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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, and in nuclear data processing and cross section libraries 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 new 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 refuelling and with very small burnup reactivity swing. The computational tools benchmarked include: MOCUP - a coupled MCNP-4C and ORIGEN2.1 utility codes with MCNP data libraries based on ENDF/B-VI evaluations; and KWO2 - a coupled KENO-V.a and ORIGEN2.1 code with ENDFB-V.2 based 238 groups library. Uncertainties in the cross sections of lead were found particularly large and deserve careful evaluation.

1. INTRODUCTION

In the next few decades, reactors that use uranium more efficiently and that can also burn their own long-lived waste are needed to make nuclear power sustainable. Lead or lead-alloy cooled fast reactors can provide this sustainability and have potential advantages regarding proliferation resistance, inherent safety, and possibly also regarding economics. Furthermore, there has been an 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 one of which is the Encapsulated Nuclear Heat Source (ENHS) that features natural circulation cooling [2]. The ENHS 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 burnup.

Without an experimental benchmark of a comparable hard spectrum lead-cooled core, a single zone ENHS core model was defined for use as a computational benchmark [3]. Two computational procedures were used for the burnup 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 second procedure is based on employment of the KENO-V.a [8] and ORIGEN2.1 codes coupled with KWO2 driver [4].

Recently, these procedures were considerably refined [4]. The fuel burnup model was improved so that MCNP-4C could handle 95 fission products (FP); proper one-group cross sections were provided for production of isotopes in metastable nuclear states; and MCNP™ cross sections libraries at more temperatures were generated. With applied 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 burnup 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 influence of cross section data for lead on $k_{eff}$ evolution.

2. COMPUTATIONAL BENCHMARK MODEL

The single zone model of the ENHS core benchmark [3] is shown in Figure 1. 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% 235U. The isotopic composition of the loaded plutonium is 67.2% 239Pu, 21.7% 240Pu, 6.4% 241Pu and 4.7% 242Pu. 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.

![ENHS core benchmark geometry (dimensions in cm)](image-url)
3. COMPUTATIONAL METHODS

The main computational tool employed consists of the MCNP-4C and ORIGEN2.1 utility codes interfaced by the MOCUP driver. In addition to calculating $k_{\text{eff}}$, 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 burnup analysis. For isotopes not included in the MCNP-4C analysis, the ORIGEN2.1 code uses cross sections from new pre-processed ORIGEN2.1 one-group cross sections library prepared for the ENHS core benchmark calculation. Although replacing the existing ORIGEN2.1 libraries, designed for fast reactor fuel burnup analysis, with the new one is not so important for the $k_{\text{eff}}$ evolution, this replacement 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. A common deficiency of both procedures is the limited number of material zones for which the fuel burnup calculation can be performed. This limitation is the consequence of the data handling of these code systems – keeping all microscopic cross sections for all nuclides in all material zones in the computer memory or in auxiliary binary files. The major advantage of using KWO2 procedure is the decrease in computation time by about a factor of 10 as compared with MOCUP procedure.

4. RESULTS

Recently improved MOCUP procedure with two new VMCCS continuous energy libraries [4] based on the ENDF/B-V1.8 and ENDF/B-V.2 evaluations has provided the reference results for comparison with the KWO2 procedure developed on the basis of the SCALE-4.4a codes and general purpose ENDF/B-V.2 based 238-group library.

Both MCNP\textsuperscript{TM} libraries were prepared 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,
- a $1/E$ spectrum from 0.125 eV to 67.4 keV,
- a fission spectrum from 67.4 keV to 10 MeV, and
- a $1/E$ spectrum from 10 to 20 MeV.

The ENDF/B-V.2 based results of $k_{\text{eff}}$ evolution, presented in Figure 2, show a large difference between the reference and KWO2 values. It has been recognized that SCALE-4.4a codes, that are based on the shielding factor method [12], do not provide the elastic down-scatter cross section correction for gross 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

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

was selected to represents the neutron flux spectrum of the ENHS core benchmark. The utilization of the new 238-group cross section data for Pb, Fe, Ni, Zr and $^{238}$U and of the general purpose 238-group SCALE-4.4a library for remainder 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.

![Fig. 2. Comparison of ENDF/B-V.2 based $k_{\text{eff}}$ calculations](image-url)

A similar conclusion was obtained with the new KWO2 procedure, modified by including the new capabilities of the SCALE-5.0 code system [13] that allow the coupling of the continuous-energy resonance self-shielding (via the CENTRM code [14]) with the multigroup transport solution. Using these capabilities it was shown that standard averaging of resonance cross sections with obtained continuous-energy scalar flux or current (without averaging of down-scatter data) can not improve the accuracy of KWO2 (SCALE-5.0/CENTRM) results, and that the ENHS benchmark is not a leakage-dominated spectra core that require current-weighted cross sections. Only the averaging of both resonance cross sections and slowing-down sources with computed space-dependent neutron spectra provided the same accuracy of newly KWO2 procedure with ENDF/B-V.2 based MOCUP calculation.

One important step for assessment of calculation results, made for the ENHS core benchmark, is a reliable examination of the accuracy of a model used in the ORIGEN2.1 code for fission products yield from fissionable nuclides without explicit fission yields. The ORIGEN2.1 code 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 the ORIGEN-S code with explicit fission yields. However, the automatic utilization of CENTRM and ORIGEN-S codes is provided only in the TRITON sequence [15], based on the two-dimensional (2D) discrete ordinates transport method.
order to achieve the comparison of the ORIGEN-2.1 code (via MOCUP and KWO2 procedures) with TRITON procedure, an infinitely long simple 2D-xy geometry model of the ENHS benchmark with equivalent core diameter equal to 105.6 cm and square lead reflector of 178x178 cm² was selected. This model does not preserve entirely the energy-dependent neutron flux of the ENHS core benchmark, and can not be recommended for an accurate representation of fuel depletion in this core benchmark. The purpose of the 2D-xy model of the ENHS core benchmark is the testing of the ORIGEN2.1 code accuracy. Results obtained for this geometry model, given in Figure 3 show:

- a good agreement between the ORIGEN2.1 code and most improved ORIGEN-S code from the SCALE-5.0 code system,
- a very good agreement between 25A+95FP and 35A+185FP fuel burnup models; and
- once again, a good agreement between ENDF/B-V.2 based MOCUP and newly KWO2 procedures.

At this stage, a comparison between the ENDF/B-V.2 and ENDF/B-VI.8 based MOCUP calculations was undertaken. This comparison is important due to significant differences in the cross sections data for lead, 238U and 239Pu in these evaluations. Because the ENDF/B-VI.8 evaluation lacks cross-sections data for 206Pb, and since the scattering cross section for 207Pb at fission energies most closely resembles that of 206Pb, the content of 207Pb was increased, atom for atom, to account for the missing 206Pb. Calculation results, presented in Figure 4 show:

- a notable difference (about 500 pcm at EOC) between the k_eff calculations based on the ENDF/B-VI.8 (from 1996), JEFF-3.1 and JENDL-3.1 evaluated cross section data for lead;
- a notable difference between the k_eff calculations based on the ENDF/B-VI.8 and ENDF/B-V.2 and ENDF/B-VI.2 (from 1989) evaluated cross section data for lead (the older evaluations give a higher values by about 700 pcm); and
- a notable difference between the k_eff calculations based on the ENDF/B-VI.8 and newest JENDL-3.3 evaluated cross section data for lead (the JENDL-3.3 evaluation gives a lower value by about 700 pcm).

Finally, the effect of the 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. In this analysis the cross section data for all remaining nuclides were used from the ENDF/B-VI.8 evaluation. Results of this analysis, given in Figures 5 and 6 show:

- a good agreement between the k_eff calculations based on the ENDF/B-VI.8 (from 1996), JEFF-3.1 and JENDL-3.1 evaluated cross section data for lead;
- 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.
Fig. 6. Comparison of reactivity calculations for different lead cross section data

5. CONCLUSION

This paper described the problems encountered in the analysis of ENHS core benchmark and the most important improvements of cross section libraries developed to overcome some of these problems. A good agreement between different neutron transport methods and different fuel burnup models were obtained. However, it has been shown that the current cross section data for lead have some inaccuracies that result in very high uncertainty of \( k_{\text{eff}} \) evolution (more than 1500 pcm at BOC).

ACKNOWLEDGEMENT

This work was supported by US Department of Energy NERI program under Award No. DE-FG03-99SF21889 and by the Ministry of Science and Environment Protection of the Republic of Serbia under Contract No. 1958 ("Transport processes of particles in fission and fusion systems").

REFERENCES


