]. This new analysis provides comparisons of calculational results with measured integral data, viz. reaction rate ratios which have been measured at the center of the test lattice, expressed relative to the principal fission rate in the lattice, i.e. that of ^{239}Pu (F9). Furthermore, the current use of a state-of-the-art stochastic method in conjunction with four different modern data libraries (based on JEF-2.2, JEFF-3.0, ENDF/B-VI.v8 and JENDL-3.3 evaluations, respectively) provides valuable additional comparisons in assessing the performance of ERANOS-2.0. The latter has been employed in association with adjusted, as well as non-adjusted, nuclear data (JECCOLIB2, based on the JEF-2.2 evaluation). It should be mentioned that the adjusted library (ERALIB1) was obtained primarily from the analysis of sodium-cooled fast-spectrum systems [7].

In the Monte Carlo calculations, a sufficient number of particle histories have been run with a fixed initial source to obtain results for which the statistical 1σ error (<0.4%) is considerably smaller than the experimental 1σ uncertainty (typically ~2%). Thus, the stochastic calculations provide reference values for the deterministic results and also permit, as indicated, an examination of the sensitivity to four different data libraries.

The paper is structured as follows: Section 2 provides comparative analyses, with respect to experimental values, of the deterministic and stochastic results, while in Section 3 use is made of "Extended Generalized Perturbation Theory" (EGPT) [8] in an attempt to explain some of the important discrepancies. Finally, Section 4 is dedicated to concluding remarks.

2. Comparison between ERANOS-2.0, MCNPX-2.5e and experimental results

Table 1 shows the comparison of calculational (C) and experimental (E) results for the various measured reaction rate ratios in the form of (C-E)/E values, together with the 1σ measurement errors.

Relative good agreement with experiment is seen to be obtained by the different calculations for the reaction rate ratios involving capture and fission of ^{238}U (C8/F9 and F8/F9, respectively) and fission of ^{235}U (F5/F9), i.e. ratios corresponding to reactions actually occurring in the MOX lattice and hence directly influencing the neutron balance.

More specifically, the observed agreement with experiment is excellent, i.e. mostly within the 1σ uncertainties, with ERANOS-2.0 using ERALIB1, and with MCNPX-2.5e using the JENDL-3.3 and JEF-2.2 libraries. The differences with respect to experimental values are, in fact, quite similar for these three sets of calculational results. Moreover, when comparing the two sets of ERANOS-2.0 calculations, the use of adjusted data is seen to yield significantly better agreement for these three important reaction rate ratios, the prediction of F8/F9 in particular improving markedly.

The second block of measured reaction rate ratios listed in Table 1 effectively represents a useful set of additional, GCFR-relevant spectral indices. The numerator, in each case, involved the measurement of an infinite-dilution reaction rate since the corresponding nuclide did not occur in the reference lattice. (The digits 2, 3 and 7 denote ^{232}Th, ^{233}U and ^{237}Np, respectively.)

Table 1: Analysis, employing modern calculational tools, of integral reaction rate ratios measured in the center of GCFR-PROTEUS Core 11 (reference test lattice), along with computed k_∞ values. For the reaction rate ratios, the results are expressed as %-deviations of the computed values (C) from the corresponding experimental values (E); the experimental uncertainty, 1σ, is given in %.

		ERANOS-2.0		**MCNPX-2.5e**			
Relative reaction rate	1σ (E),%	**JECCOLIB2**	**ERALIB1**	**JEF-2.2**	**JEFF-3.0**	**END/F-BVI.v8**	**JENDL-3.3**
		(C-E)/E, %					
C8/F9	1.2	0.4	-0.4	1.1	2.5	-2.3	0.0
F8/F9	1.4	4.0	1.1	1.0	3.2	6.0	2.8
F5/F9	1.5	1.3	-0.2	-0.6	1.2	0.0	0.6
C2/F9	1.4	-3.0	-4.1	-0.6	-8.0	-5.9	-8.3
F2/F9	2.1	-2.1	-3.6	-10.1	1.2	-1.4	-0.3
(n,2n)2/C2	2.6	-0.2	-1.0	24.2	3.9	-1.2	9.3
F3/F9	1.4	1.3	-0.4	-0.3	-0.1	0.2	-1.0
C7/F9	2.5	-4.1	-5.3	-6.6	-5.0	-7.8	-6.2
F7/F9	2.1	-4.2	-4.6	-5.6	-2.1	3.3	0.1
Parameter		C					
k_∞		1.3516	1.3591	1.3480	1.3449	1.3766	1.3576

Whereas the ratio involving the fission rate of ^{233}U, viz. F3/F9, is well predicted, there is no consistent trend as regards the other spectral indices, i.e. those involving ^{232}Th and ^{237}Np, except that the capture rates (C2/F9 and C7/F9) are systematically under-predicted by several σ-values. A surprisingly large spread of the different calculations is seen particularly for the ^{232}Th(n,2n) reaction, expressed relative to ^{232}Th capture ((n,2n)2/C2), and the fission rate ratios. In the former case, the ERANOS predictions of the experimental value appear to be the most accurate.

The computed results in Table 1 for k_∞, the important integral parameter that could not be measured in the reference GCFR-PROTEUS lattice, indicate differences in the neutron balance calculations which are again surprisingly large in certain cases. Various observations can be made, e.g. (1) there is a k_∞ difference of as much as 2.4% between the extreme Monte Carlo results, viz. those corresponding to ENDF/B6.v8 and JEFF-3.0, respectively, and (2) the ERANOS-2.0/ERALIB1 k_∞ value is very close to the MCNPX-2.5e/JENDL-3.3 value, with a difference of only 0.1%.

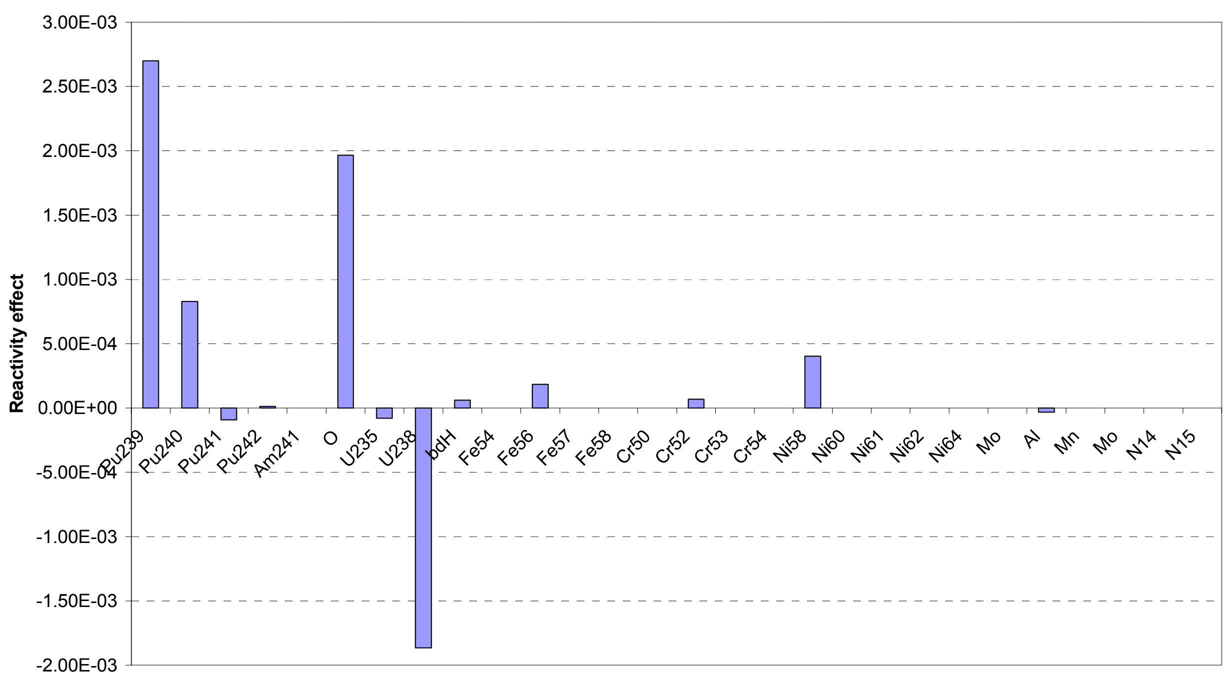
Additionally, it is seen that the data adjustment itself induces a k_∞ increase of 0.6%. This effect is studied in detail in the following section, as illustration of the influence of individual data set changes on the neutron balance of the reference lattice.

3. Analysis of k_∞ differences using "Extended Generalized Perturbation Theory"

Use has been made of the EGPT procedures available in ERANOS-2.0 to decompose the nuclear data adjustment effect on k_∞ , amounting to 404 "units" if it is formally and conveniently expressed in terms of a fictitious "reactivity" variation between the two calculations, i.e. as "$10^5 \Delta k_\infty / k_\infty$(ERALIB1)/$k_\infty$(JECCOLIB2)".

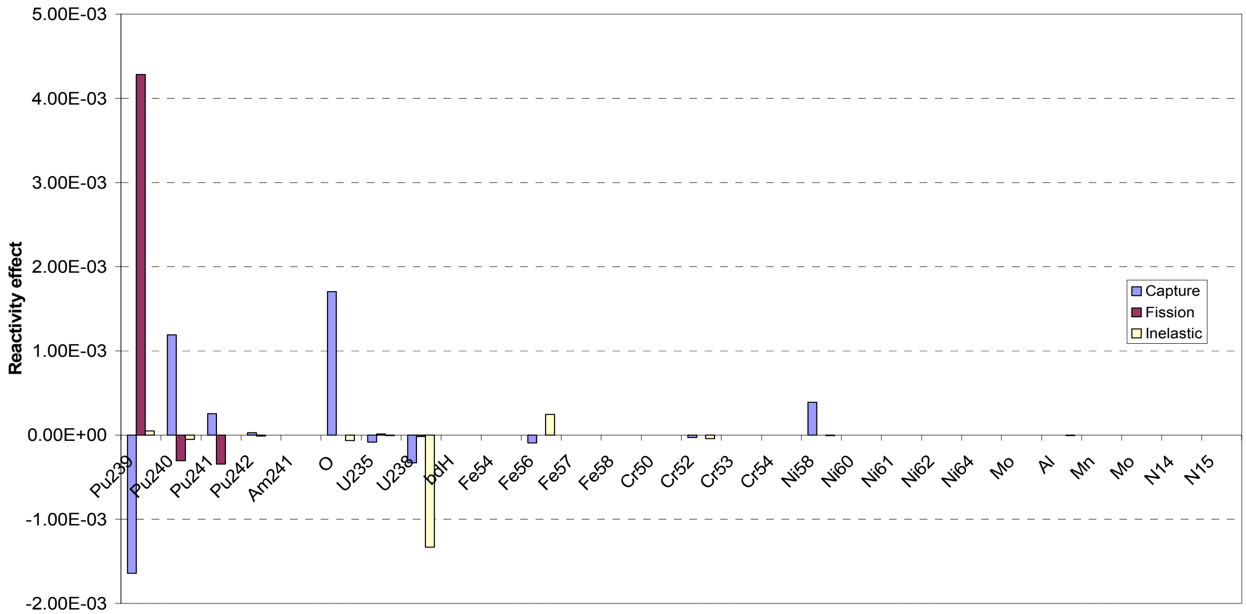
Globally, the most important contributions to the k_∞ change can be attributed to the heavy isotopes for which data have primarily been adjusted, viz. ^{239}Pu, ^{238}U, ^{240}Pu and (to a lesser extent) ^{241}Pu, as also to ^{16}O (see Fig. 1). More specifically, the principal contributors are, with decreasing magnitude, the fission related data (fission cross-section and ν [8]) for ^{239}Pu (429 "units"), followed by cross-sections for ^{16}O(n,α) (170), ^{239}Pu capture (-164), ^{238}U inelastic scattering (-133) and ^{240}Pu capture (119 "units"), as illustrated in Fig. 2. Smaller contributions have been found to come from ^{241}Pu fission (-34 "units"), ^{238}U capture (-33), ^{16}O elastic scattering (33), ^{240}Pu fission (-30) and ^{241}Pu capture (25 "units"). The adjustments made to the data for structural materials appear to play a less important role, e.g. ^{58}Ni capture and ^{56}Fe inelastic scattering cross-sections account for only 39 and 24 "units", respectively, all other effects being found negligibly small.

Figure 1: Data adjustment effects on k_∞ in terms of individual nuclides (10^5 "units")



For the five cross-section sets, adjustments for which make the largest contributions, the energy-dependent differential effects are displayed in the form of histograms in Figs 3-7.

Figure 2: Data adjustment effects on k_∞ in terms of individual reactions (10^5 "units")



By analyzing the "spectra" of Figs. 3-7, it is seen that

- The energy range of interest is above ~1 keV. Obviously, for threshold cross-sections, the lower energy bound lies much higher, e.g. for the $^{16}O(n,\alpha)$ cross-section (Fig. 4), it is ~3 MeV, corresponding more or less to the threshold of this reaction. For the ^{238}U inelastic scattering cross-section (Fig. 6), it is ~100 keV. For the latter reaction, the net effect is a decrease of the multiplication factor, a significant k_∞ decrease being observed due to adjustments above 2 MeV, whereas a smaller increase occurs due to the changes in the energy range 1-2 MeV.

- The data adjustment effects seem quite "scattered", showing a number of peaks and valleys. Although some of these are associated with the adjustment of individual resonances, large effects are also observed for significantly higher energies well above the unresolved resonance region. For example, for the ^{239}Pu fission and ^{240}Pu capture cross-sections (see Fig. 3 and Fig. 7, respectively), the dominant effects on k_∞ are observed for energies between 20 keV and 1 MeV.

Figure 3: Energy dependence of ^{239}Pu fission cross-section effects (10^5 "units")

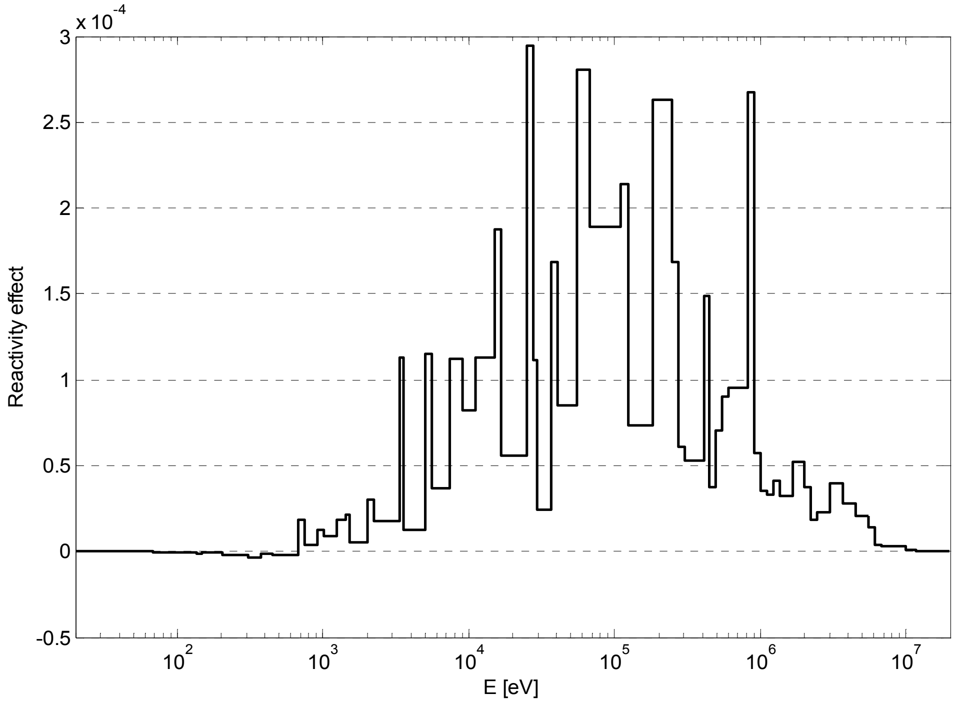


Figure 4: Energy dependence of ^{16}O(n,α) cross-section effects (10^5 "units")

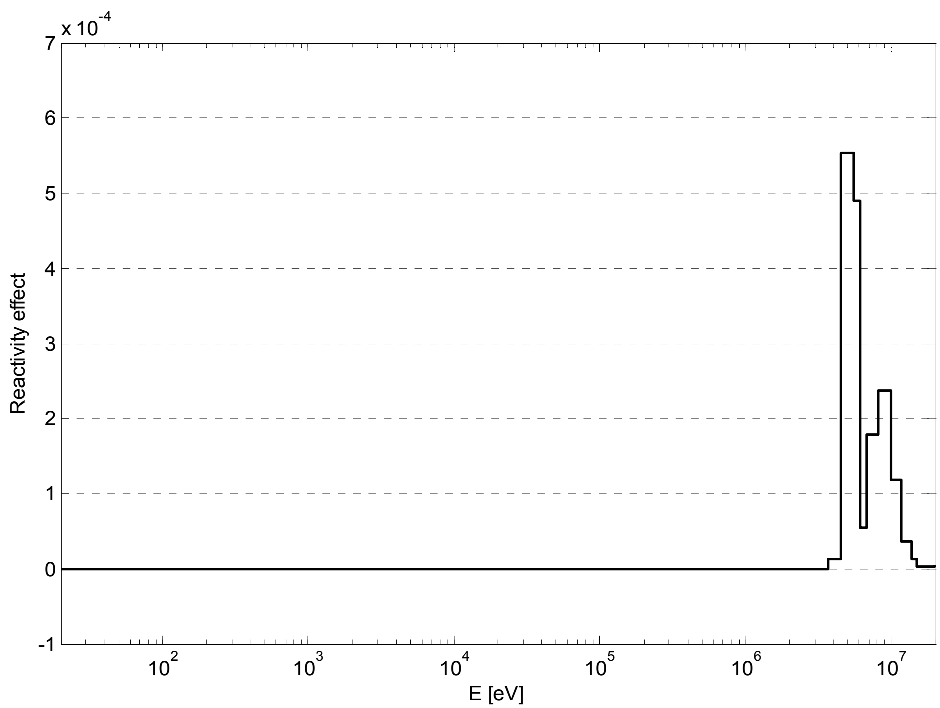


Figure 5: Energy dependence of ^{239}Pu capture cross-section effects (10^5 "units")

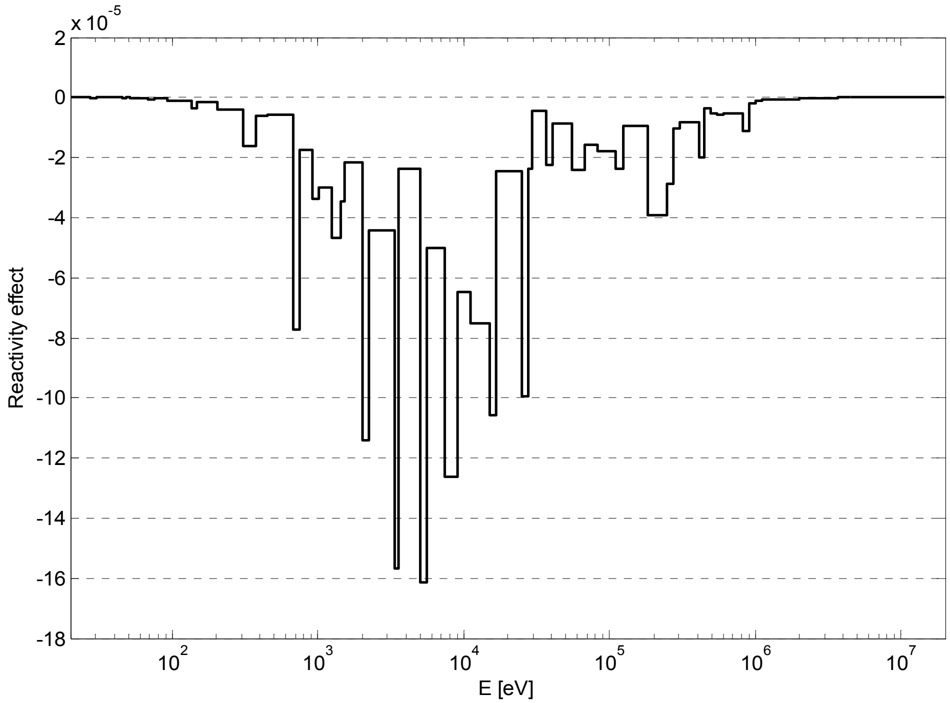


Figure 6: Energy dependence of ^{238}U inelastic scattering cross-section effects (10^5 "units")

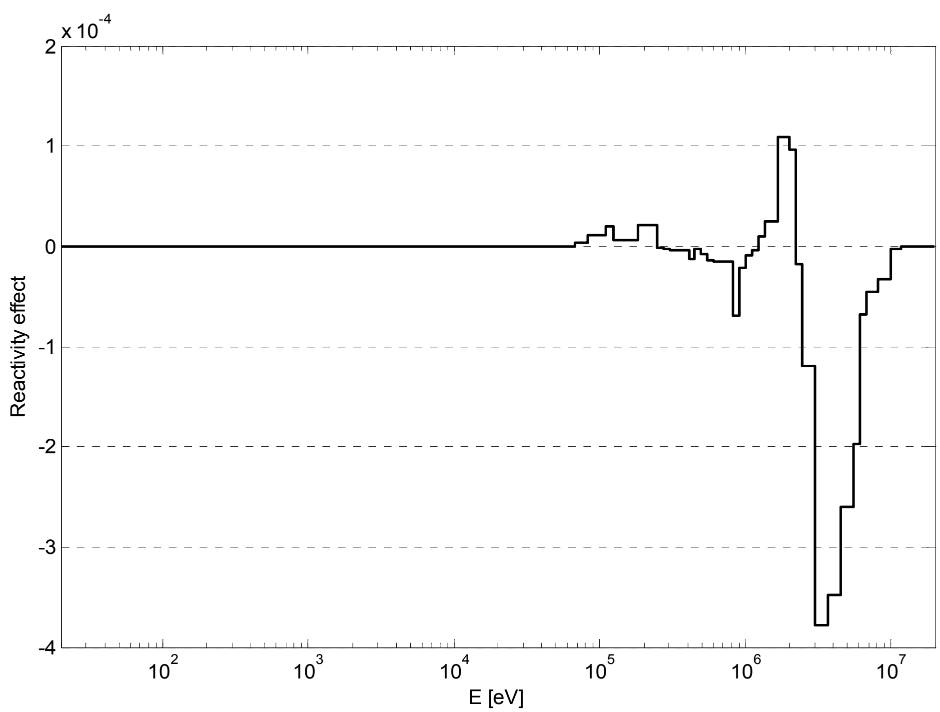
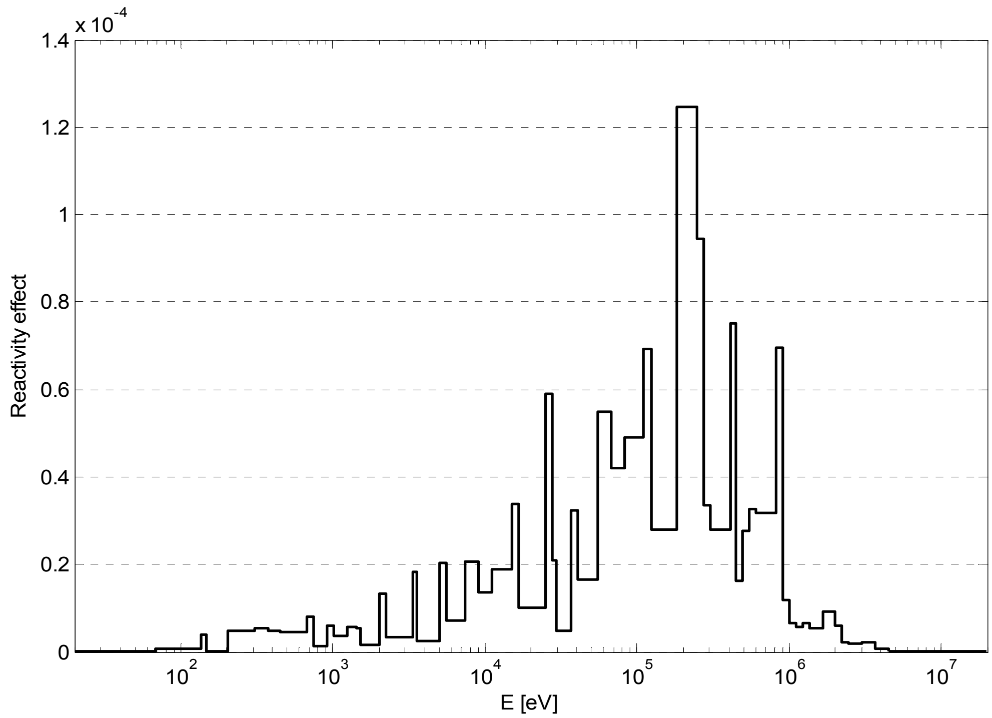


Figure 7: Energy dependence of ^{240}Pu capture cross-section effects (10^5 "units")



- The fact that the effects on k_∞ of changes in the fission and capture cross-sections of ^{239}Pu are of opposite sign (compare Figs. 3 and 5), while there is nevertheless a considerable positive net effect of ^{239}Pu (see Fig. 1), reflects the significant increase of the ν-value in the adjusted library.

4. Conclusions

This paper has summarized the results of new analyses performed for the reference test lattice of the wide range, GCFR-PROTEUS experimental program carried out at PSI during the 1970s, viz. a regular hexagonal array of steel-clad, 15%-total-Pu PuO_2/UO_2 rods in air. The calculations have been based on use of the deterministic fast-reactor code system ERANOS-2.0, as also the Monte Carlo code MCNPX-2.5e in conjunction with four different modern data libraries (JEF-2.2, JEFF-3.0, ENDF/B-VI.v8 and JENDL-3.3).

In global terms, good agreement with experiment is seen to be obtained by the different calculations for the important reaction rate ratios involving capture and fission of ^{238}U, as well as fission of ^{235}U (each expressed relative to the fission of ^{239}Pu). In particular, when comparing the ERANOS-2.0 calculations, the use of adjusted JEF-2.2 data (ERALIB1) yields a significantly better overall agreement for the three reaction rate ratios, the prediction of ^{238}U fission in particular improving markedly. In this case, the agreement with the experimental data is within the 1σ experimental uncertainty. This provides some useful indication of the adequacy of ERANOS-2.0/ERALIB1 for design studies of advanced gas-cooled fast reactors using conventional fuel pins.

Also measured in the center of the reference GCFR-PROTEUS test lattice was a set of reaction rate ratios which effectively represent additional, GCFR-relevant spectral indices. The numerator, in each case, involved the measurement of an infinite-dilution reaction rate since the corresponding nuclide, viz. either ^{232}Th, ^{233}U or ^{237}Np, did not occur in the reference lattice. Generally speaking, no consistent trend can be identified for spectral indices involving ^{232}Th and ^{237}Np, except that the capture rates appear to be systematically under-predicted (by up to several σ-values). The surprisingly large spread of the different calculations, seen particularly for the ^{232}Th(n,2n) reaction (expressed relative to ^{232}Th capture), and the fission rate ratios, is a clear indication that the data for ^{232}Th and ^{237}Np in the different libraries have undergone independent assessments in the energy range of interest. The need for revisiting the data for these nuclides, particularly from the viewpoint of analyzing fast-spectrum cores containing thorium and/or minor actinides, is thus clearly highlighted.

The computed results for k_∞, the important integral parameter that could not be measured in the reference lattice, indicate differences in the neutron balance calculations which are again surprisingly large in certain cases. An important result is that the ERANOS-2.0/ERALIB1 k_∞ value is very close to the MCNPX-2.5e/JENDL-3.3 value, with a difference of only 0.1%, providing some further indication that the adjusted library performs better than the non-adjusted one. Additionally, it was seen that the data adjustment itself induces a k_∞ increase of 0.6%. As illustration of the influence of individual data set changes on the neutron balance of the reference lattice, use has been made of the "Extended Generalized Perturbation Theory" procedures available in ERANOS-2.0 to decompose this particular effect. The main contributors are found to be the cross-sections for (1) ^{239}Pu fission (also the ν-value), (2) ^{16}O(n,α), (3) ^{239}Pu capture, (4) ^{238}U inelastic scattering and (5) ^{240}Pu capture. The data adjustment made for structural materials was seen not to play a major role in this context.

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