Effects of Uncertainties in Cross Sections and Geometric Models in Monte Carlo Analysis of Innovative Lead-Cooled Fast Reactors

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Abstract

There are numerous uncertainties in the prediction of core parameters of innovative reactor designs, arising from approximations used in the solution of the transport equation, geometrical models, and in nuclear data processing and cross section library generation. This paper describes the problems encountered in the analysis of the Encapsulated Nuclear Heat Source (ENHS) core benchmark and the new cross section libraries developed to overcome these problems. The ENHS is a lead-bismuth or lead cooled novel reactor concept that is fuelled with metallic alloy of Pu, U and Zr, and is designed to operate for 20 effective full power years without re-fuelling and with very small burn-up reactivity swing. The computational tools used include: MOCUP - a coupled MCNP-4C and ORIGEN2.1 using MCNP data libraries based on ENDF/B-VI evaluations; and KWO2 - a coupled KENO-V.a and ORIGEN2.1 using ENDFB-V.2 based 238-group library. Two geometrical models of the ENHS core were used: a detailed 2D-rz model and approximate 2D-xy mode. Uncertainties in the cross sections of lead were found to be particularly large and deserve careful evaluation.

KEYWORDS: ENHS fast reactor, lead-coolant, MOCUP and KWO2 codes, fuel burn-up, lead cross section data, uncertainties of k_{eff} evolution

1. Introduction

Lead or lead-alloy cooled fast reactors can provide nuclear power sustainability and have potential advantages in proliferation resistance, inherent safety, and possibly economics. Furthermore, there has been more than 80 reactor-year experience with lead/bismuth eutectic cooled reactors in Russia [1], and there are several new conceptual designs of small lead-bismuth or lead cooled reactors developed in the US. The Encapsulated Nuclear Heat Source (ENHS) features natural circulation cooling [2]. Its core contains uniform composition fuel rods without blanket elements and is designed to operate for 20 effective full power years without refueling by maintaining the effective multiplication factor k_{eff} nearly constant during the fuel burn-up.

A single zone ENHS core model was defined for use as a computational benchmark [3]. Two computational procedures were used for the analysis of this benchmark [4]. The first procedure is based on application of the MCNP -4C [5] and ORIGEN2.1 [6] codes interfaced by the MOCUP driver [7], and the second procedure is based on using the KENO-V.a [8] and ORIGEN2.1 codes

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coupled with KWO2 driver [4]. These procedures were considerably refined recently [4].

The fuel burn-up model was improved so that MCNP-4C could handle 95 fission products (FP); more accurate one-group cross sections were provided for production of isotopes in metastable nuclear states; and the MCNP cross sections libraries at additional temperatures were generated. With these modifications, the overall agreement between the computational tools used for single zone model calculations of the ENHS core benchmark was improved. It was found that the improved procedures do not affect the initial conclusions concerning the feasibility of designing the ENHS core to have a nearly zero burn-up reactivity swing. In addition, it was shown that depletion results strongly depend on the number of axial and radial depletion zones used.

Uncertainty analysis of new problems encountered in the analysis of the ENHS core benchmark described in this paper include: the elastic down-scatter cross section correction; modeling of fission products yield from fissionable nuclides without explicit fission yields; and effect of lead cross section data variations on k_{eff} evolution and the coolant void reactivity worth.

2. Computational benchmark model

The single zone model of the ENHS core benchmark [3] is shown in Figure 1.

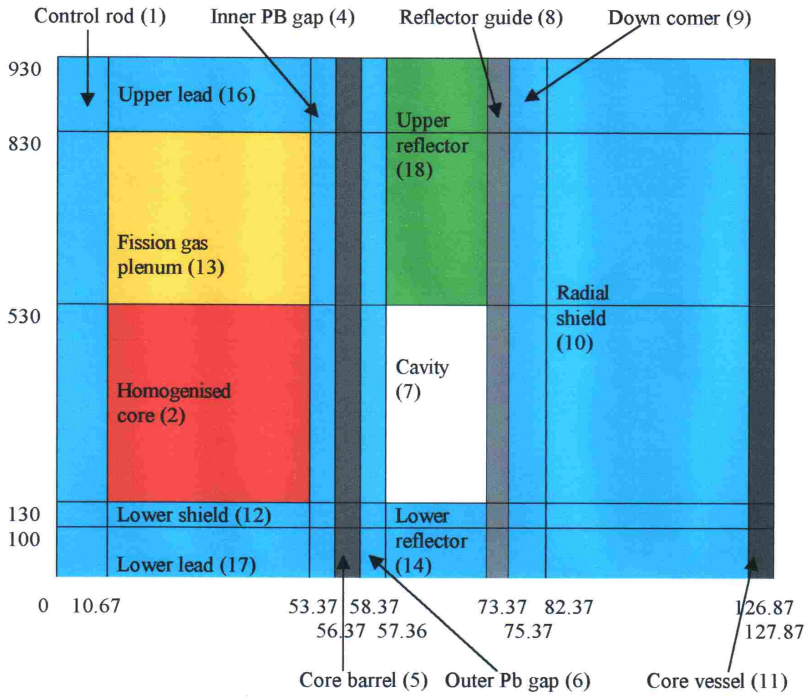

Figure 1. ENHS core benchmark geometry and dimensions (in cm)

The reactor thermal power is 250 MW and the average specific power is 14.3 W per gram of heavy metal (HM) corresponding to an average linear heat rate of 120 W cm^{-1}. The core is assumed to be homogeneous. The fuel is a metallic alloy of 90 weight % HM and 10% Zr. Its density is assumed to be 75% of the nominal density. The HM consists of 9.81% Pu and 80.19% U. The uranium is depleted to 0.2% ^{235}U. The isotopic composition of the loaded plutonium is 67.2% ^{239}Pu, 21.7%

^{240}Pu, 6.4% ^{241}Pu and 4.7% ^{242}Pu. The clad is made of ferritic - martensitic steel having 17% Cr, 14% Ni, 2.8% Mo and 1.5% Mn; the rest is Fe. The coolant is lead.

3. Computational methods

The MCNP-4C and ORIGEN2.1 codes interfaced by the MOCUP driver were used. In addition to calculating k_{eff}, neutron flux and power distribution, MCNP-4C calculates effective one-group cross-sections for the fuel constituents specified in its input. These cross sections are used by ORIGEN2.1 for fuel burn-up analysis. For isotopes that are not included in the MCNP-4C analysis, ORIGEN2.1 uses cross sections from a new pre-processed ORIGEN2.1 one-group cross sections library prepared specifically for the ENHS core benchmark calculation. Although replacing the existing ORIGEN2.1 libraries, designed for fast reactor fuel burn-up analysis, with the new one is not so important for the k_{eff} evolution, it is very important with regard to radiological characterization of the ENHS core benchmark.

Another computational tool used is KWO2; it is a variant of MOCUP in which KENO-V.a is used instead of MCNP-4C. It uses the ENDF/B-V.2 based 238-group cross section library of the SCALE-4.4a code package [9]. A predictor/corrector procedure was added instead of predictor only steps used in the MOCUP procedure. The major advantage of using KWO2 procedure is the decrease in computation time by about a factor of 10 as compared with MOCUP.

Recently improved MOCUP procedure with two new VMCCS continuous energy libraries [4] based on the ENDF/B-VI.8 and ENDF/B-V.2 evaluations has provided the reference results for comparison with the KWO2 procedure developed that uses the general purpose ENDF/B-V.2 based 238-group library. Both MCNP libraries were generated for seven temperatures (300, 500, 600, 700, 750, 800 and 900 K) by using the NJOY-99 code [10], and allow the inclusion of unresolved resonance self-shielding effects via the probability table method at these temperatures (*ptable* option). The most complete 238-group ENDF/B-V.2 library available in SCALE-4.4a was prepared with AMPX code [11] by using standard weighting function:

- Maxwellian spectrum from 10^{-5} to 0.125 eV,
- 1/E spectrum from 0.125 eV to 67.4 keV,
- Fission spectrum from 67.4 keV to 10 MeV, and
- 1/E spectrum from 10 to 20 MeV.

The ENDF/B-V.2 based results of k_{eff} evolution, presented in Fig. 2, show a large difference between the reference and KWO2 values. The SCALE-4.4a codes, that are based on the shielding factor method [12], do not provide the elastic down-scatter cross section correction for overall spectral shape. In order to analyze this effect, an additional ENDF/B-V.2 based 238-group library was prepared using the NJOY-99 code for most important elastic down-scatter nuclides, i.e., for Pb, Fe, Ni, Zr and ^{238}U. The weighting function

$$\phi_0(E) = e^{-2E} + 0.1\, e^{-0.8E}$$

was selected to represent the neutron flux spectrum of the ENHS core benchmark. Utilization of the new 238-group cross section data for Pb, Fe, Ni, Zr and ^{238}U and the general purpose 238-group SCALE-4.4a library for other nuclides, confirmed a characteristic dependence of elastic down-scatter cross sections on the spectral shape of flux weighting function, and improved the agreement between KWO2 and reference MOCUP results.

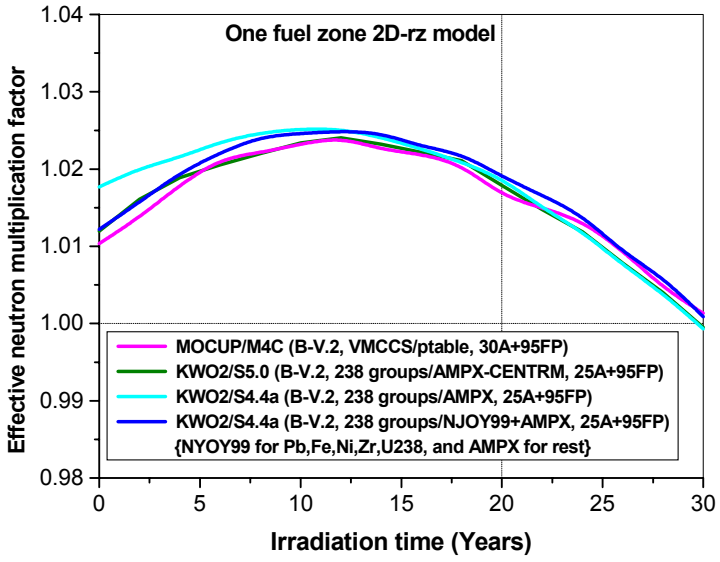

Figure 2. Comparison of ENDF/B-V.2 based k_{eff} calculations

A similar conclusion was obtained with the new KWO2 procedure, that uses capabilities of the SCALE-5.0 code system [13]. Namely, the coupling of the continuous-energy resonance self-shielding (via the CENTRM code [14]) with the multigroup transport solution was provided. It was shown: (a) that standard averaging of resonance cross sections with obtained continuous-energy scalar flux or current (without averaging of down-scatter data) cannot improve the accuracy of KWO2 (SCALE-5.0/CENTRM) results, and (b) that the ENHS benchmark is not a leakage-dominated core that requires current-weighted cross sections. In order to provide the same accuracy of the new KWO2 procedure as in the case of ENDF/B-V.2 based MOCUP calculation, the averaging of both resonance cross sections and slowing-down sources with computed space-dependent neutron spectra was necessary.

One important step for assessment of the ENHS results is a reliable examination of the accuracy of a model used in ORIGEN2.1 for fission products (FP) yield from fissionable nuclides without explicit fission yields. ORIGEN2.1 automatically substitutes yields from nearest actinides (A). The SCALE-5.0 code system extended up to 30 the number of fissionable nuclides that can be handled by ORIGEN-S with explicit fission yields. However, the automatic utilization of CENTRM and ORIGEN-S is provided only in the TRITON sequence [15], based on the two-dimensional (2D) discrete ordinates transport method. In order to test accuracy of ORIGEN-2.1 (via MOCUP and KWO2 procedures) and compare it with the TRITON procedure, an infinitely long simple 2D-xy geometry model of the ENHS benchmark was selected, having an equivalent core diameter equal to 105.6 cm and a square lead reflector of 178x178 cm^2. This model does not entirely preserve the energy-dependent neutron flux of the ENHS core benchmark, and cannot be recommended for an accurate representation of fuel depletion in this core benchmark. Results obtained for this geometry model, given in Figure 3, show: a good agreement between ORIGEN2.1 and ORIGEN-S (from the SCALE-5.0 code system), as well as between 25A+95FP and 35A+185FP fuel burn-up models. Once again, a good agreement between the ENDF/B-V.2 based MOCUP and the new KWO2 procedures was shown.

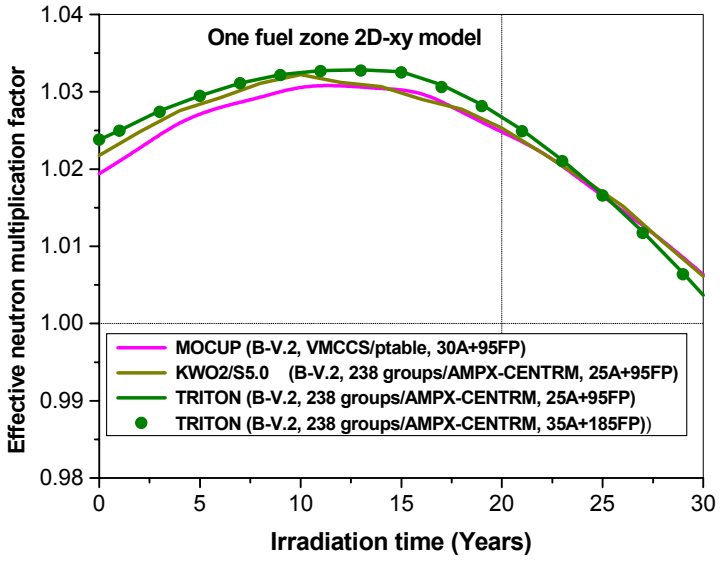

Figure 3. Comparison of ORIGEN2.1 and ORIGEN-S results

The MOCUP calculations using the ENDF/B-V.2 and ENDF/B-VI.8 cross section libraries were compared. This comparison is important due to significant differences in the cross section data for lead, ^{238}U and ^{239}Pu in these evaluations. The ENDF/B-VI.8 evaluation lacks cross-sections data for ^{204}Pb. Since the scattering cross section for ^{207}Pb at fission energies most closely resembles that of ^{204}Pb, the content of ^{207}Pb in the ENDF/B-VI.8 based calculations was increased, atom for atom, to account for the missing ^{204}Pb. The results, as presented in Figure 4 show:

- A notable difference (about 500 pcm at EOC) between the MOCUP results based on ENDF/B-V.2 and ENDF/B-VI.8;
- A small decrease of k_{eff} (for about 200 pcm) caused by introducing the JEFF-3.1 evaluated cross section data for the missing ^{204}Pb (roughly the same effect is observed with the ^{204}Pb data from the JENDL-3.3 evaluation);
- An unimportant influence of unresolved resonance self-shielding effects in the ENDF/B-VI based MOCUP calculations; and
- A negligible difference between the MCNP-4C and MCNP-5.0 based MOCUP calculations.

4. Results

The effect of lead-coolant in the ENHS core benchmark on the neutron slowing-down source was considered, and an analysis of its sensitivity to cross section data from available evaluations for lead was undertaken using MCNP-4C. The MCNP libraries were prepared by using the most modern evaluations:

- The ENDF/B-VI.8 (1996), JEFF-3.1 and JENDL-3.3 evaluations for ^{206}Pb, ^{207}Pb and ^{208}Pb nuclides, and
- The JEFF-3.1 and JENDL-3.3 evaluations for ^{204}Pb.

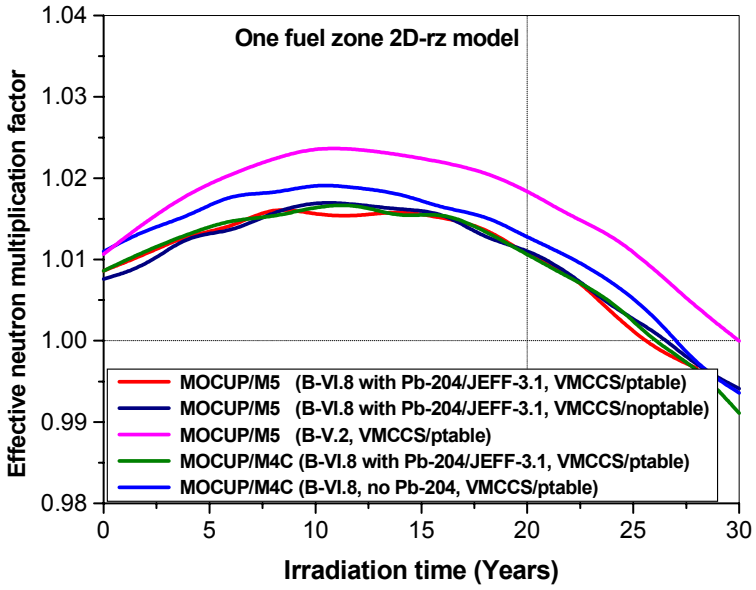

Figure 4. Comparison of the MOCUP results for various cross section libraries.

Additional MCNP libraries were prepared on the basis of some older evaluations: (a) the ENDF/B-VI.2 (1989) evaluation for ^{206}Pb, ^{207}Pb and ^{208}Pb nuclides, and (b) the ENDF/B-V.2 and JENDL-3.1 evaluations for Pb nuclide. The older evaluations of lead cross section data were included in this analysis because:

- The ENDF/B-V.2 data are used in the general purpose 238-group SCALE^{TM} libraries;
- The ENDF/B-VI.2 data were applied for the TAMU libraries preparation (widely used at California University at Berkeley); and
- The JENDL-3.1 data provided the best agreement between calculated and measured results obtained at the BFS-61, -64, -77, -85 and -87 critical configurations with lead located in the core and in the reflector [1].

The cross section data for all remaining nuclides were from the ENDF/B-VI.8 evaluation. The MCNP-4C calculations were carried out with statistical uncertainty (1σ) equal to 40 pcm. Results of this analysis using various evaluated cross section data for lead, given in Fig. 5 and 6, show: (a) good agreement between calculations based on the data from ENDF/B-VI.8, JEFF-3.1 and JENDL-3.1; (b) notable difference (about -600 pcm) between calculations based on the ENDF/B-VI.8 and older evaluated cross section data (ENDF/B-V.2 and ENDF/B-VI.2); and (c) notable difference (about 700 pcm) between calculations based on the ENDF/B-VI.8 and JENDL-3.3 data.

In order to examine the reason for a notable difference between the results obtained with the ENDF/B-VI.8 and JENDL-3.3 evaluated cross section data for lead, and to investigate the characteristics of ENHS core benchmark with non-radioactive lead coolant, i.e., with ^{206}Pb, the k_{eff} calculations were repeated replacing the lead with ^{206}Pb, ^{207}Pb and ^{208}Pb respectively.

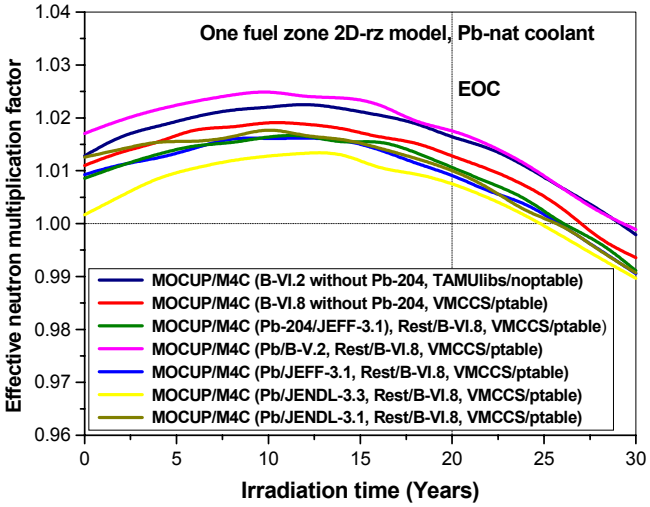

Figure 5. Comparison of k_{eff} calculations for different cross section data for lead

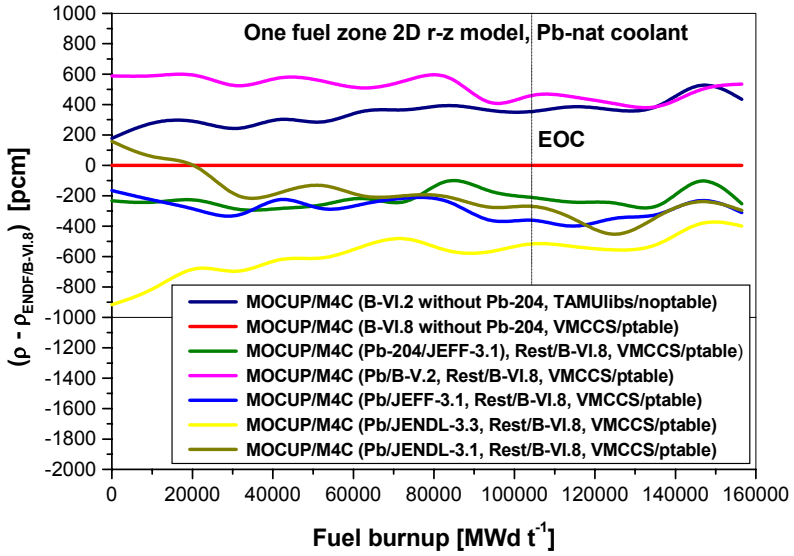

Figure 6. Comparison of reactivity calculations for different cross section data lead

Results are given in Figures 7, 8, and 9, and show: (a) good agreement (within the range of 500 pcm) between all modern evaluations for the ^{206}Pb and ^{208}Pb coolants; and (b) a significant difference (about 1500 pcm) between the ENDF/B-VI.8 and JENDL-3.3 evaluations due to a slightly higher values in the JENDL-3.3 evaluation for elastic cross section of ^{207}Pb as compared with ENDF/B-VI.8 evaluation.

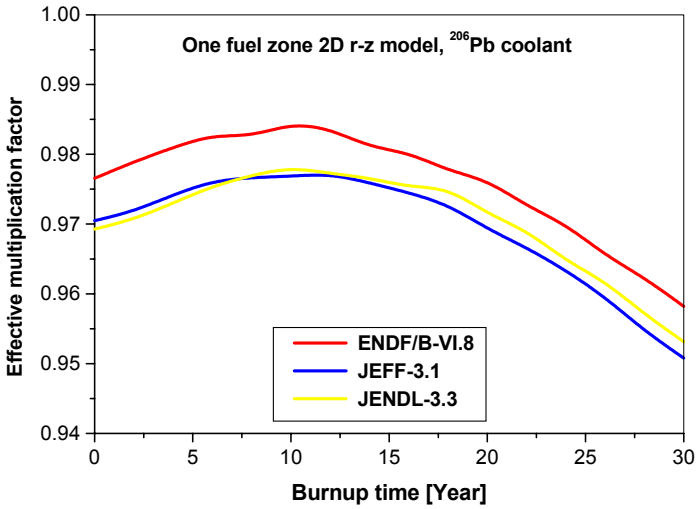

Figure 7. Comparison of k_{eff} calculations for different ^{206}Pb cross-section data

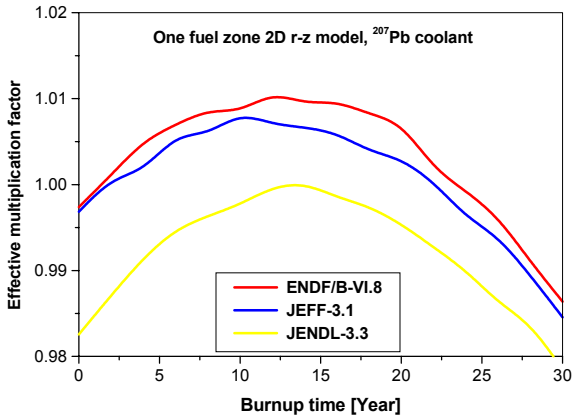

Figure 8. Comparison of k_{eff} calculations for different ^{207}Pb cross section data

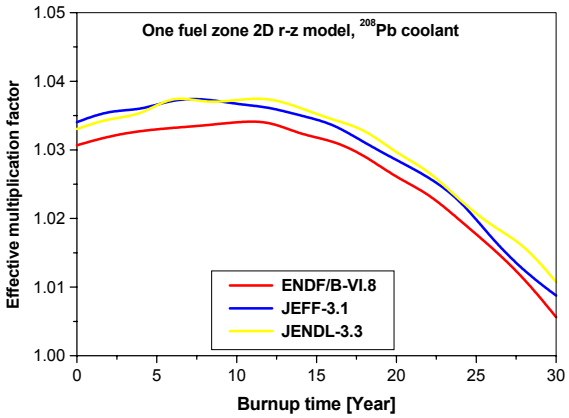

Figure 9. Comparison of k_{eff} calculations for different ^{208}Pb cross section data

Coolant void reactivity worth (calculated as the reactivity due to change of coolant density inside the core barrel from value ρ_0 to value of $0.75\,\rho_0$) is presented in Figure 9 as a function of different cross section data for lead. The observed difference in the coolant void reactivity worth is between 100 and 400 pcm.

Figure 10 shows comparison of coolant void reactivity worth as a function of various lead isotopes, using the cross section data from the same library. The observed difference when

compared with natural lead could be as high as 600 pcm

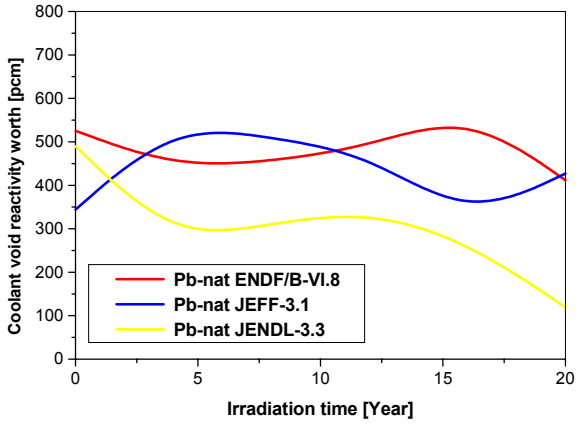

Figure 9. Comparison of coolant void reactivity worth for different lead cross section data

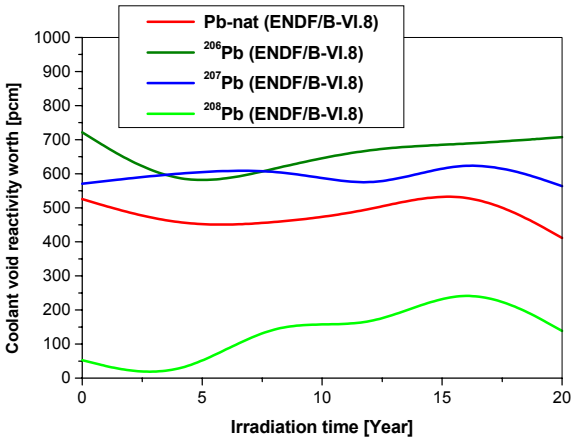

Figure 10. Comparison of coolant void reactivity worth for different lead isotopes

5. Conclusion

This paper describes the problems encountered in the analysis of the ENHS core benchmark. In order to overcome some of those problems various improvements of cross section libraries were developed and the most important improvements were presented here. Thanks to the improvements of cross sections data, a good agreement between different neutron transport methods and different fuel burn-up models were obtained. In addition, it has been shown that the current cross section data for lead differ among different cross section libraries, and that these inaccuracies result in very high uncertainty of k_{eff} and coolant void reactivity.

Acknowledgement

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