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Assesment of advanced step models for steady state Monte Carlo burnup calculations in application to prismatic HTGR

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Abstract. In this paper, we compare the methodology of different time-step models in the context of Monte Carlo burnup calculations for nuclear reactors. We discuss the differences between staircase step model, slope model, bridge scheme and stochastic implicit Euler method proposed in literature. We focus on the spatial stability of depletion procedure and put additional emphasis on the problem of normalization of neutron source strength. Considered methodology has been implemented in our continuous energy Monte Carlo burnup code (MCB5). The burnup simulations have been performed using the simplified high temperature gas-cooled reactor (HTGR) system with and without modeling of control rod withdrawal. Useful conclusions have been formulated on the basis of results.

Key words: burnup • high temperature gas-cooled reactor (HTGR) • Monte Carlo • stability • step model

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Introduction

The concept of using continuous energy Monte Carlo simulations for critical systems as a precise tool for burnup calculations is well known in the field of research and development of fuel cycle. The beginning-of-step approximation of neutron flux over the time-step is often applied by many burnup codes for its simplicity. This approach assumes constant flux/power profile during entire step, which can cause problems such as spatial instability of reaction rates in the simulated system [1]. Spatial oscillations of flux and xenon concentration appear for relatively short steps, thus affecting the core's equilibrium. Regarding fuel cycle analysis of prismatic HTGR, the spatial flux distribution of the core varies strongly in the vicinity of compensation rods, which are being slowly withdrawn in order to compensate the reactivity loss. In order to handle this problem properly, a better flux normalization procedure – so-called bridge scheme – was developed and applied in the study of PuMA project [2]. An optimal model of time-step is necessary to account for the non-constant system's behavior as well as to provide stability of burnup. Various models called predictor-corrector schemes have been suggested in the literature to compensate/reduce spatial instability of burnup. The stochastic implicit Euler method [3] was chosen for our research due to attractive convergence control features. The methodology was implemented in MCB5 code [4] and compared with existing step models. Its performance was studied

using the geometry of prismatic HTGR – the reactor type with currently most complex core and fuel. Additional stress was put on the problem of neutron source strength normalization.

Increasing computing power of the cluster computers encourages for the full-core burnup calculations using Monte Carlo methodology. The problem of oscillations in depletion procedure for the spatially large models may be a serious barrier for the research and development teams. This motivated us for to study this topic and understand the problem and compare different solutions to overcome the modeling difficulties.

In the next section, we present the overview of depletion calculations. Section 'Methodology of time-step' shows the comparison of few selected time-step models for burnup procedure and discusses their features. In section 'System and geometry', the geometry of system based on HTGR is presented. Sections: 'Results without control rod presence' and 'Results with control rod movement' show the results of the simulations in terms of spatial stability without and with modeling of control rods. Finally, we present the summary of this work in the last section.

Aspects of burnup calculation theory

Monte Carlo burnup codes are advance tools for the analysis of nuclear reactors' fuel cycle. Depletion calculation requires analytical or numerical solution of Bateman equations that can be formulated as:

$$\frac{d\mathbf{N}(\bar{r},t)}{dt} = \mathbf{M}(\phi,T)\mathbf{N}(\bar{r},t) \tag{1}$$

where: **N** – isotopic composition of fuel volume, **M** – transmutation matrix, ϕ – neutron flux, T – local temperature, t – time. Transmutation matrix can be described by the following expression:

$$\mathbf{M}(\phi) = \int_0^\infty \phi(\bar{r},E,t)\chi(T)dE + \mathbf{D} \tag{2}$$

where: E – energy of incident neutron, χ – matrix combining cross sections and fission yield, **D** – decay matrix. Notice, that such formulation assumes neutron flux and temperature field to be constant. The formal solution of this system is called 'matrix exponential' [5]:

$$\mathbf{M}(\bar{r},t) = \exp\left[\mathbf{M}(\phi,T)\,(t-t_0)\right]\mathbf{N}_0(\bar{r}) \tag{3}$$

Different numerical and analytical methods have been developed to compute the result; it is useful to mention the most prominent methodology currently used [5]:
- Runge–Kutta–Gauss solution (RGK),
- Transmutation trajectory analysis (TTA),
- Chebyshew rational approximation method (CRAM).

In general, quantities such as ϕ and T are time dependent in nuclear system even in steady state. Neutron and thermal-hydraulic computation need repetitions to account for changes. So far, the strict Bateman solution for a system with time-dependent transmutation matrix does not exist. As a result, the burnup codes are forced to divide the fuel cycle into irradiation periods of constant physical properties. Monte Carlo simulation provides statistical solution of Boltzmann equation (B):

$$B\phi(\bar{r}) = \left[L(\mathbf{N},\mathbf{N}_c) - \frac{1}{k}F(\mathbf{N},\mathbf{N}_c)\right]\phi(\bar{r}) = 0 \tag{4}$$

where: **N** describes the isotopic composition of fuel and structures, $\mathbf{N}_c$ represents reactivity control nuclides (control rods, burnable poisons etc.), L stays for operator of migration and loss of neutrons at point $\boldsymbol{r}$, F represents fission neutron production operator and k is eigenvalue of the fundamental flux mode. The output of Monte Carlo method is used to compute the coefficients of transmutation matrix. Next, the Bateman solution is computed and applied for depletion period and step procedure is repeated until the end of fuel cycle (EOC).

The approach seems simple and flexible, because the user can adjust both number of time-steps and Monte Carlo statistics to find a compromise between required precision of results and computational effort. The prominent problem of this methodology is a choice of the effective coefficients for **M** matrix. One may ask, how to find the transmutation constants representative for entire step and how to obtain spatially stable burnup procedure.

Methodology of time-step

The models of time-step described in this section relate to continuous energy Monte Carlo burnup codes (in our case MCB5, [4]). Instead of tallying neutron flux in groups of energy, the reaction rates (***R***) are scored for each isotope and reaction together with heating rate per nuclide and per source neutron (h_{nuc}). The power balance procedure is invoked to obtain neutron source intensity (S) as a function of total power in system (P) and to calculate the coefficients of the transmutation matrix. Heating balance equation may be described briefly in the following way:

$$P_{\text{core}} = S \cdot h = S \cdot \sum_{j\in VOL}\sum_{i\in NUC} h^{ij}_{nuc} V_{ij} \rho^j_{AT} \tag{5}$$

The summation over burnable zones is indexed with j and nuclides are indexed with i. The sum contains atomic density of nuclides (ρ_{AT}), volumes of fuel cells (V_{ij}) and heating rate per nuclide and per source neutron (h^{ij}_{nuc}).

The exponential solution of Bateman equation is obtained with transmutation trajectory analysis (TTA). This method breaks the nonlinear chain of equations into set of linear chains, applies analytical solution and provides strict control of numerical truncation error. The scheme of staircase model (aka. beginning-of-step constant flux approximation or Euler predictor) is presented in Table 1.

As was shown in the literature, this method may exhibit spatially unstable burnup, especially for large, loosely coupled systems like LWR geometry

Table 1. The algorithm of staircase step model (based on [3])

input: $\mathbf{N}_0$

for $i \leftarrow 0,1,\ldots,$ *do*

$\mathbf{R}$, $\mathbf{h}_{nuc} \leftarrow$ Monte Carlo B($\mathbf{N}_i$)
$S \leftarrow S(\mathbf{N}_i, \mathbf{h}_{nuc}, \mathbf{P})$ power balance
$\mathbf{N}_{i+1} \leftarrow \mathbf{N}_i \exp[\mathbf{M}(\mathbf{R}, S)\Delta t_i]$

end for

(shown on the symmetrical assembly by J. Dufek *et al.* [1], also full core instabilities by A. Grisell [6]). Even for relatively short steps of few days, the profiles of neutron flux and power begin to oscillate. This problem originates from strong feedback between neutron flux and nuclide field (especially ^{135}Xe – the strongest known neutron absorber). It was shown, that a simple increase of Monte Carlo precision is not a solution. The physical reason for these problems is the unstable model of the system (lack of compensation rod control and thermal-hydraulic feedback in simplified cases).

Next, we present the slope-step model that takes correction for neutron source intensity variation during step (so as to provide correct burnup). The scheme is presented in Table 2.

The modification presented here is useful especially for long time-steps preferred in the context of fuel cycle calculations. What is important is that the increase of computation effort is negligible, because the additional neutron calculation is not required.

The concept of using effective quantities related to middle-of-step (MOS) can be extended also to reaction rates, as a better prediction of depletion

Table 2. The algorithm of slope-step model (BOS – beginning-of-step, EOS – end-of-step)

input: $\mathbf{N}_0$

for $i \leftarrow 0,1,\ldots,$ *do*

$\mathbf{R}$, $\mathbf{h}_{nuc} \leftarrow$ Monte Carlo $B(\mathbf{N}_i)$
S^{BOS}, $h \leftarrow S(\mathbf{N}_i, \mathbf{h}_{nuc}, \mathbf{P})$ power balance BOS
$\mathbf{N}_{i+1} \leftarrow \mathbf{N}_i \exp[\mathbf{M}(\mathbf{R}, S^{\mathrm{BOS}})\Delta t_i]$
S^{BOS}, $\Delta h \leftarrow S(\mathbf{N}_i, \mathbf{h}_{nuc}, \mathbf{P})$ power balance EOS
$\bar{S} \leftarrow S^{\mathrm{BOS}} [1 - (\Delta h/2) / (h + \Delta h)]$
$\mathbf{N}_{i+1} \leftarrow \mathbf{N}_i \exp[\mathbf{M}(\mathbf{R}, \bar{S})\Delta t_i]$

end for

Table 3. The algorithm of bridge scheme (explained in [2])

Input: $\mathbf{N}_0$

for $i \leftarrow 0,1,\ldots,$ *do*

$\mathbf{R}^{\mathrm{BOS}}$, $\mathbf{h}_{nuc}^{\mathrm{BOS}} \leftarrow$ Monte Carlo B($\mathbf{N}_i$)
$S^{\mathrm{BOS}} \leftarrow S(\mathbf{N}_i, \mathbf{h}_{nuc}^{\mathrm{BOS}}, \mathbf{P})$ power balance BOS
$\mathbf{N}_{i+1} \leftarrow \mathbf{N}_i \exp[\mathbf{M}(\mathbf{R}^{\mathrm{BOS}}, S^{\mathrm{BOS}})\Delta t_i]$
$\mathbf{R}^{\mathrm{EOS}}$, $\mathbf{h}_{nuc}^{\mathrm{EOS}} \leftarrow$ Monte Carlo $B(\mathbf{N}_{i+1})$
$S^{\mathrm{EOS}} \leftarrow S(\mathbf{N}_{i+1}, \mathbf{h}_{nuc}^{\mathrm{EOS}}, \mathbf{P})$ power balance EOS
$\bar{S} \leftarrow (S^{\mathrm{BOS}} + S^{\mathrm{EOS}}) / 2$
$\bar{\mathbf{R}} \leftarrow (\mathbf{R}^{\mathrm{BOS}} + \mathbf{R}^{\mathrm{EOS}}) / 2$
$\mathbf{N}_{i+1} \leftarrow \mathbf{N}_i \exp[\mathbf{M}(\bar{\mathbf{R}}, \bar{S})\Delta t_i]$

end for

Table 4. The algorithm of SIEM model with neutron source intensity renormalization adjusted to continuous energy Monte Carlo simulation (based on [3])

input: $\mathbf{N}_0$
$\mathbf{R}_0$, $\mathbf{h}_{nuc,0} \leftarrow B(\mathbf{N}_0)$ Monte Carlo
for $i \leftarrow 0,1,\ldots,$ *do*
$S^{\mathrm{BOS}} \leftarrow S(\mathbf{N}_i, \mathbf{h}_{nuc,i}, \mathbf{P})$ power balance BOS
$\mathbf{N}_{i+1}^{(0)}$ $\mathbf{N}_i \exp[\mathbf{M}(\mathbf{R}_i, S^{\mathrm{BOS}})\Delta t_i]$

for $n \leftarrow 1,2,\ldots,c$ *do*

$\mathbf{R}_{i+1}^{(n)}$, $\mathbf{h}_{nuc,i+1}^{(n)} \leftarrow B(\mathbf{N}_{i+1}^{(n)})$ Monte Carlo
$\bar{\mathbf{R}}_{i+1}^{(n)} \leftarrow \sum_{j=1}^{n} \mathbf{R}_{i+1}^{(j)} / n$

$S^{\mathrm{EOS}} \leftarrow S(\mathbf{N}_{i+1}, \bar{\mathbf{h}}_{nuc,i}^{(n)}, \mathbf{P})$ power balance EOS
$\bar{S}^{\mathrm{EOS}} \leftarrow S(^{\mathrm{BOS}} + S^{\mathrm{EOS}}) / 2$
$\mathbf{N}_{i+1}^{(n)} \leftarrow \mathbf{N}_i \exp[\mathbf{M}(\bar{\mathbf{R}}_{i+1}^{(n)}, \bar{S})\Delta t_i]$

end for

$\mathbf{N}_{i+1} \leftarrow \mathbf{N}_{i+1}^{(c)}$
$\mathbf{R}_{i+1}$, $\mathbf{h}_{nuc,i+1} \leftarrow \bar{\mathbf{R}}_{i+1}^{(c)}$, $\bar{\mathbf{h}}_{nuc,i+1}^{(c)}$

end for

SIEM: Stochastic implicit Euler method.

coefficients. Such approach was applied in PuMA project [2] and was called a bridge scheme. As a higher order step model, it requires one additional neutron calculation at each time-step. The scheme is shown in Table 3.

The bridge scheme was developed in order to provide a better approach to control rod withdrawal and fast variation of reaction rates in uncovered fresh fuel. Similar methods have already been discussed in the literature and tested for spatial stability of burnup procedure [7].

A large variety of higher order step models called predictor-corrector methodology has been proposed by multiple authors [1, 7]. The main feature of acceptable approach is unconditional spatial stability. We have chosen, so-called, stochastic implicit Euler method (SIEM, [3]) and adjusted it to our continuous energy version of Monte Carlo. The scheme can be found in Table 4.

In this work, both staircase model and SIEM were implemented and their performance was examined on the geometry described in the next section. What is important is that, in the second scheme, the effective neutron source intensity applied for burnup step was taken as average of values from the beginning- and end-of-step as more physically correct estimation. The explanation of such assumption is presented by the following equation:

$$P_{\mathrm{core}} = \frac{1}{\Delta t}\int S(t)h(t)dt \approx \frac{1}{2}\left(S^{\mathrm{BOS}} + S^{\mathrm{EOS}}\right)\bar{h}^{\mathrm{MOS}} \tag{6}$$

The impact of this modification is supposed to be visible, especially for long time-steps, where large variation of heating per source neutron (h) occurs.

System and geometry

The system considered in this work was a single fuel column of high temperature gas-cooled reac-

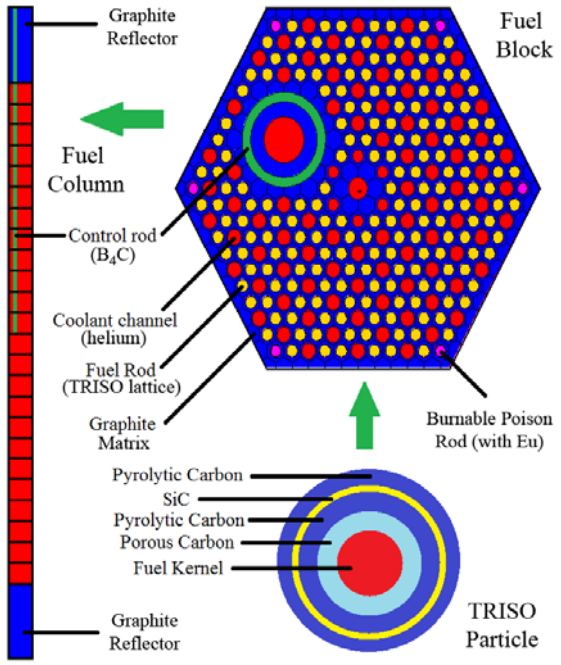

Fig. 1. The scheme of the system: fuel column (vertical section – left, horizontal section – top), structure of TRISO particle (bottom).

tor (HTGR), whose geometry was derived from the technical specification of PuMa project [2]. We chose such system in order to limit the possible phenomena of spatial oscillations to one dimension and facilitate the analysis and reduce the computation effort. Due to simplification of geometry, the results obtained in our simulations should be very cautiously extended to any full core calculations. Full double heterogeneity of the hexagonal prisms, included were lattice of TRISO particles. The reflective boundary condition was applied at XY sides of the hexagonal column. The void condition was used above top reflector and under bottom one. In order to understand better the burnup problems, the depletion simulations for different length and number of time-steps were performed both with and without realistic control rod movement modeling (stepwise withdrawal). The scheme of the system may be found in the Fig. 1.

The fuel comprised in the TRISO kernels was MOX with plutonium vector obtained from 41 GWD/t spent fuel of PWR. Active region was divided into 24 axial zones. The cross-section tables used for neutron transport simulations belong to JEFF2.2 library. The temperatures of the media were adjusted to 1500 K for the fuel, and 1200 K for graphite and rest of the components (burnable poison rods, helium coolant etc.). The power of the system was normalized to the average value per fuel column of 600 MW_{th} core.

Results without control rod presence

In this section, we present the results of burnup calculations, performed on the system without modeling of compensation rods. First, the performance of staircase step model will be compared for several

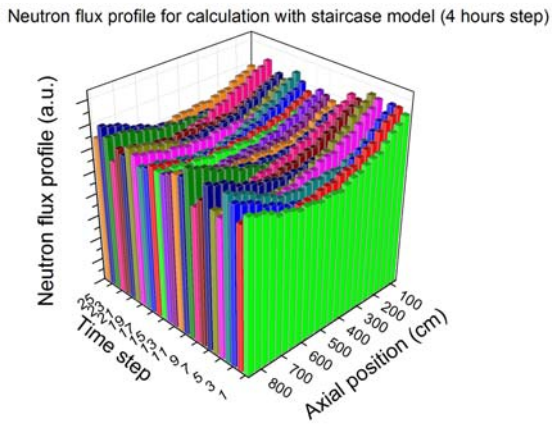

Fig. 2. The neutron flux profile for burnup calculation with staircase scheme and time-steps of 4 h.

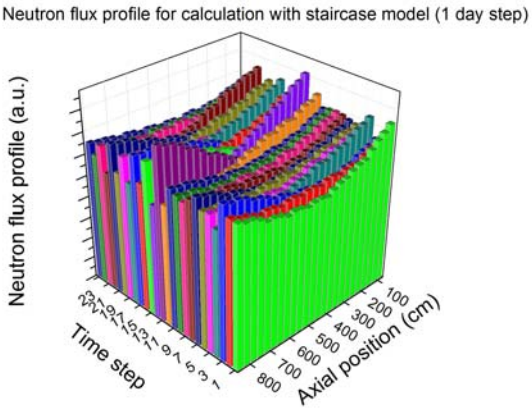

Fig. 3. The neutron flux profile for burnup calculation with staircase scheme and time-steps of 1 day.

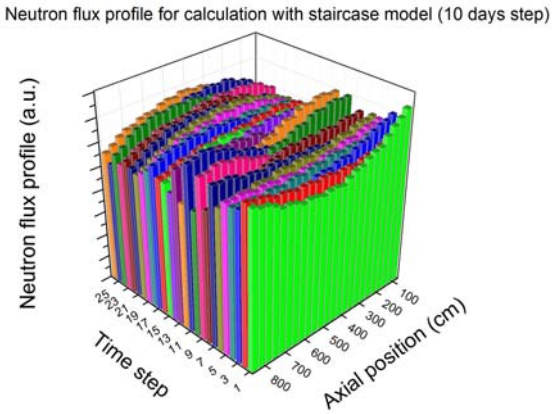

Fig. 4. The neutron flux profile for burnup calculation with staircase scheme and time-steps of 10 days.

lengths of time-step. Next, the work of the predictor-corrector model will be shown for comparison. All calculations in this section refer to Monte Carlo statistics of 10^7 particles simulated for each time-step.

The length of time-steps chosen for tests was 4 hours, 1 day, 10 days and 100 days. The stability of the burnup was monitored using flux profile; the results are presented in the Figs. 2–5.

Analysis of the figures brings information about two types of fluctuations. Statistical fluctuations are present for any step length, have limited amplitude and random behavior. As a result, it does not affect significantly the depletion procedure. On the other hand, for step length of 100 days, we can see

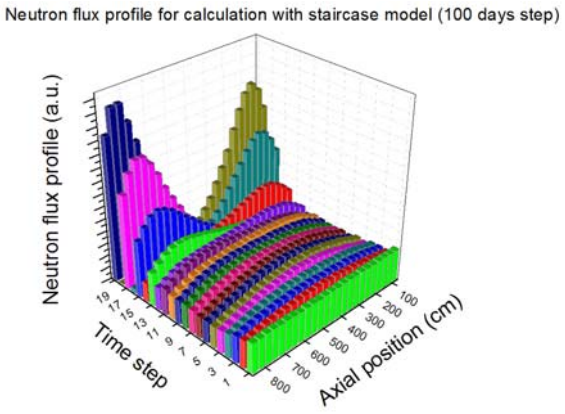

Fig. 5. The neutron flux profile for burnup calculation with staircase scheme and time-steps of 100 days.

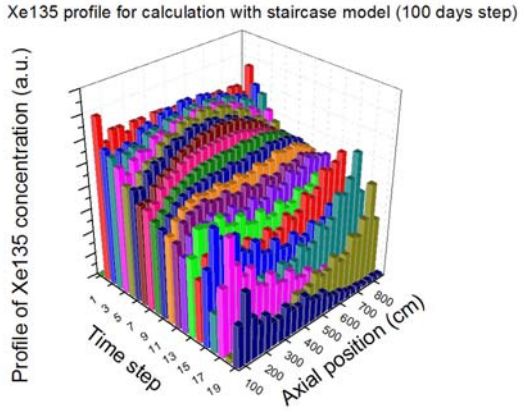

Fig. 6. The oscillations of ^{135}Xe concentration profile for burnup calculation with staircase scheme and time-step of 100 days.

the strong instabilities with increasing amplitude and strong coupling with ^{135}Xe concentration profile (see Fig. 6).

It seems that the burning out the neutron poison (^{151}Eu, ^{152}Eu) can be possibly correlated with the emerging of systematic oscillations of power profile. Figure 7 presents the consumption of burnable poison inside the system.

Complex geometry of HTGR system requires high number of simulated particles to reduce the statistical fluctuations of tallied quantities. The applied statistics (10^7 neutrons per step) appears to be insufficient. It underlines the computational difficulty in research and development for such kind of reactors with the Monte Carlo method.

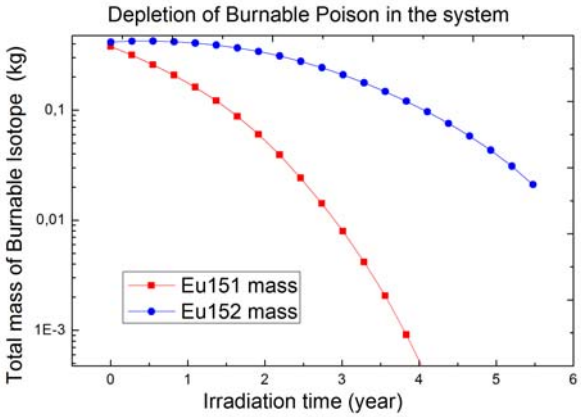

Fig. 7. The depletion of burnable poison in the system for burnup calculation with staircase scheme and time-step of 100 days.

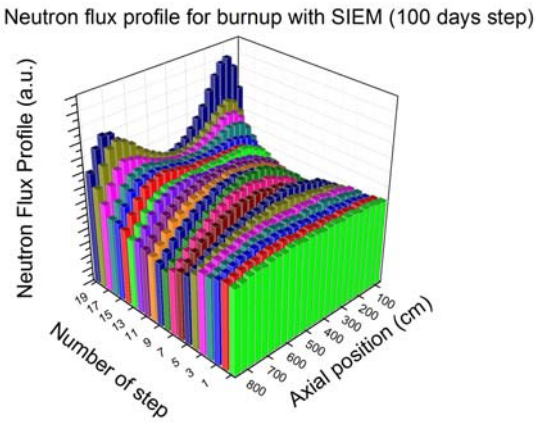

Fig. 8. The neutron flux profile for burnup calculation with stochastic implicit Euler method and time-step of 100 days.

However, the systematic oscillations are claimed to be dependent from the time-step model applied for Bateman solution. For comparison, we repeated the calculation with time-step of 100 days using the SIEM (that belongs to family of predictor-corrector schemes). We kept the number of simulated neutrons, but applied five iterations per time-step. The result is presented in Fig. 8 (different initial flux profile comes from lower burnable poison content).

The burnup seems to be stable up to about 1400 days of depletion. After this, the obtained shape of the flux (and other tallies like reaction rates) becomes symmetric but double peaked. Close investigation of corrector iterations for end-of-step quantities revealed that shape of flux does not converge to flat shape (see Fig. 9). However, it is not possible to state directly if such behavior is incorrect.

We observed the strong oscillations even between the iterations of corrector runs. Possibly, not sufficient precision of Monte Carlo or too low number of iterations can explain such a behavior. Of course, these oscillations are strongly coupled to the concentration of ^{135}Xe, which is able to dominate locally the neutron absorption in system. It seems that the problem lies in the fact that we neglect the

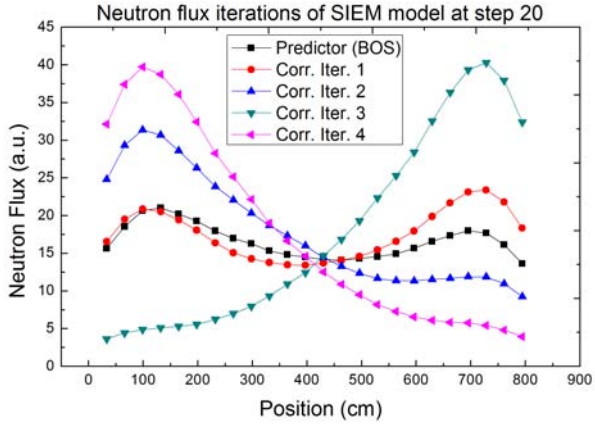

Fig. 9. The neutron flux profile for iterations of stochastic implicit Euler method model at time-step 20.

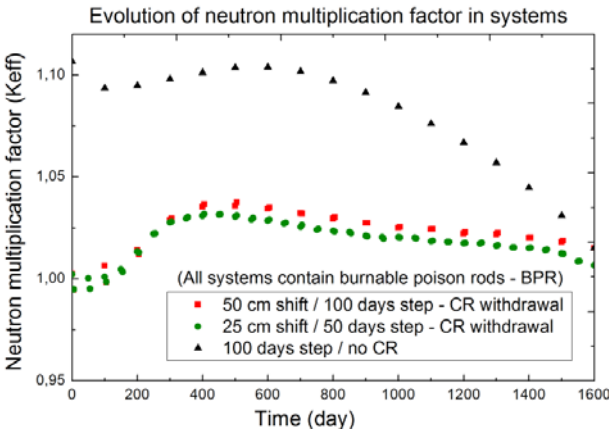

Fig. 10. Neutron multiplication factor in systems with and without control rod withdrawal (staircase model).

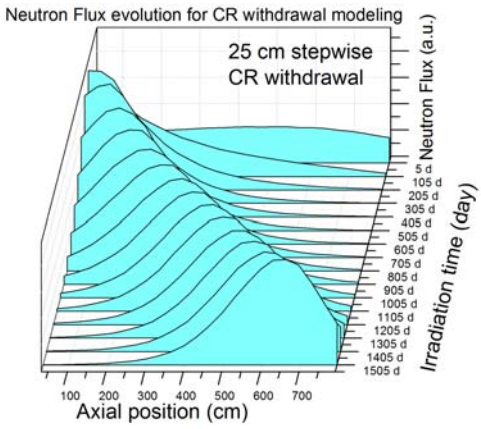

Fig. 12. Variation of the neutron flux profile for the system with 25-cm control rod withdrawal every 50 days.

variation of reaction rates inside the material during time-step (common assumption in burnup codes). The analyzed step of 100 days is much longer than 9.2 h half-life of strongest absorber in the system. As will be shown in the next section, the presence and withdrawal of compensation rods solve the problem of spatial instability in our system.

Results with control rod movement

The irradiation of 1600 days was performed for similar system, but with applied reactivity control with linear stepwise compensation rod withdrawal. The spatial model of rod was tested for two cases: 50 cm shift every 100 days and 25 cm shift every 50 days of irradiation. Additionally, after each shift of rod, short time-step of 5 days was applied for providing equilibrium profile of ^{135}Xe in system. Figure 10 shows the neutron multiplication factor evolution over time for both simulations with compensation rod modeling and calculation without reactivity control (for comparison).

The reactivity control allowed keeping the k_{eff} factor in the range of 0.99 and 1.04. As a preliminary approach to problem, such values are acceptable. The neutron flux profile evolution can be found in Figs. 11 and 12.

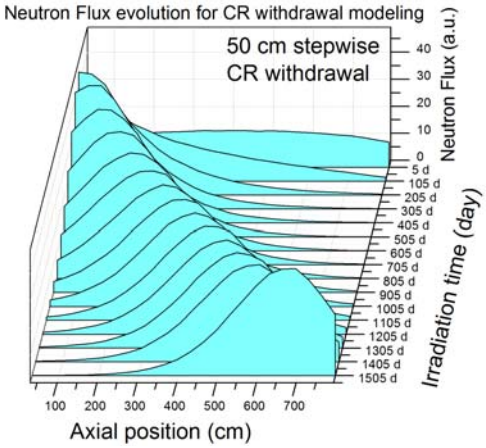

Fig. 11. Variation of the neutron flux profile for the system with 50-cm control rod withdrawal every 100 days.

The first and the most important information is lack of visible oscillation of power/flux profile. Closer examination of the profiles' evolution revealed that no significant change of peaking factor or spectra shape exists between two systems with different stepwise movement of control rod. Of course the evolution of fissile isotope concentration is totally different from case without compensation rods. The comparison is presented in the Figs. 13 and 14.

The presence of control rod introduces the asymmetry in the system. The peak of generated power

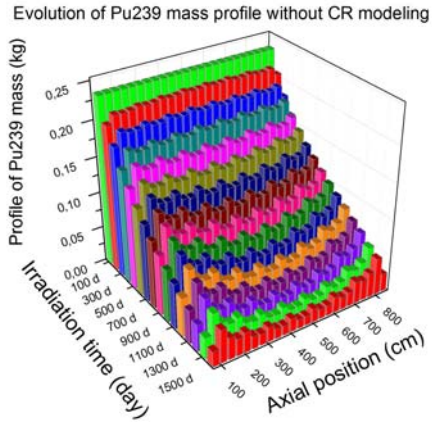

Fig. 13. Consumption of ^{239}Pu isotope in the system without control rod treatment.

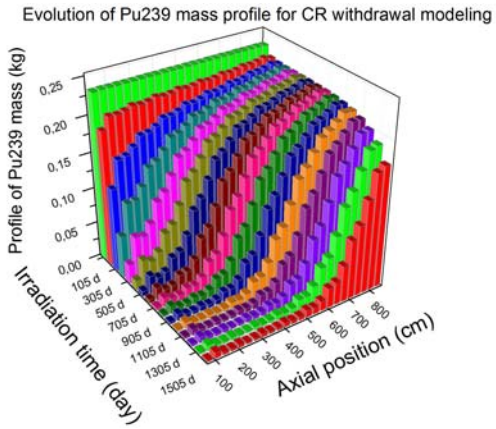

Fig. 14. Consumption of ^{239}Pu isotope in the system with control rod treatment.

stays close to the uncovered fresh fuel and shifts during the irradiation time. As we can see, the step toward realistic modeling of control rods brought the solution of instability problem. Of course the considered case is simplified and neglects, for example, the fuel batch shuffling (equilibrium cycle) and thermal feedback that provides the flattening of the power profile. However, it exposes the important aspects toward more precise and reliable reactor simulations and prediction of fuel cycle. We can refer here to the results of PuMa project [2], where full core equilibrium fuel cycle of HTGR were performed with the presence of control rod withdrawal and thermal-hydraulic coupling. No spatial instabilities were observed and burnup procedure remained at steady state equilibrium.

Summary and conclusions

The studies of simplified HTGR system with continuous energy Monte Carlo burnup code revealed the existence of burnup instability for such geometry. The statistical fluctuations of limited amplitude are visible for any considered step length in the range from 4 hours up to 100 days. The systematic instability of neutron flux profile coupled with ^{135}Xe concentration appears for depletion simulation with time-step of 100 days. Our explanation for this phenomenon is the neglect of the strong variation of reaction rates in burnable zones during steps much longer than absorber's half-life. In fact, ^{135}Xe (the strongest known neutron absorber) becomes the main feedback for the neutron transport in the Monte Carlo burnup simulation. Simplified models neglect other factors such as thermal-hydraulic feedback (impacts Doppler broadening in the fuel and neutron moderation in the graphite), which may have positive impact on the stability of depletion procedure. The presence of reactivity control via presence and withdrawal of compensation rods is a significant step toward reliable simulation and the physical impact on the computation is significant. The introduction of compensation rod modeling resulted in a stable and more realistic burnup simulation. The power peak follows uncovered fresh fuel and asymmetric system seems to be not prone to spatial oscillations. We found the simple control rod modeling a better approach than use of the predictor-corrector procedure or an increase of Monte Carlo precision.

It should be underlined, that Monte Carlo burnup simulations of thermal nuclear reactors (including HTGR) demand thorough analysis of stability. Comparison of power/neutron flux profile in the following time-steps seems to be sufficient for detection of oscillations in the depletion procedure. At present, the predictor-corrector methodology is recommended by many authors as a solution for providing stable simulation; however, these numerical schemes do not eliminate the origin of the problem, even if the results are stable.

Monte Carlo burnup methodology requires further research for estimating how much the instabilities are dependent on the model of the core itself. Especially, the full-core depletion simulations await numerical assessment of stability. Increasing efficiency of the supercomputers (clusters) have encouraged numerical tests and more advanced computations are in progress.

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