MONTE CARLO WITH FUEL BURNUP METHOD FOR THE ENHS BENCHMARK CALCULATIONS

by

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Estimates of the uncertainties arising from approximations in the methods used in different nuclear data processing and neutron transport codes are usually obtained by inter-comparing calculations made using different code systems. This paper gives details of an investigation of differences between results obtained by using different codes for a single zone model of the Encapsulated Nuclear Heat Source (ENHS) benchmark core fuelled with metallic alloy of Pu, U, and Zr. The ENHS is a new lead-bismuth or lead cooled novel reactor concept for 20 effective full power years without refuelling and with very small 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 evaluation; KENO-V.a/ORIGEN2.1 code system, recently developed by authors of this paper, with the ENDFB-V based 238 group library; the design-oriented procedure based on the simplified one-dimensional (1D) geometry model and SAS2H control module; and the well-established fast reactor neutronics design tools in use at Argonne National Laboratory. Calculations made for the ENHS benchmark have shown that the differences between the results obtained when using different code schemes are quite significant and should be taken into account in assessing the quality of the nuclear data library.

Key words: Monte Carlo, fuel burnup, ORIGEN2.1, ENHS benchmark

INTRODUCTION

The Encapsulated Nuclear Heat Source (ENHS) is a new lead-bismuth or lead cooled novel reactor concept for a nominal power of 125-250 MW_{th} [1, 2]. One of its novel design features is its core; it is to use uniform composition fuel rods, have no blanket elements and is to operate for 20 effective full power years without refuelling and with a very small reactivity swing. In the absence of an experimental benchmark of comparable hard spectrum lead-cooled cores, a computational single zone benchmark was defined by the ENHS project team to provide a reference design case.

This paper describes three procedures, being prepared for the long-life core fuel burnup analysis of defined ENHS benchmark core. The first procedure is based on the application of the MCNP-4C [3] and ORIGEN2.1 [4] codes, interfaced by the MOCUP [5] driver. The second procedure is founded on the coupling of KENO-V.a [6] and ORIGEN2.1 codes. These utility codes are designed for reference calculations of long-life cores in 2D or 3D geometry models. In the third, design-oriented procedure, the simplified 1D geometry model and control module SAS2H are used. The purpose of this paper is to describe the ENHS benchmark problem and to inter-compare the results obtained with these procedures and with fast reactor neutronics design tools in use at the Argonne National Laboratory (ANL).

COMPUTATIONAL BENCHMARK MODEL

The single zone model of ENHS benchmark is shown in fig. 1. Material compositions for this bench-

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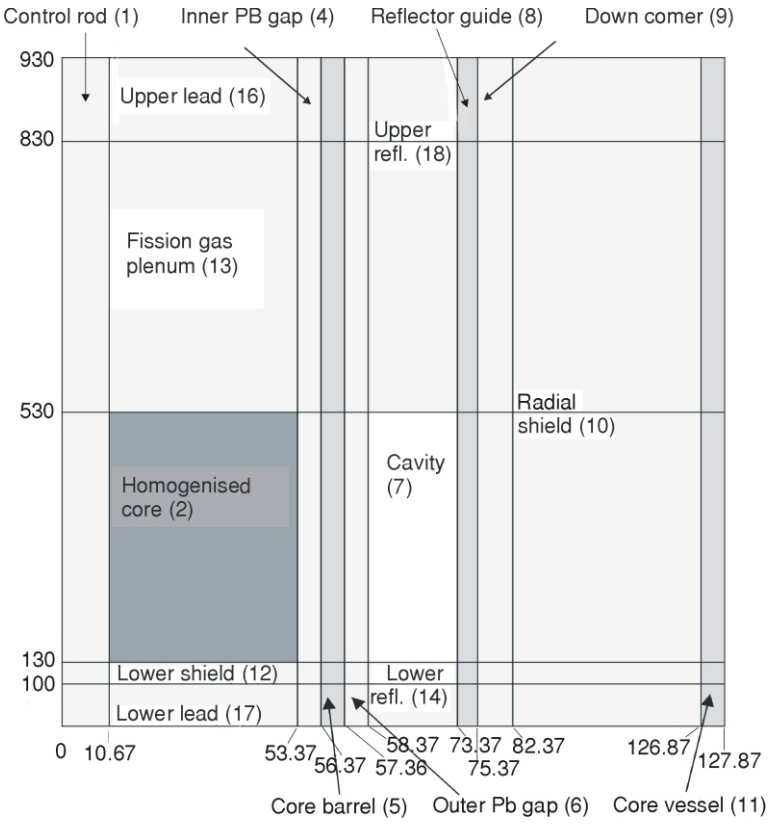

Figure 1. ENHS benchmark problem geometry and dimensions (in cm)

Table 1. Material compositions, volume fractions, and temperatures

Regions (region number)	Material, volume fraction	Temperature K
Control rod region (1)	99% Pb + 1% SS[a]	753
Core (2)	47.621% fuel + 31.425% Pb + 20.953% SS	753
Inner Pb gap (4)	100% Pb	753
Core barrel (5)	100% SS	753
Outer Pb gap (6)	100% Pb	693
Cavity (7)	100% Pb (or 10% SS[b])	693
Reflector guide (8)	70% Pb + 30% SS	693
Down comer (9)	100% Pb	693
Radial shield (10)	100% Pb	693
Core vessel (11)	100% SS	693
Lower shied (12)	100% Pb	693
Gas plenum (13)	31.4253% Pb + 20.953% SS	813
Lower reflector (14)	100% Pb	693
Upper Pb (16)	100% Pb	813
Lower Pb (17)	100% Pb	693
Upper reflector (18)	90% Pb + 10% SS	693

[a] SS denotes stainless steel
[b] When cavity is not filled with lead

mark problem are given in tab. 1, and atomic number densities for composing materials are presented in tab. 2. The reactor thermal power is 250 MW and is constant during the entire life of ENHS assumed to be even 30 years. The average specific power is 6.12 Wg^{-1} heavy metal (HM) corresponding to an average linear heat rate of 120 Wcm^{-1}. The core is assumed to be homogeneous and of annular cylindrical geometry. The fuel is a metallic alloy of 90% 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 stainless steel having 17% Cr, 14% Ni, 2.8% Mo, and 1.5% Mn; the rest is Fe. The coolant is lead.

COMPUTATIONAL METHODS

The main computational tool employed consists of MCNP-4C and ORIGEN2.1 interfaced by MOCUP driver. In addition to calculating k_{eff}, 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 burnup analysis. For isotopes not included in the MCNP-4C analysis,

Table 2. Atomic number densities for composing materials

Region (region number)	Atomic number density 10^{-24} cm^{-3}
Control rod region (1)	Pb: 3.02043-2[a], Fe: 5.55118-4, Ni: 1.14172-4, Cr: 1.56540-4, Mo: 1.37239-5, Mn: 1.30727-5
Core (2)[b]	Pu-239: 9.40189-4, Pu-240: 3.02336-4, Pu-241: 8.87696-5, Pu-242: 6.49405-5, U-235: 2.32633-5, U-238: 1.14617-2, Zr: 3.73749-3, Pb: 9.58770-3, Fe: 1.16316-2, Ni: 2.39230-3, Cr: 3.28003-3, Mo: 2.87562-4 Mn: 2.73916-4
Inner Pb gap (4)[c]	Pb: 3.05094-2
Core barrel (5)	Fe: 5.55118-2, Ni: 1.14172-2, Cr: 1.56540-2, Mo: 1.37239-3, Mn: 1.30727-3
Outer Pb gap (6)	Pb: 3.07187-2
Cavity (7)	Pb: 3.07187-2
Reflector guide (8)	Pb: 2.15031-2, Fe: 1.66535-2, Ni: 3.42517-3, Cr: 4.69619-3, Mo: 4.11718-4, Mn: 3.92180-4
Down comer (9)	Pb: 3.07187-2
Radial shield (10)	Pb: 3.07187-2
Core vessel (11)	Fe: 5.55118-2, Ni: 1.14172-2, Cr: 1.56540-2, Mo: 1.37239-3, Mn: 1.30727-3
Lower shield (12)	Pb: 3.07187-2
Gas plenum (13)	Pb: 9.52193-3, Fe: 1.16316-2, Ni: 2.39230-3, Cr: 3.28003-3, Mo: 2.87562-4, Mn: 2.73916-4
Lower reflector (14)	Pb: 3.07187-2
Upper Pb (16)	Pb: 3.03001-2
Lower Pb (17)	Pb: 3.07187-2
Upper reflector (18)	Pb: 2.76468-2, Fe: 5.55118-3, Ni: 1.14172-3, Cr: 1.56540-3, Mo: 1.37239-4, Mn: 1.30727-4

[a] Read as 3.02043 10^{-2}
[b] Fuel density: 15.85 0.75 gcm^{-3}; SS density: 7.95 gcm^{-3}
[c] Pb density: 11.3 gcm^{-3} (solid); (11072-1.2 T)/1000 gcm^{-3} (liquid), for T from 400 to 700 C

ORIGEN2.1 uses cross sections from its pre-processed standard libraries.

The first MOCUP results for the ENHS benchmark core was obtained by using the fuel burnup model with 26 actinides (A) and 47 fission products (FPs). Then, the UCB (University of California at Berkeley) model with 45 A and 67 FPs was applied. In this model different MCNP-4C cross section libraries were used. For example:

– for the ^{235,238}U and $^{238–242}$Pu the Texas A&M library is used (.86c at 750 K, based on the ENDF/B-VI evaluation);

– for Th, Pa, Np, ^{241,243}Am and Cm the FSXJ3R2 library is used (.37c at 300 K, based on the JENDL-3.2 evaluation);

– for ^{242m}Am the RMCCS library is used (.51c at 300 K, based on ENDF/B-V evaluation);

– for fission products two libraries are used, the ENDF60 (.60c at 300 K based on the ENDF/B-VI evaluation) and FSXJ3R2 library (.37c at 300 K, based on the JENDL-3.2 evaluation); and

– for constructional material the ENDF60 library is used (.60c at 300 K based on the ENDF/B-VI evaluation).

For reason of decreasing CPU time, the ENHS benchmark calculations with this model was performed with (50 + 250) 1000 source neutrons.

A modified procedure of interfacing MCNP-4C and ORIGEN2.1 was developed to bypass the limitation of the number of fission products that can be handled by MCNP-4C. In addition to the 67, all other fission products for which we had cross sections in the MCNP-4C format were specified in the input to MCNP-4C and taken into account for the calculation of k_{eff}. However, MCNP-4C did not generate the effective one-group cross sections for these extra fission products. An algorithm was written to transfer the number density of these extra fission products into the MCNP-4C input in addition to the number densities MOCUP was set to transfer from ORIGEN2.1 to MCNP-4C. By using this new procedure we were able to account for additional 111 fission products in MCNP-4C calculations. In this procedure the one-group cross section data for fission products not included in MCNP-4C were taken from AMORUUUC [4] library prepared by using the energy spectrum of neutron flux in the typical Fast Breeder Reactor with sodium.

In order to use the MCNP-4C cross section data for temperatures which are as close to the benchmark specification (tab. 1) as possible, we selected the VMCCS library [7] based primarily on ENDF/B-VI data, but, if that is not available, on JENDL3.2 and BROND2 data. At present, this library contains cross section data for light elements, actinides and fission products at three temperatures (300 K, 600 K, and 900 K). It allowed us to use MCNP-4C cross section data at 900 K for all actinides and fission products, and at 600 K for all constructional materials and coolant. For decreasing the statistical uncertainties, a model with (50 + 500) source neutrons was used. Also, the new ORIGEN2.1 one-group cross-section library, *i. e.*, the ENHSB library for the ENHS benchmark core calculation was prepared. Although, replacing the existing ORIGEN2.1 library with the ENHSB library for the benchmark core is not so important with regard to criticality calculation, this replacement is very important with regard to the

radiological characterisation of ENHS benchmark core. The first results with VMCCS library were obtained with the so-called UCB model with 45 A and 67 FPs [8].

Another computational tool is a variant of MOCUP in which KENO-V.a is used instead of MCNP-4C. It uses the ENDF/B-V based 238-group cross section library of the SCALE-4.4a code package [9]. The initial version of KENO-V.a/ORIGEN2.1 procedure was similar to the MOCUP utility since the MOCUP codes origenPRO for preparing input and for running the ORIGEN2.1 code and compPRO for preparing the atomic number densities of actinides and fission products were used. Later this procedure was simplified; the new modules were prepared, and the existing origenPRO and compPRO codes from MOCUP utility code were replaced. Also, the possibility to use the predictor/corrector steps was added instead of predictor steps that are used in the MOCUP procedure. Although, this new KENO-V.a/ORIGEN2.1 procedure can handle any number of actinides and fission products for which the cross sections exist in the SCALE multigroup libraries (instead of total 130 nuclides, actinides plus fission products, in the MOCUP utility code), and although this procedure is much faster than MOCUP, the common characteristic of these procedures (MOCUP and KENO-V.a/ORIGEN.2.1) is a limited number of material zones in which fuel burnup calculation can be performed. This limitation is the consequence of the feature of these procedures to keep, at the same time, all microscopic cross sections for all nuclides in all material zones in the computer memory or in auxiliary binary files. In cases of high number of material zones (*i. e.* nodes) this requirement cannot be satisfied with the present version of MOCUP and KENO-V.a/ORIGEN.2.1 procedures. The major advantage of using KENO-V.a/ORIGEN2.1 procedure is the decrease in computation time by about factor 20 compared with MOCUP. Therefore, we used KENO-V.a/ORIGEN2.1 procedure:

– for choosing the fuel burnup model (*i. e.* for selection of actinides and fission products that we must include in one-group cross section calculations),

– for examination of the influence of handling the corrector steps in fuel burnup analysis,

– for the testing of accuracy of different geometrical models, and

– for selection of the number of source neutrons per generation and number of generations which can provide a reliable space distribution of fission power.

Recently, we applied the same fuel burnup model in both methodologies MOCUP(MCNP-4C/ORIGEN2.1) and KENO-V.a/ORIGEN2.1. In this new model we selected 95 most important fission products (in the sense of neutron absorption in the ENHS benchmark core), which represent the 99.5% of total fission products absorption (including 180 FPs) or 99.97% of total actinides and fission products absorption (including 30 A and 180 FPs). This model leads to a negligible overestimation of k_{eff}, less than 30 pcm (1 pcm = 10^{-5}). The application of this model has resulted in better agreement between these two methodologies during fuel burnup. Using the new model with 95 FPs and KENO-V.a/ORIGEN2.1 procedure we found that the difference between the results obtained only with predictor time steps equal to 2 years and those obtained with predictor/corrector time steps also equal to 2 years is negligible (less than 30 pcm). This means that the model with only predictor time steps, which we used in the MOCUP utility code is appropriate for ENHS cores calculations.

The REBUS-3 code system [10] was used at ANL for the benchmark calculations [8]. The DIF3D code [11] was used with 230-energy group structure for calculating space and energy dependence of neutron flux using finite-difference RZ diffusion theory method. Burnup chains spanning the range from ^{232}U to ^{248}Cm were taken into consideration. The multigroup cross sections are based on ENDF/B-V data and were generated by using the MC^2-2 code [12]. A resonance "screening" procedure was applied to pre-process broad resonance into MC^2-2 "smooth data" library at 2082 group level. Self-shielding effects of the remaining resonance were explicitly evaluated in MC^2-2 by narrow resonance approximation. For individual core-region materials of given nuclide density and temperature, homogeneous ultra-fine-group flux calculations were performed by using MC^2-2. The consistent P_1 method was applied in group-independent buckling search for fundamental mode spectrum using 2082 groups. From the homogeneous ultra-fine MC^2-2 calculations (2082 energy groups), 230-group cross sections were generated for individual materials of given nuclide number density and temperature as specified for the ENHS benchmark problem at the beginning-of-cycle (BOC). A lumped fission product approach, based on cross section data for 180 individual FPs, was used to model the pseudo fission products (PFPs) from five different actinides. The PFPs were created from fission yields based on ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu fission, and subsequent transmutation in a typical fast reactor spectrum.

At this stage we tried to find explanation for a large difference in evolution between UCB results (obtained by MCNP-4C/ORIGEN2.1 and KENO-V.a/ORIGEN2.1 utility codes) and ANL results (obtained by REBUS-3 code package). Among other reasons, we observed a significant deficiency in the MOCUP utility code. First, this deficiency was observed in ^{241}Am, and then in all nuclides (light elements, actinides and fission products) that produce a product nuclide in an excited (metastable) nuclear state in (n,) reaction. For these nuclides, the MOCUP offers two possibilities (that will be explained for the ^{241}Am and ^{242m}Am):

– the first option, in MCPN-4C tally specification for one-group cross section preparation pro-

vides that neutron capture (n,) on ^{241}Am will produce ^{242}Am (*i. e.* the calculation of atomic number density for ^{242m}Am is omitted), and

– the second option in MOCUP utility code, designed for (n, γ) reaction that produces a product nuclide in an excited (metastable) nuclear state enables to produce ^{242}Am with the one-group cross section $_{n,}$ calculated with MCNP-4C code during fuel burnup, while the fixed cross section $^{*}_{n,}$ taken from the specified ORIGEN2.1 library (AMORUUUC.LIB or ENHSB.LIB in the case of ENHS benchmark core) will be used to produce ^{242m}Am. This means that atomic number density of ^{242}Am will be overestimated, and the changes of the $^{*}_{n,}$ cross section during fuel burnup will be omitted.

In order to remove this deficiency, we made a simple correction of MOCUP utility code. It was found that the simplest way for this correction is to change the input file (TAPE5.INP) for the ORIGEN2.1 code after its preparation with the origenPRO code. For this purpose we wrote a new simple code FNG1. The FNG1 code uses data file FNG1.INP which contains the fraction $f_{\gamma 1}$ of radioactive capture (n,) reactions that produce a product nuclide in an excited (metastable) nuclear state for all light elements, actinides and fission products, and allows us to divide the (n, γ) cross section $_{n,}$ (calculated with MCNP-4C code during the fuel burnup) into:

– the cross section $_{n,}$ $(1 - f_{1})$ for production of nuclide in ground nuclear state, and

– the cross section $_{n,}$ $f_{\gamma 1}$ for production of nuclide in excited nuclear state.

The f_{1} fraction data are taken from the XSECTPHO library, prepared for the ORIGEN-S [13] code in the SCALE-4.4a code system.

To provide an independent check of evolutions during fuel depletion, based on the approximate model with five PFPs (at ANL) and the rigorous model used in the ORIGEN2.1 code (in both MOCUP and KENO-V.a/ORIGEN2.1 procedures), we created a simple 1D cylindrical model of the ENHS benchmark core for the application in the ORIGEN-S code (via the SAS2H [14] control module of the SCALE-4.4a code system). It was found that a simple two-zone 1D cylindrical model with core radius equal to 52.29 cm (calculated so that core volume is preserved) and with 47.71 cm thick lead (99% PB +1% SS) reflector, where axial neutron leakage is modelled with actual core height (*i. e.* with height equal to 400 cm), is good enough for k_{eff} evolution. That was confirmed by comparison of k_{eff} results obtained with KENO-V.a/ORIGEN2.1 utility code for the proposed 1D model and for an exact model (*i. e.* the 2D r-z model). The compared results are shown in fig. 2. To use the SAS2H code, designed for fuel burnup analysis with ORIGEN-S code in lattice cell problems with the white boundary

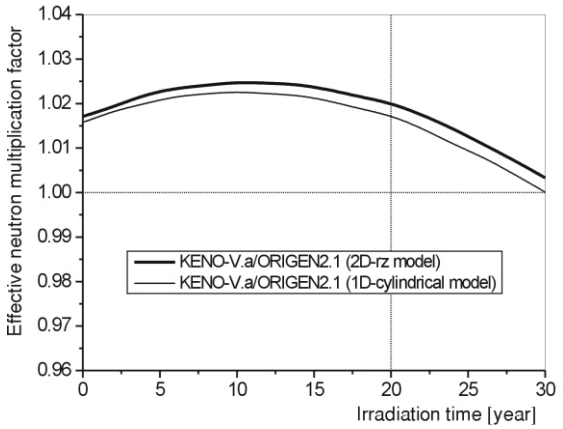

Figure 2. Comparison of the KENO-V.a/ORIGEN2.1 calculations of 2D (r, z) and 1D cylindrical single zone models of the ENHS benchmark core. Results obtained for (100 + 750) 5000 source neutrons with ENDF/B-V based 238 groups library, and fuel burnup model with 25 A and 95 FPs, corrected for fraction of (n,) reaction that produces nuclide in an excited nuclear state

condition at the outer lattice cell surface, we extend the proposed two-zone 1D model by a third zone of effective thickness equal to 10 cm. This zone contains lead and added 1/v absorber (with high atomic number density, equal to 10^{-18} atoms cm^{-3}), and serves for the simulation of vacuum boundary condition at the outer reflector surface of the proposed 1D model. The results obtained by the proposed 1D model and SAS2H (used with the ENDF/B-V based 238-group cross section library and ORIGEN-S BASLMFBR library, designed for the LMFBR cores analysis) were corrected for the difference between 2D and 1D models, that was found with the KENO-V.a/ORIGEN2.1 utility code.

RESULTS

The MOCUP (MCNP-4C/ORIGEN2.1) results obtained for the single zone model of ENHS benchmark core with all fuel burnup models used at UCB are given in fig. 3. As we can see from fig. 3, the influence of $f_{\gamma 1}$ -correction that separates the (n,) cross section (calculated by MCNP-4C code during fuel burnup) into the cross section for production of nuclides in ground and in excited nuclear states is not significant, *i. e.* this influence cannot explain the difference in k_{eff} between the UCB and ANL results.

The final results for the single zone model of ENHS benchmark core, obtained with both procedures based on ORIGEN2.1 code (corrected for the fraction of (n,) reaction that produce a product nuclide in an excited nuclear state), and SAS2H and REBUS-3 utility codes are given in fig. 4. In these calculations the temperature equal to 750 K for the benchmark core was used, except the MOCUP evo-

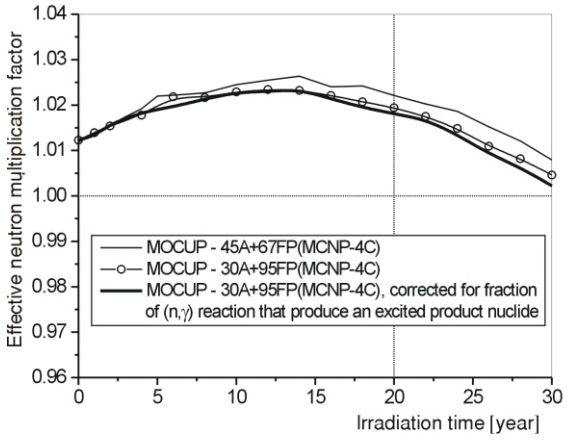

Figure 3. MOCUP (MCNP-4C/ORIGEN2.1) results for 2D (r, z) single zone model of the ENHS benchmark core (obtained with VMCCS library for (50 + 600) 1000 source neutrons and different fuel burnup models)

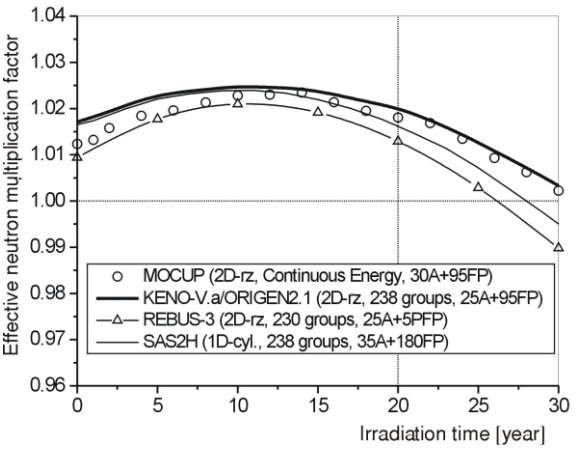

Figure 4. Comparison of k_{eff} calculations of single zone model of the ENHS benchmark core (MOCUP and KENO-V./aORIGEN2.1 cross sections are corrected for fraction of (n,) reaction that produces a product nuclide in an excited nuclear state)

lution, where the core temperature equal to 900 K was applied. When the same cross section data are used (as in case of KENO-V.a/ORIGEN2.1 and SAS2H utility codes calculations), these results confirm a good agreement between ORIGEN2.1 and ORIGEN-S codes in fuel burnup range from the BOC to the EOC (end-of-cycle), equal to 20 years, *i. e.* 120,000 MWd/tHM. There is also a good agreement between MCNP-4C/ORIGEN2.1 and KENO-V.a/ORIGEN2.1 procedures, although these results do not decline with burnup as ANL results. The difference between two ORIGEN2.1 results, which is still present, is mostly a consequence of various cross section evaluations that we used (ENDF/B-VI in MOCUP, and ENDF/B-V in KENO-V.a/ORIGEN2.1 procedure).

Results for the macroscopic cross sections obtained for the single zone model of the ENHS benchmark core with KENO-V.a/ORIGEN2.1 procedure and REBUS-3 utility code (both using ENDF/B-V evaluation), and with MOCUP procedure (using ENDF/B-VI evaluation) are given in tab. 3. KENO-V.a/ORIGEN2.1 and REBUS-3 calculations overestimate both macroscopic fission and capture cross sections when compared to MCNP-4C results. However, KENO-V.a code overestimates much more the fission than capture cross section, while ANL procedure overestimates much more the capture (particularly in construction material, *i. e.* stainless steel) than the fission cross section. This means that accuracy of resonance absorption calculation in KENO-V.a (via CSAS25 module) and in ANL codes are not the same. The cross sections of nuclides Cr, Mn, Fe, Ni, Mo, and Zr have windows below each scattering resonance where the cross section becomes very small over a small energy range, so that the procedure for modelling of resonance self-shielding effect on these nuclides in the ENHS core must be very rigorous. It was recognized that even the 238-group SCALE-4.4a library is not good enough to account for this effect. That's why we tried to use the best option for modelling of resonance

Table 3. BOC macroscopic one-group cross sections in single zone model of the ENHS benchmark core

Reaction rate	MCNP-4C (ENDF/B-VI.7)	KENO-V.a (ENFB/B-V)	REBUS-3 (ENFB/B-V)
Fission (Difference to MCNP-4C in %)	2.299-3[a] (0.000)	2.339-3 (1.752)	2.325-3 (1.148)
Capture of all nuclides (Difference to MCNP-4C in %)	3.164-3 (0.000)	3.208-3 (1.384)	3.237-3 (2.298)
Capture of actinides (Difference to MCNP-4C in %)	2.898-3 (0.000)	2.933-3 (1.222)	2.945-3 (1.637)
Capture of construction materials (Difference to MCNP-4C in %)	2.660-4 (0.000)	2.744-4 (3.151)	2.913-4 (9.502)
Ratio of total fission and absorption (Difference to MCNP-4C in pcm)	4.208-1 (0.000)	4.217-1 (209.8)	4.180-1 (– 654.6)

[a] Read as $2.299\ 10^{-3}$

Table 4. The influence of Fe cross section data on k_{eff} at BOC state of single zone model of the ENHS benchmark core

Case	MCNP™ library Fe cross section data evaluation	Temperature K	k_{eff} (1 = 0.00025)
1	VMCCS (VINČA Institute) (^{54}Fe, ^{56}Fe, ^{57}Fe, and ^{58}Fe) from ENDF/B-VI.7	600	1.01393
2	VMCCS (VINČA Institute) (^{54}Fe, ^{56}Fe, ^{57}Fe, and ^{58}Fe) from ENDF/B-VI.7	300	1.01395
3	ENDF60 (LANL) (^{54}Fe, ^{56}Fe, ^{57}Fe, and ^{58}Fe) from ENDF/B-VI.2	300	1.01265
4	RMCCS (LANL) (Fe-Nat) from ENDF/B-V	300	1.00930
5	Auxiliary library [a] (F-Nat) from ENDF/B-V	300	1.01079

[a] The MCNP-4C library for Fe-Nat was obtained with NJOY97 [15] code by using the same principles as for the VMCCS library preparation (*i. e.* without cross section thinning)

self-shielding effect in the ENHS benchmark core with CSAS25 module. We found that the best option for accounting for these effects in KENO-V.a calculation (via the CSAS25 module) is: to use for stainless steel a specially prepared cross sections for Fe, Ni, and Cr available in ENDF/B-V SCALE libraries; and for zones which contain a mixture of stainless steel and other materials to use so-called *more data* option for approximate 1D geometry of these zones with Dancoff factors equal to zero.

Assuming in the first approximation that the product of average ¯ in the ENHS benchmark core and neutron leakage probability from the core has the same value in both KENO-V.a (CSAS25) and REBUS-3 calculations, we found that the difference of the ratio of total fission and absorption (capture plus fission) of these codes and the MCNP-4C code is the same as the difference that we found with these codes.

The importance of Fe (^{54}Fe, ^{56}Fe ^{57}Fe, and ^{58}Fe) cross section data is illustrated in tab. 4, which presents the results of MCNP-4C calculations of a single zone model of the ENHS benchmark core for BOC state. These results were obtained with VMCCS library (based on the ENDF/B-VI.7 evaluation), but with different iron cross-section data. As we can see from tab. 4, the influence of different Fe cross sections evaluations is a quite high (up to 460 pcm).

The continuous energy libraries VMCCS (from VINČA Institute of Nuclear Sciences) and ENDF60 (from Los Alamos National Laboratory – LANL) did not provide for the self-shielding effect in the unresolved resonance energy region, although the code MCNP-4C was designed to include this effect by using the probability table method (the most rigorous method for the treatment of the unresolved resonance self-shielding effect in the Monte Carlo calculations). The only library that contains probability table (ptable) data is the LANL library URES 3 , prepared for the most important uranium and plutonium nuclides at room temperature (300 K). We used this library to examine the self-shielding effect in the unresolved resonance energy region of single zone model of the ENHS benchmark core at 300 K. The obtained results are shown in tab. 5. Since the MCNP-4B code does not include the probability table option, the results shown in tab. 5 allow us to conclude that the difference between the results obtained with MCNP-4C and MCNP-4B codes with URES library for uranium and plutonium nuclides represents the effect of self shielding in the unresolved resonance region. This effect has the value equal to 330 pcm at room temperature. Since this effect has a lower value at working temperature (equal to 750 K), the omission of unresolved resonance self-shielding effects in the current MCNP-4C calculation is not responsible for the observed difference between MCNP-4C and REBUS-3 results.

In order to investigate the effects of space dependent depletion in the ENHS benchmark core, as a further step of fuel burnup analysis for the ENHS core, the following division types of the core are used:

Table 5. Results of self-shielding effect calculations in the unresolved resonance region at BOC (300 K) state for single zone model of the ENHS benchmark core

Code	MCNP™ library	k_{eff} (1 = 0.00050)
MCNP-4C	URES – for U and Pu nuclides; ENDF60 – for the rest nuclides	1.01988
MCNP-4C	ENDF60 – for U and Pu nuclides; ENDF60 – for the rest nuclides	1.01687
MCNP-4B	URES – for U and Pu nuclides; ENDF60 – for the rest nuclides	1.01657
MCNP-4B	ENDF60 – for U and Pu nuclides; ENDF60 – for the rest nuclides	1.01629

– single zone (the space dependent depletion is ignored),

– three radial zones with equal zone volumes, and

– three radial zones and five axial zones with equal zone volumes (total fifteen zones).

The results obtained with improved MCNP-4C/ORIGEN2.1 procedure, corrected for the fraction of (n,) reaction that produces a product nuclide in an excited nuclear state, are shown in fig. 5. These results were obtained by the MCNP-4C code with the VMCCS cross section data at 900 K for all actinides and fission products, and at 600 K for all constructional material and coolant. As usually, we used the KENO-V.a/ORIGEN2.1 procedure to examine the influence of the number of source neutrons per generation on the space dependent depletion. It was found that the 1500 source neutrons per generation (with initial 50 discarded generations and 600 active generation) are sufficient to include the effects of the space dependent depletion in the ENHS core. The results given in fig. 5 show the existence of a considerable gradient of fuel depletion in the radial and axial direction. This means that the use of single zone model for the fuel depletion of ENHS benchmark core is not adequate. Nevertheless, the single zone model of the ENHS core represents a simple computational benchmark for testing of accuracy of different codes and cross section data libraries designed for the fact reactor calculations.

All MOCUP and KENO-V.a/ORIGEN2.1 results were obtained on a Pentium III PC (2 733 MHz, with the FreeBSD unix). The typical CPU time for single zone model of the ENHS benchmark core with 16-fuel burnup steps is 17 days for MOCUP, and 1 day for KENO-V.a/ORIGEN2.1 procedure.

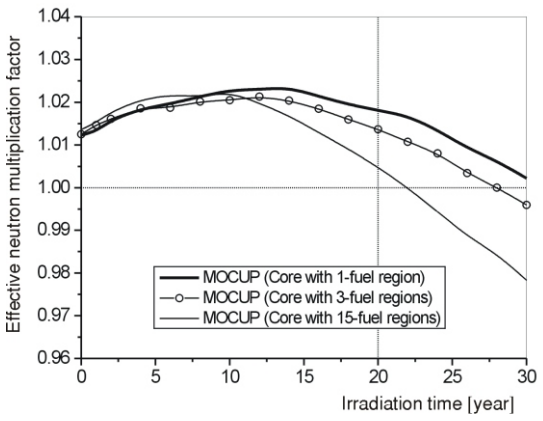

Figure 5. MOCUP calculations of 2D (r, z) models of the ENHS benchmark core with different number of fuel regions. Results obtained with the VMCCS library for (50 + 600) 1500 source neutrons and fuel burnup models with 30 A and 95 FPs, corrected for the fraction of (n,) reaction that produces a product nuclide in an excited state

CONCLUSIONS

The overall agreement between the computational tools used for single zone model calculations of the ENHS benchmark core is satisfactory. In particular, the disagreements found would not affect the conclusions concerning the feasibility of designing the ENHS core to have a nearly constant k_{eff} for 20 effective full-power years.

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ПРИМЕНА МОНТЕ КАРЛО МЕТОДА ЗА АНАЛИЗУ ИЗГАРАЊА ГОРИВА У БЕНЧМАРК ЈЕЗГРУ ENHS РЕАКТОРА НА БРЗЕ НЕУТРОНЕ

У раду су описане три процедуре за праћење ефективног фактора умножавања неутрона (k_{eff}) и просторне расподеле фисионе снаге у реакторима на брзе неутроне у зависности од средњег изгарања горива. Две су засноване на спрези Монте Карло програма MCNP-4C и KENO-V.a из пакета програма SCALE-4.4a (којима се одређује расподела фисионе снаге и једногрупни неутронски пресеци) и програма ORIGEN2.1 (за детаљне анализе састава горива) и намењене су за референтне прорачуне у вишедимензионалним (2D и 3D) геометријским моделима. У трећој процедури, заснованој на примени упрошћених једнодимензионалних (1D) модела и контролног модула SAS2H, једногрупни неутронски пресеци одређују се помоћу методе дискретних ордината, а изгарање горива се прати програмом ORIGEN-S. Приказане процедуре примењене су за анализу нове генерације ENHS реактора на брзе неутроне код којих се као хладилац користи течно олово (или смеша олово-бизмут) и од којих се очекује да обезбеде непрекидан рад (без измене горива) током 30 година. Резултати ове анализе упоређени су са резултатима других лабораторија у свету, добијеним применом постојећих програма заснованих на вишегрупној дифузионој апроксимацији.