

MCNP5 STUDY ON KINETICS PARAMETERS OF COUPLED FAST-THERMAL SYSTEM HERBE

by

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New validation of the well-known Monte Carlo code MCNP5 against measured criticality and kinetics data for the coupled fast-thermal HERBE System at the Reactor B critical assembly is shown in this paper. Results of earlier calculations of these criticality and kinetics parameters, done by combination of transport and diffusion codes using two-dimension geometry model are compared to results of new calculations carried out by the MCNP5 code in three-dimension geometry. Satisfactory agreements in comparison of new results with experimental data, in spite complex heterogeneous composition of the HERBE core, are achieved confirming that MCNP5 code could apply successfully to study on HERBE kinetics parameters after uncertainties in impurities in material compositions and positions of fuel elements in fast zone were removed.

Key words: HERBE experiment, kinetics parameters, RB reactor

INTRODUCTION

Extensive studies on fast neutron fields at the Vinča Institute of Nuclear Sciences in 1979-1988 resulted in design and construction of a complex, coupled fast-thermal core at the Reactor B (RB) critical assembly [1], called the HERBE System [2].

Basic purpose of the HERBE System was application in experimental validation of computer codes for calculation of reactor complex lattice cells in especially designed experiments in this coupled fast-thermal core and study of fast neutron fields. The HERBE System is described elsewhere [3] as the well as the results of calculations and experimentally measured kinetics parameters [4, 5] in various HERBE configurations. In this paper, the horizontal cross-sections of the full three-dimension (3-D) model RB critical assembly with selected HERBE configuration (RB77/1995) with a vertical central channel (VCH) in the fast core centre and the HERBE fast zone are shown in figs. 1 and 2, respectively. Vertical cross-section of 3-D model of RB critical assembly with same HERBE configuration is shown in fig. 3.

Initial results of calculations of the HERBE criticality and kinetics parameters, carried out by standard reactor diffusion and transport codes did not agree

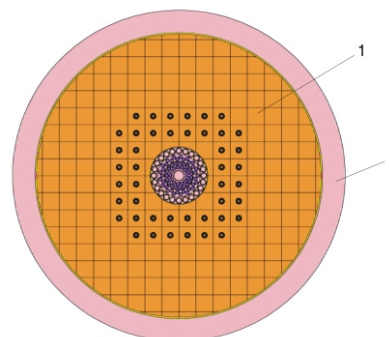


Figure 1. Horizontal cross-section of the RB with the HERBE system (1 – heavy water; 2 – air)

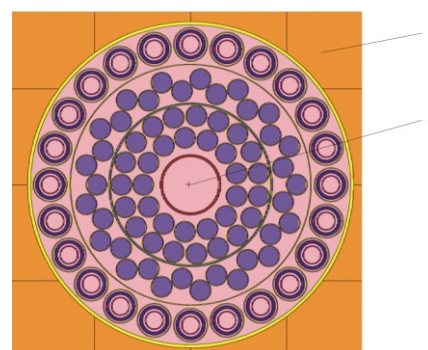


Figure 2. Horizontal cross-section of the fast zone of the HERBE system (1 – heavy water; 2 – air)

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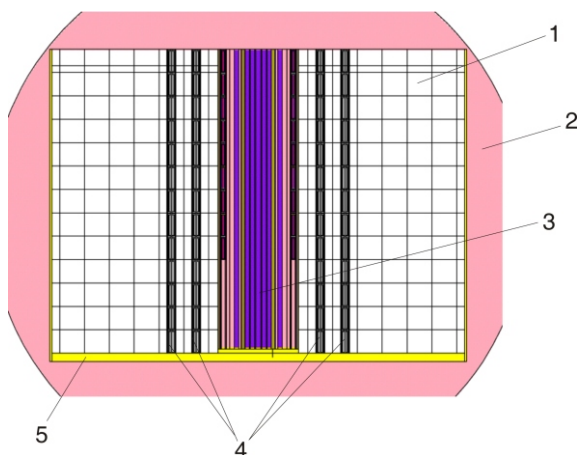


Figure 3. Vertical cross-section of the RB with the HERBE system (1 – heavy water; 2 – air; 3 – fast zone; 4 – thermal core; 5 – aluminium construction material)

quite well with experimental results. To improve models and calculation methods applied, new codes were developed or existing ones were modified to include large heterogeneous effects in the HERBE System due to existence of void (air zones) and neutron high-absorption (cadmium layer) regions in the fast zone [2].

Complete new, detailed 3-D geometry model of the RB critical assembly with coupled fast-thermal core HERBE, based on new 3-D geometry model of the highly enriched uranium fuel slug [6], is developed for the Monte Carlo based MCNP code. The latest information on compositions of materials utilised in the RB critical assembly are used. Calculations of static parameters – criticality data – and neutron spatial and energy distribution inside the HERBE System are carried out [7, 8] by using the MCNP4B2 code [9]. Neutron continuous-energy library VMCCS [10], developed in the Vinča Institute, and TMCCS library for neutron scattering at thermal energies at H and D atoms connected in molecules of light and heavy water, respectively, are used with the MCNP code. Acceptable calculation results for fast neutron spectrum in the centre of fast core and spatial two group neutron distributions, compared to measured ones, are obtained.

Studies on HERBE System safety operations were carried out with increased attentions to a great extent, *e. g.* in reference [11-14], since the possible accident of flooding (by moderator) of the fast zone is accepted as the design basis accident.

MATERIALS AND METHODS

Recent studies on impurities in RB reactor materials [16], development of new version 1.4 [15] of MCNP5 computer code and associated nuclear data libraries, as well as, increasing computation power of

PC, offered a possibility to re-study the kinetics parameters of HERBE System.

As it is shown in fig. 2, the fast zone (FZ) of the HERBE System consists of an outer ring of 24 highly enriched uranium (HEU) fuel assemblies in air that acts as a neutron converter (NC). Uranium in HEU elements (slugs) is in the form of uranium dioxide and enriched to 80% ^{235}U . Fuel slugs cladding is produced as high purity aluminum known in Russia as SAV-1 [6]. External diameter of the NC is 400 mm and inner diameter of the NC is 300 mm. Each fuel assembly of the NC consists of 9 HEU slugs, placed above inner (low purity, YuAl) aluminum supporter (430 mm high), and inserted in an aluminum (fuel assembly) tube. The assembly tubes are closed at the bottom in aim to prevent heavy water to enter in, in a case of possible fast zone flooding accident. Medium ring of the fast zone is made of 32 natural uranium metal rods in air with cadmium sheet (thick 1.6 mm) at inner side and acts as the neutron filter (NF). External diameter of the NF is 300 mm and inner diameter of the NF is 200 mm. The inner ring of the fast zone, made of 32 natural uranium metal rods in air around the vertical central channel (VCH), acts as the fast core (FC). Outer diameter of the FC is 200 mm, while inner diameter of the VCH, made of ANSI 403 stainless steel with wall thickness 3 mm, is 70 mm.

This HERBE fast core is driven, as it is shown in fig. 1, by a thermal core (TC) designed from 44 highly enriched uranium fuel assemblies (each with 13 fuel slugs in aluminum tube) placed around the FZ in heavy water moderator and reflector in square lattice with pitch of 120 mm. Diameter of RB tank is 2000 mm and the critical level of heavy water for the RB77/1995 configuration is 1386.6 ± 0.2 mm, determined experimentally at 19.3 ± 0.2 °C. In real HERBE System (and in the model) the cylindrical tank (made of low purity aluminum) of the critical assembly is surrounded by air. Two detectors of moderator leaking, placed in the FZ (in NC and NF), are neglected in the 3-D model.

MCNP42B was applied for HERBE System 3D geometry configuration in 2000 using neutron cross-section data library VMCCS (based on neutron cross-section data from the ENDF/B-VI) for the most of natural occurred elements in HERBE System materials. If ENDFB60 nuclide library are used, for some impurities (*e. g.*, Cr, Fe, Ni, Cu, Cd) neutron cross-section library from RMCCS (based on neutron cross-section data from EBDF/B-V) was applied because the appropriate cross sections in ENDFB60 were missing. For interaction of neutrons in thermal range of energies with H and D atoms in molecules of heavy water with small amount light water at 20 °C are applied TMCCS (based on ENDF/B-V) neutron thermal cross-sections libraries HWTR.01c and LWTR.01c for heavy water and light water, respectively. For neutron interaction with argon in air and with zinc impurity in the high purity aluminum

(SAV-1) new cross-sections are evaluated in VMMCS, or used independently from older BMCCS neutron cross-section continuous energy library (based on the ENDF/B-IV cross-sections), and ENDF60 library, respectively, because the evaluations of those cross-sections were missing in ENDF60 library.

New MCNP5 release 1.4 code is run for HERBE System 3-D geometry configuration with all material data cross-sections for nuclides (in natural occurring elements) from ENDF66 neutron cross-section continuous energy library at room temperatures, based on ENDF/B-VI release 6. For neutron interactions with H and D atoms in molecules of heavy water with contents of 1.6% (molar) fraction of light water at 20 °C last available SAB2002 neutron thermal cross-sections libraries HWTR.60c and LWTR.60c for heavy water and light water, are applied, respectively. Only for interaction with argon in air it is still applied the ENDF60 (based on neutron cross-section data developed in Lawrence Livermore National Laboratory at room temperatures in 1992) neutron cross-section continuous energy library, since cross-sections in ENDF66 for that element were still missing in cross-sections libraries distributed with the MCNP5 code. All ENDF/B-VI (release 60c or 66c), including older RMCCS (based of ENDF/B-V) and BMCCS (based of ENDF/B-IV) neutron cross-section libraries as well as TMCCS and SAB2002 neutron cross-section data are developed in Los Alamos National Laboratory. Last available gamma ray interaction library MCPLIB.04P and electron interaction library EL03 are applied for calculations in option MODE N P for MCNP5 code.

Main uncertainty in material composition of HERBE System comes from contents of impurities of neutron highly absorbing elements, like boron in aluminum of low purity produced in ex Yugoslavia in late 1950-ies, labelled as YuAl or LpAl [16], and uncertainties of exacted positions of fuel elements in the fast zone. To compensate this uncertainties, the simplest way was to adjust boron concentration in YuAl to a value (0.028%) within reported measured range (0.01-0.03%) to obtain effective factor of neutron multiplication in the system, k_{eff} , as close as possible to criticality (*i. e.*, 1) to get reliable values of kinetics parameters for the HERBE System.

RESULTS AND DISCUSSION

Obtained k_{eff} values for different neutron cross-section libraries and computer codes, compared to experimental data, are shown in tab. 1. After running MCNP5 code (in MODE N P) for adjusted values of boron concentration in YuAl for contribution of prompt neutrons from fission only (k_p , code option TOTNU NO) and for contribution of all neutrons from fission (k_{eff} , code option TOTNU) it is possible to determine effective fraction of delayed neutrons (and photoneutrons) β_{eff} and compare it to previously determined values in earlier calculations and experiment (tab. 2). The β_{eff} is determined from, either relation between k_{eff} and k_p , or from relation between number of prompt neutrons ν_p and total neutrons ν_{tot} emitted from fission nuclides as

$$\beta_{\text{eff}} = 1 - \frac{k_p}{k_{\text{eff}}} = 1 - \frac{\nu_p}{\nu_{\text{tot}}}$$

Table 1. HERBE System criticality data

Code	Dominant neutron library	KCODE/H(D ₂ O)	k_{eff} σ
Twenty grand [17]	Vinča 2 group	$H(\text{D}_2\text{O}) = 1380$ mm	0.99837
Galer [18]	Vinča 4 group	$H(\text{D}_2\text{O}) = 1380$ mm	0.99763
Triton [20]	Vinča 4 group	$H(\text{D}_2\text{O}) = 1380$ mm	1.00326
MCNP4B2	VMCCS	$H_c = 1386.6$ mm	1.00249 0.0027
MCNP5 1.4/MCNB4B2	ENDF60	2000 (100 + 1000)	1.00477
MCNP5 1.4	ENDF66 [16]	2000 (200 + 1000)	1.01182 0.00055
MCNP5 1.4	ENDF66, adjusted ¹⁰ B in YuAl	2000 (200 + 1000)	1.00021 0.00058
Experiment [5]	$H_c = 1386.6 \pm 0.2$ mm at $T = 19.3 \pm 0.2$ °C		

Table 2. HERBE System effective fraction of delayed neutrons

Code	Dominant neutron library	KCODE	ν_p and ν_{tot} or k_p and k_{eff}	β_{eff} σ
–	Precursors data from jendl3.1, endf/b-iv,-v,-vi, vmccs1, vmccs2	–	–	Range from 0.007699 to 0.008499 dependent on library [20]
MCNP5 1.4/MCNB4B2	ENDF60	2000 (100 + 1000)	$k_p = 0.99713$ 0.00058 $k_{\text{eff}} = 1.00477$ 0.00055	0.00760 0.00079
MCNP5 1.4	ENDF66, adjusted ¹⁰ B in YuAl	5000 (200 + 4000)	$\nu_p = 2.428$ $\nu_{\text{tot}} = 2.445$	0.00695
MCNP5 1.4	ENDF66, adjusted ¹⁰ B in YuAl	5000 (200 + 4000)	$k_p = 0.99243$ 0.00017 $k_{\text{eff}} = 0.99957$	0.00714 0.00025
Experiment [20]	$\beta_{\text{eff}} = 0.00791$ 0.00028			

Table 3. HERBE System reactivity data

Code	Dominant neutron library	KCODE	$d\rho/dH \quad \sigma \text{ [cm}^{-1}\text{]}$
Twenty grand	Vinča 2 group	-	$194 \cdot 10^{-5}$ at $H = 138$ cm
Galer	Vinča 4 group		$195 \cdot 10^{-5}$ at $H = 138$ cm
MNCP5 1.4	ENDF66, adjusted ^{10}B in YuAl	5000 (200 + 4000)	$204.05 \cdot 10^{-5}$
Experiment [2]	$d\rho/dH = (191.6 \quad 1.5) \cdot 10^{-5} \text{ cm}^{-1}$		

The value of change of reactivity with moderator level (reactivity gradient) near critical level in the HERBE System was determined after the MCNP5 code is run for two values of moderator level, critical level of 1386.86 mm and water level that is 10 mm less. The obtained value is compared to previously determined values in earlier calculations and the experiment (tab. 3).

The value of the prompt neutron lifetime l_p is determined from the value of prompt neutron decay constant α_p and prompt neutron multiplication factor k_p using well known relation [21]

$$\alpha_p = \frac{k_p - 1}{l_p} \frac{\rho}{\Lambda}$$

where ρ is the reactivity of the system with total fraction of delayed neutrons β and neutron generation time Λ determined as $\Lambda = l_p/k_p$.

Before determining value of the prompt neutron lifetime l_p from the value of prompt neutron decay constant α_p , in a complex configuration like HERBE System with the running MCNP5 code in time domain, the value l_p is determined for a simple system of the "Lady Godiva" reactor [21, 22], which is homogeneous unreflected sphere (radius 8.7407 cm) designed from high purity uranium (weight fraction 0.9371 ^{235}U). The calculated value of α_p at the criticality and room temperature, given as $\alpha_p = -(1.22 \pm 0.02) \cdot 10^6 \text{ s}^{-1}$ is in good agreement with declared, experimentally determined [22], value $\alpha_p = -(1.11 \pm 0.02) \cdot 10^6 \text{ s}^{-1}$ under the same conditions. The obtained value for $l_p = 5.97 \text{ ns}$ is in an excellent agreement with the declared experimental value for $l_p = 6.04 \text{ ns}$ [21].

The value of the prompt neutron lifetime l_p in HERBE System is determined, for the first time, after run of MCNP5 code in the source (SDEF) option for simulation of time dependence of the prompt neutron populations (code option TOTNU NO) detected by (simulated) three BF_3 counters. The counters are placed in VCH in the FC, middle of the TC and outside of the reactor tank in air. The HERBE System is perturbed at sub-critical heavy water level of 1365.0 mm by a neutron pulse generated in the point that is at the centre at the half height critical level in the VCH (680 mm). It is assumed that 1 s wide isotropic neutron pulse of neutron energy 14 MeV is generated by a D-T neutron pulse generator in time zero and neutron population time decay in the system is monitored by BF_3 counters, as (n, α) reaction rates, from 100 s to 90 ms in time bins wide 1 ms. The code is run for near 1.7

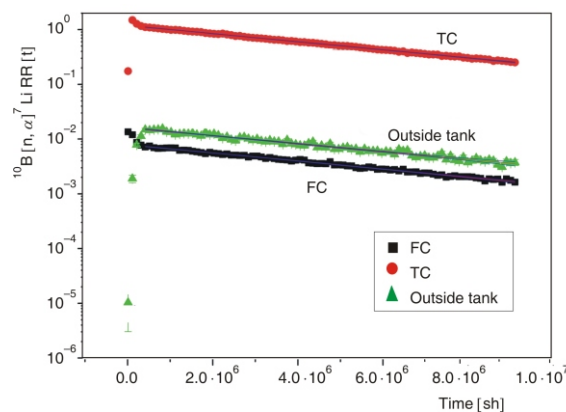


Figure 4. MCNP5 results of neutron population time decay in HERBE System (nps = 1.676 M; D-T 1 μs pulse; HERBE $H(\text{D}_2\text{O}) = 136.50$ cm; $k = 0.99467 \quad 0.00018$ ^{10}B detector at $h = 68$ cm; case prompt neutrons – TOTNU NO)

million neutron histories (pulses from the neutron generator) in aim to obtain acceptable statistical uncertainty for the time bin of 0.5%. The results of run of MCNP5 code are shown in fig. 4, where MNCP code time unit is given in shakes (1 sh = 10 ns).

Time decay of neutron population in three BF_3 detectors is fitted at an exponential decay curve and prompt decay constant α_p is determined from the fitted curve for the BF_3 detectors in TC and outside from the reactor tank, to be sure that origin pulse neutrons do not contribute reaction rates directly into the detectors. From obtained α_p and prompt neutron multiplication factor k_p , obtained for the code run for option TOTNU NO at heavy water sub-critical level, a value of the prompt neutron lifetime l_p is determined, that is compared to values found in earlier calculations and experiment (tab. 4).

Table 4. HERBE system neutron lifetime data

Code	Dominant neutron library	KCODE/NPS	$l_p \quad \sigma \text{ [ms]}$
Twenty grand	Vinča 2 group	-	0.636
Galer	Vinča 4 group		
MNCP5 1.4	ENDF66	nps = 1.676 milion	0.707 0.068
Experiment [2, 3]	$l_p = 0.621 \quad 0.05 \text{ ms}$		

After comparison of the results obtained by new calculations to the results of the experimental measurement and earlier calculations, the progress can be reported in determination of the kinetics parameters of the HERBE System (effective fraction of neutrons, reactivity gradient near critical level and prompt neutron lifetime), while the results of new calculations of the static parameters (criticality level) still require study on material impurities and geometry uncertainty evaluations for the components in the HERBE fast zone.

CONCLUSION

Coupled Fast-Thermal Core HERBE System at RB reactor was selected for verification of Monte Carlo code MCNP5 on determination of kinetics and static parameters of this complex core. After adjustment of ^{10}B impurity concentration in YuAl material to obtain criticality at experimentally determined critical heavy water level, reactivity gradient was calculated. Fraction of delayed neutrons (beta effective) was determined in two separate runs of MCNP5 code for contributions of prompt and all neutrons to criticality (k_{eff}). Prompt neutron lifetime was determined by simulation of neutron population time decay in the HERBE System after perturbation at a sub-critical level by a neutron pulse in MCNP5 run in time dependent mode. All new kinetics and static parameters, obtained by using the latest available version of MCNP5 code and library data in the Vinča Institute, are compared to previously calculated and experimentally determined data. Satisfactory agreement was achieved. Progress can be reported in obtained results of new calculations by using MCNP code with ENDFB66 data library. This study shows that, if uncertainty in material composition and HERBE Fast Core fuel assembly's position are removed expected results can be achieved after application MCNP5 code and associated nuclear cross-section data. So, further study on understating material impurities and geometry uncertainties in the HERBE System will be done in aim to propose this system as a new and complex benchmark facility with fast-thermal spectra.

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**MCNP5 СТУДИЈА КИНЕТИЧКИХ ПАРАМЕТАРА У
СПРЕГНУТОМ БРЗО-ТЕРМИЧКОМ СИСТЕМУ ХЕРБЕ**

У раду је приказана нова провера познатог Монте Карло програма MCNP5 на измереним статичким и кинетичким параметрима брзо-термичког система ХЕРБЕ направљеног на критичном реактору РБ. Резултати ранијих прорачуна ових статичких и кинетичких параметара, урађених комбинацијом транспортних и дифузионих програма у дводимензионом геометријском моделу, упоређени су са резултатима нових прорачуна извршених помоћу програма MCNP5 у тродимензионој геометрији. Задовољавајућа слагања добијених нових резултата са експерименталним мерењима, упркос комплексне хетерогене структуре брзе зоне ХЕРБЕ система, показују да MCNP5 програм може да се примени на анализу ХЕРБЕ кинетичких параметера уз отклањање неодређености у учешћу примеса у материјалима као и неодређености у погледу геометријских података за положај горива у брзој зони.

Кључне речи: ХЕРБЕ експеримент, кинетички параметри, реактор РБ
