Dear Sir or Madam,

Thank you for the valuable reviews. The necessary clarifications, corrections and improvements were added to the manuscript. The main aim of the paper is to present the results in the development of the MCB code as a scientific tool. The key results of the MCB validation, and of the presented numerical simulations were provided. The detailed results of the MCB modelling for presented cases, with full data sets, methodology descriptions and interpretation of the results are available for the scientific community in the supplementary references provided in the paper.

Yours sincerely,

Mikołaj Oettingen

Development and application of the Monte Carlo Continuous Energy Burnup Code

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1. Introduction

The paper presents the stat of the art in the development of the Monte Carlo Continuous Energy Burnup Code (MCB), dedicated for radiation transport and burnup numerical simulations [1]. The MCB code is developed at the AGH University of Science and Technology, Faculty of Energy and Fuels, Krakow, Poland. The code is suitable for the modelling of any critical or subcritical nuclear system with arbitrary geometry. The code was used in many studies on IIIth and IVth Generation nuclear reactors as well as on other innovative nuclear systems like Accelerator Driven Systems (ADS).

2. Methods and Results

The section presents the main achievements in the development of the MCB code. The key features of the code and its usage for advanced numerical simulations are shown. The examples of obtained key results for defined numerical models are presented.

2.1 Linear chain method

The MCB code applies the Monte Carlo methods, developed in the frame of the Monte Carlo N-Particle Transport Code (MCNP), for radiation transport calculations. However, for the calculations of the isotopic changes in matter it uses linear chain method, for the first time derived by Cetnar [2,3]. Nowadays, the method is treated as a reference point for other mathematical methods used for burnup calculations, like exponential matrix methods. The liner chain method provides more information about transmutation process and allows deep understanding of isotopes formation process. The method solves first order differential Bateman equation, governing nuclear transmutations, by its decomposition to a set of linear equations.

2.2 MCB implementation

The MCB code is the coupling of the MCNP and Transmutation Trajectory Analysis (TTA) codes at the level of the FORTRAN source code. The TTA code incorporates the liner chain method used for burnup calculations. The coupling is performed before the code compilation using PATCH utility. The code is able to use arbitrary nuclear data libraries prepared in the Evaluated Nuclear Data File (ENDF) format. In addition, the four set of nuclear data libraries describing nuclide formation and decay properties were merged with the MCB code. The libraries contain incident energy fission product yields for 36 isotopes, decay schema for about 2400 isotopes, branching ratios to metastable states for americium isotopes, dose data for about 740 isotopes, formation ratios due to (n, 2n) reactions. The MCB code is equipped in a capability of multiprocessing calculations using the Message Passing Interface (MPI), which allows its execution on High Performance Computers (HPC). It was already implemented on the supercomputer Prometheus of the Academic Computer Center ACK Cyfronet of the AGH University. The code was also successfully implemented on a few smaller computing clusters.

2.3 MCB Functionalities

The MCB code has many functionalities, related to the neutron transport and burnup calculations. In principle, all capabilities of the MCNP code and additional options related to the burnup calculations are available. In the development of the code efforts were taken to coupled it with the other numerical tools, especially for the mutual radiation transport, burnup and thermo-hydraulics calculations. The code was successfully coupled with the Fluent code and customized 2D thermo-hydraulic code for core analysis of the block type High Temperature Gas-Cooled Reactor (HTGR). The main functionalities of the MCB code are:

a) Possibility of coupled radiation transport and burnup calculations for an arbitrary three-dimensional geometry of the nuclear system. The functionality allows modelling of the complex nuclear systems, like cores of nuclear reactors, using a few levels of embedded geometry. This capability is especially useful in modelling of the TRi-structural ISOtropic (TRISO) fuel matrices in the fuel compacts of HTGR reactors.

b) Capability for actions related to the material processing for arbitrary time step. The functionality allows numerical modelling of reactivity control systems, like movement of control rod banks and adjustment of the boron concentration. In addition, the modelling of the fuel reloading and shuffling is available within one calculation run. The decay

calculations for the discharged fuel batches may be automatically performed for the multi-cycling nuclear fuel cycles.

c) Ability for the user to control the calculation process using dedicated cards implemented in the input file. The user can control key parameters for the neutron transport and burnup calculations as well as statistical of the simulation. The first two areas comprise mainly the control of the numerical procedures defining irradiation and decay times; material actions; number of burnup zones; number, size and format of output files. The latter allows control of the precision of the Monte Carlo simulations for tallies and system eigenvalue. Moreover, the additional statistical apparatus for the independent external Monte Carlo calculation starting with the different initial seeds, was introduced for k_{eff} convergence studies.

2.4 Validation and benchmarking

The MCB code was mainly validated using destructive assay data from the 17x17 fuel assembly irradiated in the Japanese Westinghouse 4-loop Pressurized Water Reactor (PWR) of Ohi-2 nuclear power plant [4]. Five fuel samples were extracted from the dedicated fuel assembly irradiated to burnup of 31.5 GWd/t for two consecutive reactor cycles. The 104 measured isotopic concentrations for 20 actinides were used in the validation. The data were chosen because large availability of information, not just about isotopic measurements, but also about irradiation history of the fuel assembly. Additionally, the MCB code was successfully benchmarked with other numerical tools for inventory calculations like SWAT, FISPACT, MONTEBURNS, which is presented in the reference papers [4-6]. Moreover, the sensitivity studies to the various sets of cross section libraries were performed (JEFF, JENDL, ENDF) [4,5].

Table I presents the main results of the MCB validation using Ohi-2 spent fuel assay data. The results are presented as Calculated-to-Experimental ratio (C/E) for calculated and measured isotopic concentrations. The comprehensive description of the applied methodology and obtained results are presented in the paper of Oettingen [4].

Table I: Results of MCB burnup validation using Ohi-2 samples [4].

Sample	89G01	89G03	89G05	89G08	89G10
Type	Gd	Gd	Gd	U	U
FIMA [%]	2.211	2.95	2.585	3.129	3.98
Isotope	C/E				
^{232}U	0.12	0.13	0.11	0.82	1.04
^{234}U	1.00	1.01	1.00	1.00	0.99
^{235}U	1.05	1.08	1.08	1.05	1.05
^{236}U	1.01	1.00	0.99	0.99	0.99
^{238}U	1.00	1.00	1.00	1.00	1.00
^{237}Np	1.01	1.02	1.06	1.03	1.08
^{236}Pu	1.54	1.28	1.29	1.32	1.20
^{238}Pu	0.97	0.95	0.96	0.92	0.95
^{239}Pu+^{239}Np	1.01	0.99	1.00	1.01	1.00
^{240}Pu	1.02	1.00	1.00	1.01	0.98
^{241}Pu	1.01	0.99	0.99	0.99	0.99
^{242}Pu	1.03	0.98	0.97	0.99	0.97
^{241}Am	0.90	0.98	1.15	0.89	0.92
^{242m}Am	1.11	0.98	1.37	1.01	1.22
^{243}Am	1.11	1.03	0.90	1.06	1.02
^{242}Cm	0.80	0.90	1.00	0.80	0.94
^{243}Cm	0.91	0.85	0.79	0.67	0.89
^{244}Cm	1.08	0.93	1.02	1.02	1.00
^{245}Cm	1.18	0.99	1.11	1.13	1.04
^{246}Cm	0.97	0.82	0.93	0.91	0.88
^{247}Cm	0.94	0.75	N.A.	0.76	1.03

2.5 Sample results

The section shows the example key results of the MCB numerical simulations for various nuclear systems staring from the most recent ones. The detailed results with methodology description, data presentation and interpretation are available for scientific community in the presented references.

a) Modelling of the block type HTGR. The MCB system was used for core design and optimization of the HTGR reactor with TRISO fuel. The analysis of the core focused mainly on the thermo-hydraulic coupling, design of control rods and adjustment of TRISO fuel for the initial and reloaded cores.

The results on control rod design demonstrate that the radial division of control rods made of tungsten can effectively compensate for the reactivity loss during the irradiation cycle of HTGR while flattening the core power distribution. In the investigated model the radial distribution parameter at BOL equals 0.91 and starts to increase moderately, not to grow above 1.02, and then drops to a value of 0.95 at EOC [7]. The results on HTGR modelling with thorium fuel shows that the application of volumetric homogenization method can be effectively applied for modelling of the double heterogeneity of HTGR core. The analysis shows that k_{eff} increases to its peak value at about 200 days of irradiation due to the breeding of ^{233}U, ^{239}Pu and ^{241}Pu from residual ^{232}Th and ^{238}U [8].

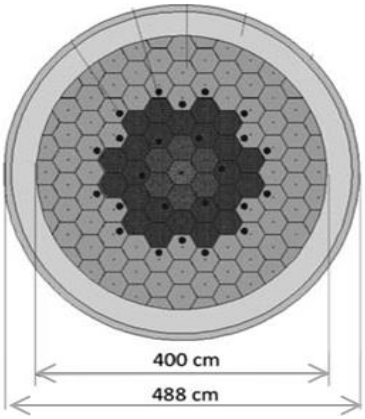

Fig. 1. MCB model of the HTGR reactor core [8].

b) Modelling of Lead-Cooled Fast Reactor (LFR). The activity was related to the design of the European Lead-Cooled Fast Reactor. The MCB was applied for the design of the pool-type core with nitrate fuel. The significant effort was taken to design LFR working in the adiabatic equilibrium state as well as to design thermo-hydraulic coupling with the Fluent code.

The results of MCB modelling of nitride LFR core containing Pu and MAs show that maximum axially integrated power peaking factor of about 1.2 occurs at BOL in fifth fuel region [9]. The modelling of LFR in adiabatic equilibrium state presents that the average core burnup over both investigated cycles was 52.40 MWd/kg (5.71% FIMA) while the achieved peak burnup was 90.21 MWd/kg (10.02% FIMA) [10].

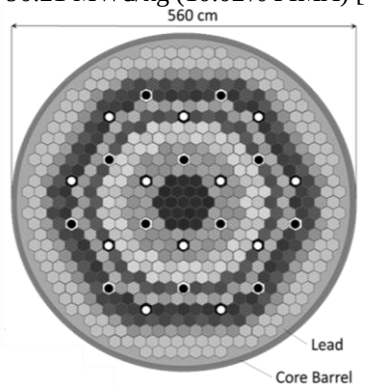

Fig. 2. MCB model of the LFR reactor core [10].

c) Modelling of PWR. The PWR analysis focused mainly on the characterization of the Westinghouse 4-loop plant for the benchmarking and validation purposes. In addition, the study on the thorium fuel cycle was performed. The core of the reactor was redesigned for the introduction of Th fuel assemblies according to the Seed Blanket Unit concept by Alvin Radkovsky.

The results of burnup validation with Ohi-2 spent fuel assay data show good consistency with the experimental measurements, see Table I [4]. The modelling of Seed Blanket Unity fuel assembly for PWR reactor shows that the concentration of bred of ^{233}U reaches maximum at 120 day of irradiation and then decreases until EOC [11].

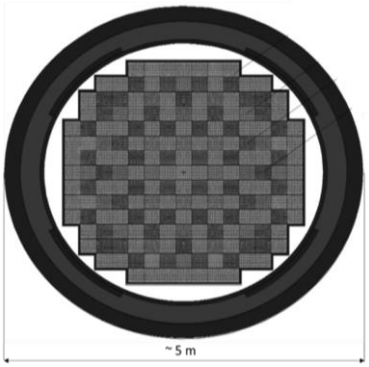

Fig. 3. MCB model of the PWR reactor core [11].

d) Modelling of Th subcritical assembly. The assembly constructed with Th fuel rods and Pb reflector rods is available at the AGH University, Krakow, Poland. The assembly was applied in 90's for the irradiation experiments using the Cf neutron source. The MCB code was used recently for the characterization of the redesigned assembly's core and design of new irradiation experiments.

The results show that the final concentrations of bred ^{233}U after 25 days of irradiation using 43 μg Cf neutron source in dedicated sample is about $2 \cdot 10^{10}$ atoms [12]. In addition, the rearrangement of the assembly for fast and thermal irradiations is possible. In the first case the maximal fast neutron flux of $6.6 \cdot 10^6$ n/cm^{2}s is achieved in the first radial zone. In the second case the maximum thermal flux of $1.0 \cdot 10^5$ n/cm^{2}s is achieved in the fourth radial zone [13].

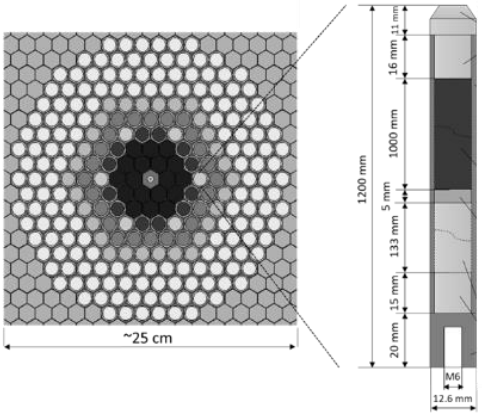

Fig. 4. MCB model of Th-Pb fuel assembly [12].

e) Modelling of early nuclear accidents. The MCB code was used for the criticality analysis of the early critical accidents of Harry Daghlian and Louis Slotin. The work was initiated by the author's curiosity due to the fact that there are no available open reliable sources of information about both accidents. In the study the numerical model of the human body for Monte Carlo radiation transport calculations was developed.

The results of criticality analysis of Harry Daghlian accident have shown that maximal k_{eff} for JEFF3.1 nuclear data library is 0.99883; therefore, even for the most reactive core, the supercritical state could not be achieved, which indicates to the missing elements in the available descriptions of the experimental setup [14]. In case of the Louis Slotin accident, the critical angel of the Be hemisphere over Pu core estimated using MCB is 0.28 – 0.29°. The results also show that the body of Louis Slotin has significant influence on criticality of about 200 pcm [15].

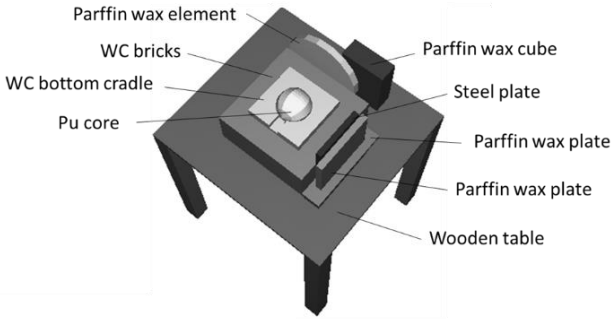

Fig. 5. MCB model of experimental set-up for LA-1 accident [8].

3. Conclusions

The MCB code is a robust tool for the radiation transport and burnup simulations. It was applied in many scientific projects related to the design of various nuclear systems. However, some improvements and developments of the code are foreseen for the future:

a) The MCB code is written in the FORTRAN computing language. The developers plan to rewrite and sort out the source code to make it more users friendly and thus more effective for implementation of improvements. The more efficient algorithms for the multiprocessing using HPR computers are foreseen for implementation. The MCB also lacks customized Graphical User Interface (GUI), which development is also considered in the future.

b) The most challenging task in the MCB development is the implementation of the uncertainty propagation modules for the coupled neutron transport and burnup simulations. This will allow for the estimation of the final actinide concentrations with the associated uncertainties. The task is quite complex since final uncertainties have to comprise impacts of many factors, especially related to the reactions cross sections, which in turn influence reaction rates in neutron transport calculations. The initial trails for application of the perturbation theory for the task were already performed.

c) The last task is related to the numerical modelling of the modern Generation III+ PWR reactors. The major activities in the usage of the MCB code were related to the numerical modelling of Generation IV nuclear reactors and in lesser extend to the numerical modelling of Light Water Reactors (LWR). Therefore, in the near future the MCB code will be used for the analysis of the Korean Advanced Power Reactor (APR1400).

Acknowledgements

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REFERENCES

[1] M. Oettingen, J. Cetnar, T. Mirowski, The MCB code for numerical modelling of fourth generation nuclear reactors, Computer Science, 16, 329–350, 2015.
[2] J. Cetnar, P. Stanisz, M. Oettingen, Linear Chain Method for Numerical Modelling of Burnup Systems, Energies, 14, 1520, 2021.
[3] P. Stanisz, M. Oettingen, J. Cetnar, Development of a Trajectory Period Folding Method for Burnup Calculations. Energies 15, 2245, 2022.
[4] M. Oettingen, Validation of fuel burnup modelling with MCB Monte Carlo system using destructive assay data from Ohi-2 PWR, Kraków, Wydawnictwa AGH, 174, 2016.
[5] M. Oettingen, C. Döderlein, E. D'Agata, K. Tuček, J. Cetnar, Comparison of MCB and FISPACT burn-up performances using the HELIOS experiment technical specifications, Nuclear Engineering and Design, 242, 399, 2012.
[6] A. Talamo, W. Ji, J. Cetnar, W. Gudowski, Comparison of MCB and MONTEBURNS Monte Carlo burnup codes on a one-pass deep burn, Annals of Nuclear Energy, 33, 1176–1188, 2006.
[7] M. Górkiewicz, J. Cetnar, Flattening of the Power Distribution in the HTGR Core with Structured Control Rods, Energies, 14, 7377, 2021.
[8] M. Oettingen, J. Cetnar, Numerical modelling of modular high-temperature gas-cooled reactors with thorium fuel, NUKLEONIKA, 66(4),133-138,2021.
[9] J. Cetnar, M. Oettingen, G. Domańska, On the neutronics of European lead-cooled fast reactor, NUKLEONIKA 55(3), 317−322, 2010.
[10] P. Stanisz, M. Oettingen, J. Cetnar, Monte Carlo modeling of Lead-Cooled Fast Reactor in adiabatic equilibrium state, Nuclear Engineering and Design, 301, 341-352, 2016.
[11] M. Oettingen, K. Skolik, Numerical design of the seed-blanket unit for the thorium nuclear fuel cycle, E3S Web of Conferences, 10, 1-5, 2016.
[12] M. Oettingen, Numerical design of thorium and uranium fuel samples irradiation in lead environment EPJ Nuclear Sciences & Technologies, 6, 1-11, 2020. X
[13] M. Oettingen, P. Stanisz, Monte Carlo modelling of Th Pb fuel assembly with californium neutron source, NUKLEONIKA, 63(3), 87-91, 2018.
[14] M. Oettingen, A criticality study on the LA-1 accident using Monte Carlo methods, Nuclear Engineering and Design, 359, 1-10, 2020.
[15] M. Oettingen, Criticality analysis of the Louis Slotin accident, Nuclear Engineering and Design, 338, 92-101, 2018.