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Advancements in reactor physics modelling methodology of Monte Carlo Burnup Code MCB dedicated to higher simulation fidelity of HTR cores

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Abstract – *The recent development of MCB - Monte Carlo Continuous Energy Burn-up code is directed towards advanced description of modern reactors, including double heterogeneity structures that exist in HTR-s. In this, we exploit the advantages of MCB methodology in integrated approach, where physics, neutronics, burnup, reprocessing, non-stationary process modeling (control rod operation) and refined spatial modeling are carried in a single flow. This approach allows for implementations of advanced statistical options like analysis of error propagation, perturbation in time domain, sensitivity and source convergence analyses. It includes statistical analysis of burnup process, emitted particle collection, thermal-hydraulic coupling, automatic power profile calculations, advanced procedures of burnup step normalization and enhanced post processing capabilities.*

I. INTRODUCTION

As some features of various nuclear reactors are similar, the other differs thus requiring an additional attention. The core of an HTR reactor is characterized by specific features, which imposes particular requirements on analytical tools and models that are to be used for analysis of its physics and safety along with fuel cycle analysis. The major differences, as compared to other systems like LWR or FBR, that need to be taken into consideration in analysis of nuclear transmutation in deep burn mode are concerned with high temperature of the fuel, different fuel form and different moderator. These specific features are:

• high operational temperature of the fuel and graphite, which necessitates the thermal-hydraulic and neutronic coupling;

• high level of core heterogeneity caused by a fine structure of fuel compacts filled with TRISO particles, for which a highly structured geometrical model is needed in order to account for neutron spectra effects that occur in the fuel due to resonant cross sections;

• deep neutron thermalisation, which imposes few important neutronic effects like: shortening free path length, higher flux gradients, stronger influence of reflectors, and as a consequence needed attention for spatial effects particularly in the vicinity of control rods or reflectors;

• large core size in terms of free path length as well as of the core fine structure length (i.e. TRISSO kernel size), which is primarily caused by relatively low average power density;

• operation of CR significantly influences axial distribution of power and burnup and reverses the effect of the temperature impact on the power profile;

• modelling of CR operation is necessary for a proper evaluation of axial power profile and power peaks.

Due to the existing complexity of burnup process, it is effective to apply an integrated calculation system, which will allow the user taking into consideration the spatial effects of full heterogeneous reactor model with continuous energy representation of cross section and the thermo-hydraulic coupling. For this purpose, an integrated Monte Carlo burnup calculation code MCB is very suitable. However, statistical fluctuations, which are intrinsically present

in Monte Carlo methods, need to be discriminated from an expected real solution. In case of HTR Monte Carlo modelling, flux oscillations and convergence problems with fission source may be brought about.

II. MONTE CARLO BURNUP CODE SYSTEM - MCB

MCB is Monte Carlo Continuous Energy Burn-up code, which extends the MCNP[1] capabilities to fuel cycle analysis, yet it enables the user to model time dependent reactor core setups like fuel reloading, reshuffling or CR operation. The transmutation modules exploit the general solution of Bateman equation for nuclear transmutation chain, while system analysis modules offer extended options for the reactor physics modelling in Monte Carlo approach. From the first release (version MCB1C[2]) through NEA Data Bank in 2002 the code is being constantly developed and applied to neutronic and fuel cycle analysis in frame of European projects on ADS and Gen-IV reactors, which include HTR-s in deep-burn concept for plutonium and MA burning. Currently, the code extended options are under development in frame of Polish national program for HTR application – HTR-PL. The recent development is directed towards advanced description of modern reactors, including double heterogeneity structures that exist in HTR-s, and is dedicated for design improvements in terms of safety and performance. In this, we exploit the advantages of MCB methodology in integrated approach, where physics, neutronics, burnup, reprocessing, non-stationary process modeling (control rod operation) and refined spatial modeling are carried in a single flow. This approach allows for implementations of advanced statistical options like analysis of error propagation, perturbation in time domain, sensitivity and source convergence analyses.

II.A. General features of MCB

The main goal of a burnup code is to calculate the evolution of material densities. It concerns all possible nuclides that may emerge in the system after nuclides decays, transmutations, or particles emissions. Transmutation process includes fission product breakdown into nuclides as well as helium and hydrogen atoms formed from emitted α particles and protons respectively. There is no required predefined list of nuclides under consideration since all transmutation chains are being formed automatically on-line basing on physical conditions that constrain the system under the control of user-defined thresholds. These thresholds concern contribution to the nuclide mass change from constructed transmutation trajectories. In a real system under irradiation or decay, the nuclide composition undergoes evolution that generally can be described with a continuous function of time. An approximation of this function is obtained in MCB throughout time the step procedure which starts from assessing reaction and decay probabilities of every possible channel by means of stationary neutron transport calculations. In the next step, the transmutation chain is formed and then solved to produce nuclide density table in required time points. The main features of the code can be outlined as follows below.

- The decay schemes of all possible nuclides and their isomeric states are formed and analyzed on the basis of the decay data taken from two sources. The first one – TOI.LIB, which is based on Table of Isotopes [3], describes decay schemes for over 2400 nuclides including formation of nuclides in the excited states.
- Numerous cross-section libraries and data sets can be loaded into computer memory to calculate adequately reaction rates and nuclide formation probabilities. It includes possibility of separate treatment of cross section for different burnable zones, to account for thermal effects, employment of energy dependent distribution of fission product formation, and energy dependent formation of isomer nuclides.
- Thermal-hydraulic coupling with FLUENT® or POKE[4] is available for prismatic HTR.
- Reaction rates are calculated exclusively by continuous energy method with the usage of the point-wise transport cross-section libraries and, in case of lack of proper library, by using the dosimetry cross section library.
- Fission product yield is calculated from incident energy dependent distributions of fission products prepared separately for every fissionable nuclide.
- Heating is automatically calculated in a similar way as the reaction rates during neutron transport simulation by using KERMA. factors included in standard cross section tables. The natural decay heat is included, what allows for consideration of afterheat effects. The energies of decays are taken from the ORIGEN library[5].
- Time evolutions of nuclide densities are calculated with the complete set of linear transmutation chains that is prepared for every zone and time step so it is being automatically adjusted to the transmutation conditions evolving with time.
- The code uses extended linear chain method, which is based on the Bateman approach, to solve prepared-on-line a set of linear chains that noticeably contribute to nuclide formation.
- Detailed analysis of transmutation transitions from nuclide to nuclide is performed. The transmutation chains that are formed by the code can be printed for nuclides of interest.
- Material processing is available along with material allocations to geometry cells during the

burnup. Using this feature the user can simulate the fuel shuffling or CR operation.

III. BATEMAN EQUATIONS

MCB adopts general solution of Bateman equations derived from linear chain method. The general transmutation chain, which is nonlinear, is resolved into series of linear chains using methodology of transmutation trajectory analysis. MCB is free from producing and using one-group neutron cross section. It uses transmutation probabilities instead, which are assessed directly in the process of neutron transport calculation executed independently for every transmutation zone and every time step.

Transmutation constants can be expressed as follows:

$$\lambda_{i,j} = b_{i,j}^{d} \cdot \lambda_j^{d} + \int \Phi(E)\sigma_{i,j}(E)dE \qquad \text{(eq. 1)}$$

where the symbols denote:
λ_j^d - decay constant of *j*-th nuclide,
$b_{i,j}^d$ - branching ratio of *j*-th nuclide decay into *i*-th nuclide formation,
$\Phi(E)$- neutron flux ,
$\sigma_{i,j}(E)$- cross section for production of *i*-th nuclide from *j*-th nuclides.

The transmutation constants appear as the coefficients of the Bateman equations describing the general, non-linear transmutation chain for *w* nuclides as follows

$$\frac{dN_i}{dt} = \sum_{j=1,w} \lambda_{i,j} \cdot N_i\,, \quad (i = 1, w) \qquad \text{(eq. 2)}$$

III.A. Solution of Bateman equations

Usually, in the commonly applied numerical methods the set of linear chains is prepared arbitrarily, which is sufficient for well-defined cases. However, for a more general case the application of procedure that resolves the non-linear chain into a set of linear chains is necessary to assure the mass flow balance and the numerical solution stability. In order to derive the solution of a general case basing on the known solution of a linear decay case, it is convenient to focus on the transmutation transition from one nuclide to the other one after elapsing time *t*. The transmutation transitions can lead through many paths, which possibly branch, forming a non-linear chain. Now, let us define a transmutation trajectory as a sequence of direct nuclide-to-nuclide transitions, starting from the first nuclide and ending at the last, *n*-th nuclide. The transmutation trajectory is almost equivalent to a decay chain, but due to an occurrence of branching in the non-linear chain, the mass flow is not preserved on a single trajectory level. It is preserved, however, over all the trajectories that can be extracted from the non-linear chain. The Bateman equations for transmutation trajectory representing a linear chain will have the following form:

$$\frac{dN_1}{dt} = -\lambda_1 N_1 \qquad \text{(eq. 3)}$$

$$\frac{dN_i}{dt} = b_i\,\lambda_{i-1}N_{i-1} - \lambda_i N_i\,, \quad (i = 2, n) \qquad \text{(eq. 4)}$$

where

$$\lambda_i = \sum_{\substack{j=1,w \\ j\neq i}} \lambda_{i,j}\,, \quad b_i = \frac{\lambda_{i,i+1}}{\lambda_i}\,, \qquad (i = 1, n)$$

The solution is following:

$$N_n(t) = \frac{N_1(0)}{\lambda_n} \sum_{i=1}^{n} \lambda_i \alpha_i\, e^{-\lambda_i t} \qquad \text{(eq. 5)}$$

where

$$\alpha_i = \prod_{\substack{j=1,n \\ j\neq i}} \frac{\lambda_j}{(\lambda_j - \lambda_i)}\,, \quad (i = 1, n) \qquad \text{(eq. 6)}$$

In a general case when certain transition can appear in the chain m_k times the solution takes more complicated form [6]:

$$N_n(t) = \frac{N_1(0)}{\lambda_n} \sum_{i=1}^{n} \lambda_i \alpha_i\, e^{-\lambda_i t} \cdot \sum_{m=0}^{\mu_i} \frac{(\lambda_i t)^m}{m!} \Omega_{i,\mu_i - m} \qquad \text{(eq. 7)}$$

where

$$\alpha_i = \prod_{\substack{j=1,n \\ j\neq i}} \left(\frac{\lambda_j}{\lambda_j - \lambda_i}\right)^{m_j} \; for \;\; (i = 1, n), \qquad \text{(eq. 8)}$$

and

$$\Omega_{i,j} = \sum_{h_1=0}^{j} \cdots \sum_{h_n=0}^{j} \prod_{\substack{k=1,n \\ k\neq i}} \binom{h_k + \mu_k}{\mu_k} \left(\frac{\lambda_i}{\lambda_i - \lambda_k}\right)^{h_k} \delta_{jp}\,,$$

$$\mu_k = m_k - 1, \qquad p = \sum_{\substack{l=1,n \\ l\neq i}} h_l\,, \qquad \text{(eq. 9)}$$

for $(i = 1, n), (j = 0, \mu_i)$. Symbol δ_{jp} is Kronecker's delta.

Basing on the formula for nuclide concentration evolution over single trajectory the entire transmutation chain. Every trajectory is quantitatively described by transition and passage parameters where the passage stands for the sum of the nuclides

concentrations of formed in the disintegration process of the *n*-th nuclide or their daughters after being produced from the transition along considered trajectory. The transition and passage functions are important for the mass balance of transmutations, which is an ultimate parameter for checking correctness and convergence of any numerical algorithm for calculation of time evolutions of concentrations in a transmutation system. They are used to control the numerical algorithm of breaking down a non-linear transmutation chain into a series of transmutation trajectories for which the concentration can be calculated.

IV. MCB CAPABILITIES FOR HTR CORES

Due to existing complexity of burnup process and reactor physics itself in an HTR, in order to ensure high quality of design, particularly with its safety features, it is reasonable to apply few different tools of reactor core analysis. This can bring about results obtained from few different perspectives. Here, the Monte Carlo methods, although demanding more computer power, are characterized by higher level of model complexity and fidelity, thus the results can be obtained in an integrated way, possibly displaying important effect that can be hidden or neglected in another approach. For this purpose, an integrated Monte Carlo burnup calculation code MCB is very suitable. It is fully integrated calculation system, which allows the user taking into consideration of spatial effects of full heterogeneous reactor model with continuous energy representation of cross section and the thermo-hydraulic coupling. Here, a particular importance lays in a proper assessment of the power distribution, but not merely at BOL but as a function of burnup with consideration of the CR operation. The power distribution affect many core safety features, therefore a simplified approach can lead to biased conclusions. As Monte Carlo approach presents some benefits, it is not free from their intrinsic problems, which need to be treated accurately. Namely, statistical fluctuations, which are intrinsically present in Monte Carlo methods, need to be discriminate from an expected real solution. In case of HTR Monte Carlo modelling, flux oscillations and convergence problems with fission source may be brought about.

IV.A. Thermal-hydraulic coupling

Introduction of thermal hydraulic calculations into Monte Carlo simulations was done by coupling MCB with the POKE code. The POKE code was written in GA; its original version was designed for the geometry and parameters of Ft. St. Vrain reactor, and later it was used for GT-MHR analysis as well. POKE determines fuel and coolant temperature distributions as well as coolant mass flow in the steady state. The reactor configuration consists of a number of parallel coolant channels connected to common inlet and outlet plenums. The reactor between the inlet and outlet plenums is divided into inlet reflector, core and outlet reflector. All heat is assumed to be generated in the core. For calculation purposes the reactor is divided into a number of cylindrical regions, which extend from the inlet to the outlet plenum. The POKE code iteratively solves three one-dimensional equations that express the conservation of mass, momentum and energy for each channel modelled. The coolant mass flow rate results from balancing the pressure drop from the inlet to the outlet plenum.

The code coupling was done on the level of source code, where the modified version of POKE has been incorporated into the MCB code, but all the data exchange between codes has been left on external files, in order to allow the user to recalculate. The thermal-hydraulic specification is read in from the POKE input file, which describes the reactor geometry and other parameters, whereas MCB delivers only the power distribution profile. The temperature profile at BOL is to be defined by the user after arbitrary assumptions or using the results obtained in earlier calculations. Invoked POKE calculates the required thermal hydraulic parameters as well as the new temperature profiles. On that basis the new temperatures of all regions together with the cross sections adjusted to the temperature are used for new power profile iteration, and the subsequent burnup calculations provides more realistic isotope production results.

IV.B. Multithread sampling and error propagation on k-eff

Statistical analysis of burnup in MCB is enhanced by possibility of multithread sampling of neutron populations in criticality calculations. Every statistical sample of neutron population starts from different random numbers thus we obtain statistically fluctuating results of burnup calculations. Every sample is lead from the beginning to the very end of burnup calculations without going into interference with other samples. The evolution of the densities as well as reaction rates statistically fluctuate from sample to sample which allows for error propagation analysis. The average results are produced at every step of burnup calculation, using the sample results, only for the purpose of their printout to the output files.

At every time step where k_{eff} f is calculated there are obtained two kinds of distributions. One is the Monte Carlo distribution of k_{eff}, which is generated in every calculation sample. It is characterized by the estimated variance, standard deviation of k_{eff} and the average (mean) k_{eff} value itself as calculated by an MCNP module – KCODE.

Although the mean k_{eff} differ from sample to sample as a result of their distribution, the variances of k_{eff} Monte Carlo distributions are supposed to be close to each other, which means that Monte Carlo distributions for the same steps differ only in the mean value. For the purpose of further analysis we need one value representing the variance. Naturally, it will be the average over all samples as follows.

$$\overline{var^{(MC)}} = \frac{1}{n}\sum_{i=1/n} var_i^{(MC)} \qquad \text{(eq. 10)}$$

The second kind of distribution concerns the sampling distribution of k_{eff} mean values. Every sample generates one mean k-eff value but all samples forms the distribution of k_{eff} mean values. This is the sampled k-eff means distribution. From the sampled k-eff means distributions the variance and standard deviation are calculated. The standard deviation of Monte Carlo distribution concerns only fluctuation in the last Monte Carlo process of k_{eff} evaluations, whereas the standard deviation of sampled k-eff means distribution concerns all sources of errors, including propagation from reaction rates and density fluctuations of the previous steps. There are the k_{eff} mean of the means:

$$\overline{k_{eff}} = \frac{1}{n}\sum_{i=\frac{1}{n}} k_{eff,i} \qquad \text{(eq. 11)}$$

where $k_{eff,i}$ is the average (mean) value of k_{eff} in the *i-th* Monte Carlo sample.

The variance of k_{eff} sampled means distribution is as follows:

$$var_{keff} = \frac{1}{n-1}\sum_{i=1/n}\left(k_{eff,i} - \overline{k_{eff}}\right)^2 \qquad \text{eq. 12)}$$

Since the variance k_{eff} Monte Carlo distribution (1) is free from error propagation, whereas the variance of k_{eff} sampled means distribution (3) account for the error propagation from previous steps we can write the following relation:

$$var_{keff} = \overline{var_{keff}^{(MC)}} + var_{keff}^{(prop)} \qquad \text{(eq. 13)}$$

The standard deviation of the mean k_{eff} (mean of the means) is calculated from variance (3):

$$\sigma_{\overline{k_{eff}}} = \sqrt{\frac{var_{keff}}{n}} \qquad \text{(eq. 14)}$$

The reaction rates error propagation on k_{eff} can be expressed as the ratio of propagated error variance to the final variance:

$$f_{prop} = \frac{var_{keff}^{(prop)}}{var_{keff}} = 1 - \frac{\overline{var_{keff}^{(MC)}}}{var_{keff}} \qquad \text{(eq. 15)}$$

The error propagation can be actually measured if the propagation occurs and the variances estimated in the sampling process are estimated with a sufficient precision. It is obvious that the higher user defined number of samples will provide a better precision. In cases of week error propagation or poor statistics, the estimated Monte Carlo distribution variance can be larger than the estimated variance of k-eff sampled means distribution. In any case the final estimation of k-eff standard deviation includes all sources of errors. If standard deviations of k-eff Monte Carlo distribution is smaller than the standard deviation of k-eff sampled means distribution at BOL it means that there are other sources of statistical errors that for the case in hand were not accounted for in the MCNP modules of error estimation. In such cases the error propagation listed by MCB is not only due to reaction rates but also due to undisclosed sources.

IV.C. Perturbation in time domain

Any perturbation invoked in MCNP generally influences the neutron flux thus changes the reaction rates and material composition globally. In burnup system the perturbation will be propagated from one initial material to all burnable materials, therefore there is no sense of following one perturbation but a union of perturbation mast be followed. Implementation of burnup perturbation is concerned with tracing of propagation of the initial perturbation, which after burnup is replaced by a union of perturbations. The burnup perturbation can start from just one perturbation in a union, but since perturbation changes the reaction rates and possibly the composition after a time step, all burnable materials will vary in perturbed composition as compared to the unperturbed one. This quite complex perturbation system needs to be kept under control. Invoked burnup perturbation is propagated through all time steps, and the perturbations involved in the perturbation union change material composition due to burnup. It should be noted that after the first burnup step every perturbation union will be rearranged and most likely will contain the number of constituting perturbations greater than or equal to the number of burnable zones. This in a system with larger number of burnable zones will require an additional memory allocation.

IV.D. Burnup Calculation System oscillations

Statistical fluctuation in Monte Carlo modelling should in general follow the law of large numbers of the probability theory. On this assumption, the standard formulations of statistical measures of

probability distribution are used in Monte Carlo neutron transport calculations. However, in some nuclear reactor systems like HTR, the fluctuation of the calculated power distribution contains a systematic term, which is propagated in consecutive neutron generations through the fission source distribution. In burnup calculations scheme the process of source normalization to the constrained power is done usually using the neutron heating rate as evaluated at the beginning of step. In this treatment, the systematic term (in the fluctuation of power distribution) tends to conserve itself or to form increasing oscillations. This process of creating oscillations is linked with production and depletion of Xe135 in a deeply moderated HTR core. Here we do not mean the real physical oscillations, which can be created also, but the numerical oscillations in the calculated density distribution. Another source of systematic term is related directly to the neutron source convergence problem, which occurs when the fundamental distribution of the source is difficult to achieve, even if the reactivity converges early. This behavior occurs in large HTR cores.

The magnitude of both effects can be reduced when advanced time step algorithms are introduced. They are based on predictor-corrector schemes and improved source normalization procedure.

The weakness of staircase model comes from the fact, that reaction rates per nuclide are not constant during step length. Neutron source intensity should vary in order to provide constant power of the system. This results in bias in isotopic composition evolution, especially for long time steps preferred for whole fuel cycle calculations.

IV.E. Advanced schemes of time steps

In order to overcome these problems, the variety of advanced step models have been suggested in the literature. As the magnitude of the system oscillations lowers with shorter time step, choosing refined time steps would stabilize time and spatial distributions of neutron flux dependent characteristics but on the expense of calculation time. Therefore an increase of efficiency should be searched in improving the time step schemes with limited number of neutron transport calculations, which are the most time consuming, while less demanding depletion calculations can be made more often. Step model improvement involves a better estimation of transmutation constants $\lambda_{i,j}$, which appears in Eq. 1, by more or less elaborated iteration procedure using their BOS and EOS values in subsequent iteration. The source of the problem lays in the fact that some of transmutation constants can become time dependent transmutation variable thus disturbing the assumption of Bateman equations. The transmutation variable for every needed reaction in every depletion cell can be described in the following form.

$$\lambda(t) = \int \Phi(E,t)\sigma\,(E)dE = \\ = S(t)\int \Phi^*(E,t)\,\sigma\,(E)dE = S(t)r(t), \quad \text{(eq. 16)}$$

where $S(t)$ is global fission neutron source intensity, $\sigma(E)$ is the microscopic cross section for the considered reaction, $\Phi^*(E,t)$ is neutron flux in the considered cell per unit neutron source intensity, and $r(t)$ is microscopic reaction rate of the considered reaction in the considered cell per unit neutron source intensity. The neutron source intensity is constrained by the defined system thermal power P and global heating rate per unit neutron source intensity $h(t)$.

$$S(t) = P/h(t) \quad \text{(eq. 17)}$$

The system thermal power is specified by the user – typically fixed separately for each time period. while The heating rate per source neutron which generally is time dependent can be expressed as:

$$h(t) = \sum_{i\in\{cell\}} \sum_{j\in\{nucl\}} H_{i,j}(t)\, V_i\, N_{i,j}(t) \quad \text{(eq. 18)}$$

where $N_{i,j}(t)$ is cell atomic density (the number density), V_i is cell volume, $H_{i,j}(t)$ is heating per source neutron generated on single $j-th$ nuclide in $i-th$ cell. The first simplest way of improving the time scheme is to assume the heating rate on single nuclide fixed overt the time step and take into consideration time dependent concentrations that result from depletion calculations. Since in the current methodology of solving Bateman's equation fixed transmutation constant are required one needs to input their step average values. In our case the neutron source intensity is the parameter that needs this treatment in a simple iterative procedure. In the first step we assume that the step average values are equal to the ones on beginning of step (BOS):

$$h(t) = h(0) = h_0, \quad \text{(eq. 19)}$$

and thus

$$_{(1)}S_{av} = \frac{P}{h_0} = S_0, \quad \text{(eq. 20)}$$

where the left subscript denotes the iteration number. The heating rate h_0 is obtained from neutron transport calculations at BOS. The solution of Bateman's equation in the first approximation brings the values of concentrations $N_{i,j}(t_K)$ after step time t_K, which is denote symbolically as the result of integration of Eq. 7 over all meaningful transmutation trajectories:

$$_{(1)}N_{i,j}(t_K) = g(N_{i,j}(0), S_0, r_0, t_K) \quad \text{(eq. 21)}$$

which allows us to calculate the heating rate at end of step (EOS). When heating rate at BOS differs from that at EOS the correction of the average source intensity is needed in order to adjust the approximation value of the step burnup ${}_{(1)}B$ to the required one - B. The new approximation of heating rate ${}_{(1)}h_{av}$ which is approximated by the average of BOS and EOS values, obtained using Eq. 18, in the first approximation needs additional correction after the step burnup adjustment which finally leads to the neutron source intensity correction for new approximation as follows:

$$ {}_{(2)}S_{av} = \frac{P}{{}_{(2)}h_{av}} = S_0 \left(1 - \frac{\frac{{}_{(1)}\Delta h}{2}}{h_0 + {}_{(1)}\Delta h} \right) \quad \text{(eq. 22)} $$

The new approximation of neutron source intensity is then used for repeated calculation of nuclide density evolution.

$$ {}_{(2)}N_{i,j}(t_K) = g(N_{i,j}(0), {}_{(2)}S_{av}, r_0, t_K) \qquad \text{(eq. 23)} $$

This process does not involve additional transport calculation since the heating rate from BOS is involved. The Bateman's equation solution is much less computer time demanding, therefore repetition of this process does not bring substantial penalty on the calculation cost. Described above calculation step scheme is called the slope scheme as it effectively corrects the effect of sloping radiation heating during single time step as an effect of fissionable nuclides depletion. In case of HTR reactors its useful for cases of deep-burn cores when depletion rate can be observed at significant rates. Neglecting the source intensity correction would result in an underestimation of the actually modeled system burnup comparing to the required constrained one. This also would be propagated on the time evolution of the nuclide densities and thus nuclide depletion which would correspond to lower than requited the burnup values. It should be noted that the above formalism take into accounts correction of a global parameter such as the neutron source intensity, but still it is calculated using spatial distributions of the heating rates per source neutron as well as of the number density.

More advanced step scheme are needed in order to account for variation of nuclide heating rates $H_{i,j}(t)$ with the time steep, which also involves their spatial dependences. So-called bridge scheme of burnup step, is characterized by source normalization using the step average functions that involve the reaction rates from BOS and EOS in the first approximation as of the slope scheme. This procedure involves repeated neutron transport calculations at both BOS and EOS, in which of the neutron heating rates and reaction rates as obtained. The diagram of bridge scheme is shown in Figure 1.

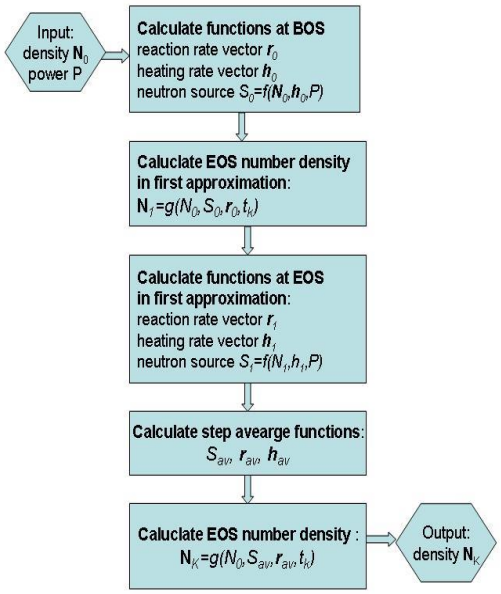

Fig. 1: Diagram of bridge scheme of burnup step with neutron source normalization

Comparing to the slope scheme the bridge scheme involves averaging of the reaction rates were the simple average of two values: at BOS and at EOS is applied after correction. This correction can be made iteratively few times but that is case dependent since each recalculation of the neutron transport modules is time consuming. After every EOS calculations new approximation of heating rate at EOS ${}_{(k)}h_K$ is obtained and then new step average values for heating rates ${}_{(k)}h_{av}$ is calculated:

$$ {}_{(k)}h_{av} = {}_{(k-1)}h_{av} + \frac{({}_{(k)}h_K - {}_{(k-1)}h_K) \cdot {}_{(k-1)}h_{av}}{(h_0 + {}_{(k)}h_K)}. \qquad \text{(eq. 24)} $$

Similarly, the neutron source intensity ${}_{(k)}S_{av}$:

$$ {}_{(k)}S_{av} = \frac{P}{{}_{(k)}h_{av}} \qquad \text{(eq. 25)} $$

and the reaction rates ${}_{(k)}r_{av}$ are obtained:

$$ {}_{(k)}r_{av} = {}_{(k-1)}r_{av} + \frac{({}_{(k)}r_K - {}_{(k-1)}r_K) \cdot {}_{(k-1)}h_{av}}{2 \cdot {}_{(k)}h_{av}}, \qquad \text{(eq. 26)} $$

and then they are used for the new approximate of the number density at EOS ${}_{(k+)}N_{i,j}(t_K)$ as follows:

$$ {}_{(k+1)}N_{i,j}(t_K) = g(N_{i,j}(0), {}_{(k)}S_{av}, {}_{(k)}r_{av}, t_K) \quad \text{(eq. 27)} $$

The final algorithm is combination of *stochastic implicit Euler method* (SIEM) and slope scheme, where the predictor-corrector procedure is applied for iterative approximation of the step average heating

and reaction rates. SIEM method was diagnosed to provide stability of burnup irrespectively of time step length[7]. A correct calculation of final number density requires the average values of the neutron source strength and reaction rates. The process of averaging uses a simple average of two values: at BOS and at EOS after correction. The EOS correction in done in a step predictor module, in which the reaction rates and source strength of the first approximation are scaled by the ratio of the burnup constrained to its first approximation. The neutronic calculation is repeated and results averaged at the EOS until convergence. In this iterative procedure the new approximations of heating and reaction rates, which are used in the corrector module are the averages of all previous iterations:

$$\overline{{}_{(n)}h_K} = \sum_{i=1}^{n} \frac{{}_{(i)}h_K}{n}, \qquad \overline{{}_{(n)}r_K} = \sum_{i=1}^{n} \frac{{}_{(i)}r_K}{n}, \text{(eq. 28)}$$

This algorithm is supposed to merge unconditional stability of *stochastic implicit Euler method* and improved accuracy for long steps due to neutron source intensity averaging. Detailed investigation about the performance of SIEM algorithm on HTR core were carried out using single block column model that usually reveals strong oscillations[8]. The major observation from this analysis is that flux distribution in fuel cycle analysis in simplified reactor models can lead to strong oscillations from step to step due to inadequate ^{135}Xe evolution modelling as shown on Figure 2.

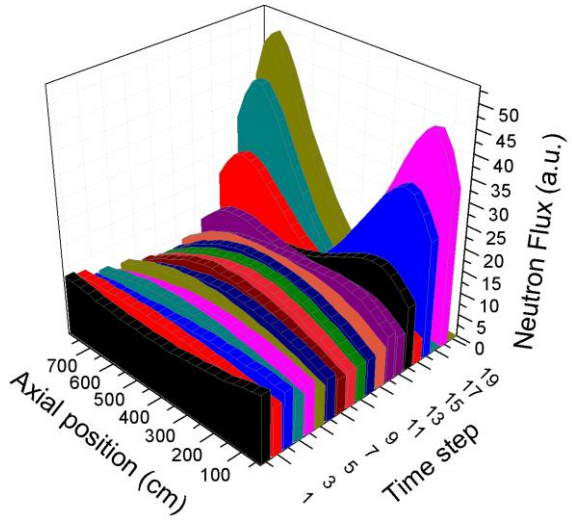

Fig. 2. The neutron flux profile for burnup with time steps of 100 days in HTR simplified model[8].

SIEM model improves situation by eliminating the oscillations in time domain but spatial power profile loses its expected buckling as shown in Figure 3.

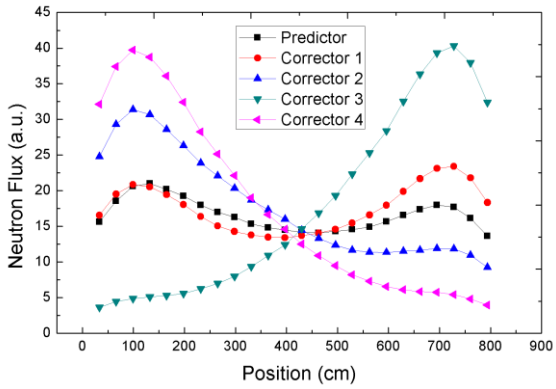

Fig. 3. Power profile correction in SIEM model at step 20[8].

Introduction in to the model the simulation of CR withdrawal for compensation of the burnup brings a big advantage by strong reduction of oscillations as shown in Figure 4.

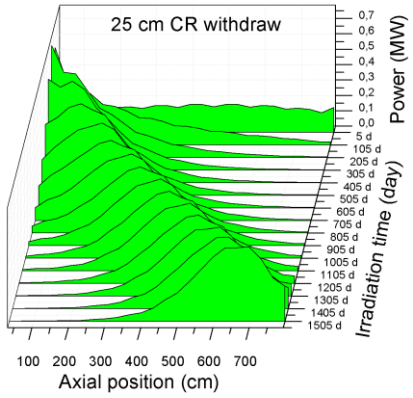

Fig. 4. Variation of power profile for system with 25 cm control rod withdraw each 50 days [8].

V. HTR FULL CORE CALCULATION MODEL

Reference model of HTR prismatic core for MCNP/MCB calculations was prepared to comply with axial-only fuel shuffling and 4-batch refueling scheme[9]. We pay a particular attention to the modelling of CR operation as the CR insertion level is adjusted along with the reactivity loss during burnup. The reference core comprises five radial rows of fuel blocks in eight axial block layers. For the power distribution analysis and burnup calculations, the active core is divided into burnup zones. Every fuel block row is divided radially into two halves, while axially every block layer is divided into three regions, which altogether constitute 240 fuel zones.

The core was filled with fuel compacts containing TRISO in 18% volume fraction. The active core is model with high level of fidelity with full description of details including the fuel double heterogeneity. The fragment of the core model is shown in Figure 5, where different colors denote different zones with their materials and corresponding temperatures.

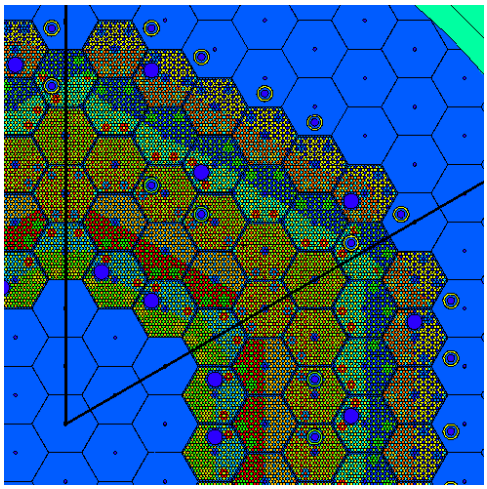

Fig. 5. Core regions with fuel rods and CR/RS holes

It can be observed that the core structure is already very complicated, but in fact each fuel rods has its own internal structure. In the applied model, apart from the fuel, also burnable poison rods constitute burnable zones in 10 radial regions times 8 axial zones. The CR channels are also axially divided in order to allow for modelling of CR operation, which follows the reactivity loss with burnup. Concerning the fuel shuffling, we have applied recommended axial-only shuffling scheme with the mirror symmetry in respect to the core middle plane. This is one of the simplest schemes, which reduces the space of an operator error and shortens the outage time required for shuffling, as compared with radial or mixed axial-with-radial shuffling schemes.

V.A. Reduction of power spatial oscillations

Applied burnup calculation model includes the bridge scheme of burnup in order to account for numerical oscillation of the neutron flux, as well as to adjust the power normalization to the heating rates, calculated as step average values instead of BOS values. The occurring power oscillations shown in Fig. 6. have a collective nature; areas of power oscillations in the same direction exceed the fuel block dimensions.

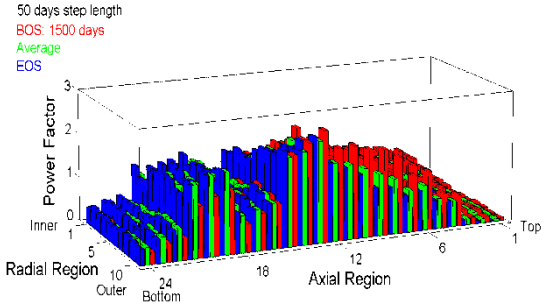

Fig. 6. Power spatial distributions in the bridge scheme of burnup step

Since the average values have been used for the burnup step, these power oscillations have been reduced in our results of power distribution.

V.B. Influence of CR operation on power distribution

Modelling of CR operations is not often being included in core performance assessments, due to complexity it involves. However, locations of power peaks and assessments of power and temperature peak values can be strongly affected by the CR operations, particularly in HTR-s, due to the short neutron transport length. Moreover, the influence of CR operation on the power distribution might be stronger in fuel batch reloading schemes. Therefore, before any optimization of fuel refueling and shuffling can be undertaken, the assessment of CR operation needs to be accomplished. As the axial only shuffling scheme has positive influence on the power distribution by leading to reduction on power peaking near reflectors, we need to assess how the CR operation influences it. This analysis has been carried out, where CR operation were modelled by changing the CR insertion level stepwise linearly in 100 cm bins along with the fuel burnup. The time evolution of power profile is depicted in Figure 7, which concerns equilibrium cycle of 350 days with the second reference fuel. The graphs apart from the first one on the figure show the step average distributions, where the basic step duration of 50 days has been used. At the cycle beginning, two shorter steps were applied in order to stabilize Xe135. At BOC the operational CR were fully inserted while the start-up CR were fully withdrawn. The power distribution then was quite well balanced; the BPR suppressed power peaking close to the inner reflector while in the central location of axial direction the power peak is reduced due to the fuel partially burned.

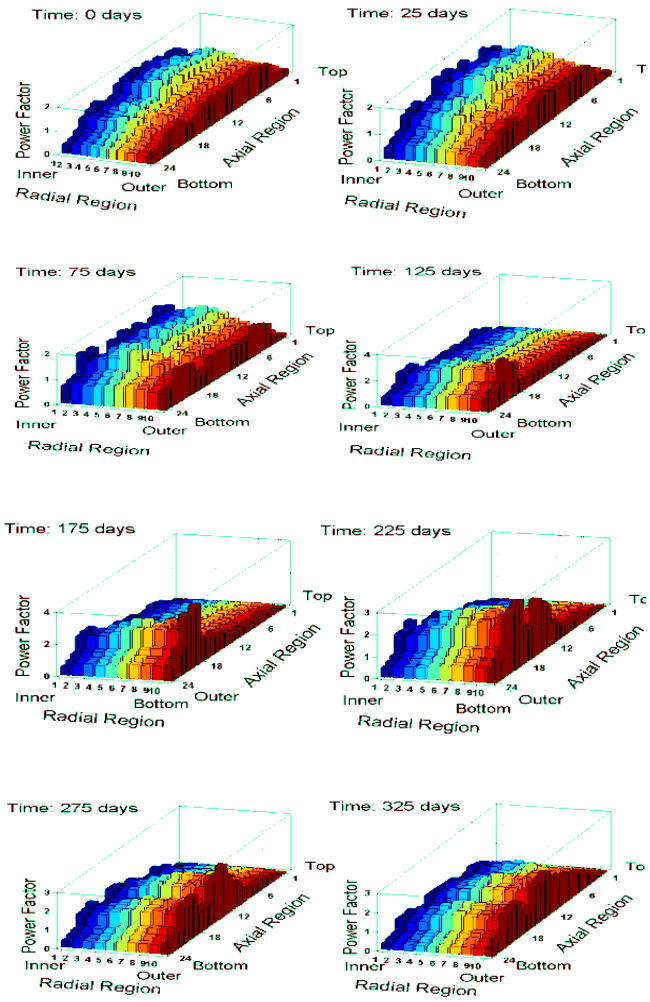

Fig. 7. Power profile in cycle with CR operation modelled; Pu+MA fuel, 350- day 4-batch equilibrium cycle in axial only shuffling.

The power generated in the upper core half is greater than in the lower. This results from lower temperature in the upper part, which negatively changes the reactivity. The power ratings in radial outer regions are generally lower than the average, due to CR influence, which reduced the reflector significance. In the next steps the CR have been gradually shifted, which brings about a significant change in the axial power profile.

VI. CONCLUSIONS

The recent development of MCB code is directed towards advanced description of modern reactors, including double heterogeneity structures that exist in HTR-s, and is dedicated for design improvements in terms of safety and performance. In this, we exploit the advantages of MCB methodology in integrated approach, where physics, neutronics, burnup, reprocessing, non-stationary process modeling (control rod operation) and refined spatial modeling are carried in a single flow. This approach allows for implementations of advanced statistical options like analysis of error propagation, perturbation, sensitivity and source convergence analyses and it brings a higher simulation fidelity of HTR cores.

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