Introduction

Fuel cycle is a major part of service and maintenance of nuclear reactors. We distinguish several industrial processes such as mining, milling, conversion, purification, enrichment and fabrication, that refers to preparation of nuclear fuel before insertion inside core. On the other hand spent material undergoes treatments such as cooling, chemical reprocessing, recycling and disposal storage. Most of mentioned procedures requires complex transport procedures due to radioactive properties of nuclear materials. Logistics of reactor fuel is strictly connected with isotopic composition of material and total mass loaded into system. Computer simulation is the basic tool for precise reference information about fuel content before, during and after irradiation.

In the following paper, the problems of Monte-Carlo based burnup codes are presented on the example of typical PWR fuel assembly depletion. The stable solution of neutron transport problem and Bateman equations’ solution are necessary for precise estimations of time and space dependent material content. The stability of numerical algorithms is crucial for industrial applications and logistics profits from its development.

First two sections: Depletion Procedure and Existing Algorithms describe the physical and numerical apparatus of fuel depletion. Next section Simulated Systems presents the geometry and content of simulated systems. The Burnup Instabilities section shows typical problems encountered with common methodology and section New Algorithm shows preliminary results for new step model. The summary of the study and comment on helpfulness for logistics is presented in section Conclusions.

Depletion procedure

Burnup calculations for fuel in critical or subcritical nuclear systems bases on numerical or analytical solution of Bateman equations governing the isotopic evolution of the medium:

$$\frac{dN(\vec{r},t)}{dt} = M(\phi,T)N(\vec{r},t)$$  \hspace{1cm} (1)

where

$N_i$ – isotopic vector in considered volume at $i$-th time step,

$M$ – transmutation matrix dependent from particle (neutron) flux $\phi$ and local temperature $T$.

It can be written as

$$M(\phi) = \int_0^{\infty} \phi(\vec{r},E,t)\chi(T)dE + D$$  \hspace{1cm} (2)
The Bateman equation has formal solution:

\[ N(r,t) = N_0(r) \exp\left[ M(\phi, T)(t-t_0) \right] \]

(3)

however solution above requires, the neutron flux \( \phi \) at given point. The required quantity is provided by Boltzmann transport equation for critical system:

\[ B(\phi)(\vec{r}) = [L(N) - \frac{1}{k} F(N)]\phi(\vec{r}) = 0 \]

(4)

where \( B \) stays for shortened equation operator, \( L \) stays for operator of migration and loss of neutrons at \( r \) and \( F \) represents fission neutrons production operator. The variety of methods for point depletion exponential solutions [2] have been found. All calculations in this work are based on analytical solution of Bateman equation (Transmutation Trajectory Analysis), that bases on breaking non-linear chain of equations into set of linear chains [3]. Such method provides numerical error control and is relatively fast in computation cell-by-cell. In the presented work we consider performance of stochastic solution for fundamental flux mode (Monte-Carlo method). Currently used burnup codes work in so called point depletion mode. That means exponential solution for \( N \) and the Monte-Carlo run are repeated at each time step.

Approach presented above seems to be simple and reliable tool for burnup calculations. However, it suffers from two strong drawbacks: conditional spatial stability and assumption of beginning-of-step (BOS) constant flux approximation (aka. Staircase model).

The first drawback becomes apparent especially for nuclear systems with loosely coupled regions (LWR core, single fuel assembly). After several initial steps, the oscillation of neutron flux profile develops inside system. Such instability is strongly coupled with Xe\(_{135}\) concentration – the strongest known neutron absorber. The origin of this phenomena is stochastic mechanism of the Monte-Carlo simulation. Even for large number of neutron generations and particles per batch, random fluctuations occur and provide numerical seed for oscillations in following steps. As was shown in literature [1], this effect is especially inconvenient for systems without thermal-hydraulic (TH) feedback and without realistic control rods modeling. That means the modeled system is instable itself.

The second weakness of staircase model comes from the fact, that reaction rates per nuclide are not constant during step length. This results in bias in evolution of isotopic composition, especially for long time steps preferred for whole fuel cycle calculations.

In order to overcome these problems, the variety of advanced step models have been suggested in the literature [1]. Each of them requires at least one additional neutronics calculation as a penalty for better model. Interestingly, so called, \textit{Stochastic Implicit Euler Method} was diagnosed to provide stability of burnup irrespectively of time step length [4]. That is why it was chosen for closer examination in this work.

\textbf{Existing Algorithms}

Simple \textit{staircase} model can be described by simple scheme (Table 1). As it will be shown, this algorithm can cause non negligible burnup instabilities.
The stochastic implicit Euler method (SIEM) uses EOS neutron flux approximation to replace BOS constant flux approximation of staircase model. The neutronic calculation is repeated and results averaged at the EOS until convergence. The flux from EOS is later used as BOS depletion input. The scheme of this model was prepared by Dufek et al. (Table 2). This algorithm is supposed to be unconditionally stable and its performance was tested in simulations described in the following chapters.

Table 2. The algorithm of Stochastic Implicit Euler Method [4]

<table>
<thead>
<tr>
<th>i</th>
<th>( N_i^{(0)} )</th>
<th>( \phi_i )</th>
<th>( \phi_i^{(n)} )</th>
<th>( \bar{\phi}_i^{(n)} )</th>
<th>( N_i^{(c)} )</th>
<th>( \phi_i^{(c)} )</th>
<th>( N_{i+1} )</th>
<th>( \phi_{i+1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( N_0 )</td>
<td>( \phi_{B(N_0)} )</td>
<td>( \phi_{B(N_i)} )</td>
<td>( \sum_{j=1}^{n} \phi_{i+1}^{(j)} / n )</td>
<td>( N_i^{(c)} )</td>
<td>( \phi_i^{(c)} )</td>
<td>( N_{i+1} )</td>
<td>( \phi_{i+1} )</td>
</tr>
</tbody>
</table>

This algorithm basically does not indicate the type of the Monte-Carlo simulation for which it is dedicated. Especially in our case, the model scheme was adjusted for MCB5 methodology approach (Continuous Energy Monte-Carlo code). Because MCB5 does not automatically tally the neutron flux, the new procedure was converted to operate on natural quantities for this code: reaction rates \( R \), heating per nuclide \( H_{\text{nuc}} \) and power in zone \( P \).

Simulated Systems

The systems chosen for reference and comparison calculations were based on the fuel assembly of 17x17 fuel rods lattice, 25 rods replaced by guide tubes. The physical properties of the lattice are presented in Table 3.
Table 3. The characteristics of fuel assembly lattice used for burnup calculations

<table>
<thead>
<tr>
<th>Characteristics of fuel lattice</th>
<th>Value and unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel rod radius</td>
<td>0.41 cm</td>
</tr>
<tr>
<td>Uranium enrichment in fuel</td>
<td>3.5%</td>
</tr>
<tr>
<td>Fuel density (UO$_2$)</td>
<td>10.4 g/cm$^3$</td>
</tr>
<tr>
<td>Helium density in gap</td>
<td>0.00222 g/cm$^3$</td>
</tr>
<tr>
<td>Cladding inner radius</td>
<td>0.418 cm</td>
</tr>
<tr>
<td>Cladding outer radius</td>
<td>0.475 cm</td>
</tr>
<tr>
<td>Cladding density (Natural Zr)</td>
<td>6.57 g/cm$^3$</td>
</tr>
<tr>
<td>Density of moderator (H$_2$O)</td>
<td>0.712 g/cm$^3$</td>
</tr>
<tr>
<td>Lattice pitch</td>
<td>1.262 cm</td>
</tr>
<tr>
<td>Temperature of fuel</td>
<td>900 K</td>
</tr>
<tr>
<td>Temperature of cladding</td>
<td>700 K</td>
</tr>
<tr>
<td>Temperature of moderator</td>
<td>600 K</td>
</tr>
<tr>
<td>Reflector height (if concerns)</td>
<td>20 cm</td>
</tr>
<tr>
<td>Reflector density (homogenized H2O+PE16 steel)</td>
<td>2.825 g/cm$^3$</td>
</tr>
</tbody>
</table>

Source: Own work

Two types of geometry were used as an input for simulations (Fig. 1):
1) Fuel assembly (3.66 m total height, left picture) divided axially into 10 fuel zones with XYZ reflective boundary condition.
2) Planar lattice of assemblies (20 cm height, right picture) $N \times N$ cells (from 10 to 15). Reflective boundary condition for Z direction, void at XY boundary.

The considered geometry of assembly was prepared to visualize the spatial Xe$^{135}$ and flux oscillation, especially in Z-axis direction. Planar lattice of assemblies was designed to expose this phenomenon in XY-plane as well.

Source: own work
The cross-section tables used for all Monte-Carlo calculation refer to the JEFF3.1. Thermal collision tables were used for moderating media. Details of simulation settings will be given with the calculation results.

**The Burnup Instabilities**

In order to present and expose a problem of the spatial oscillation of burnup procedure, the depletion calculations were performed for 2 geometries described in previous chapter. The average generated power was fixed to 14MW\textsubscript{th} per nominal assembly length. The simulations were performed for various time step lengths, particle statistics and size of the system.

First, the numerical oscillations in 1-st type of system will be shown on Fig. 2, Fig. 3 and Fig. 4. The neutronic calculations with 5000 neutrons per generations were done in 400 inactive and 1600 active particle cycles. Point depletion calculus was done for time steps of 5 days. Full symmetry of the system should result in flat distribution of all measured quantities and characteristics of assembly.

![Fig. 2. The power in assembly zones at time steps (system 1, staircase step model)](source)

*Source: own work*

Strong, periodic oscillation of power profile is visible on the Fig. 2. Initial asymmetry increases with each step and results as value close to 0 at one axial end of assembly. Analogical behavior is present for neutron flux profile.

![Fig. 3. The concentration of Xe\textsuperscript{135} in zones at time steps (system 1, staircase step model)](source)

*Source: Own work*

Fig. 3 presents the shape of Xe\textsuperscript{135} distribution in axial zones. This strong neutron absorber decreases the value of power/flux in zones with higher concentration. Strong coupling with flux profile develops the oscillations in following steps of depletion.
The asymmetric burning of fissile isotope $^{235}$U inventory is shown on the Fig. 4. Such non-physical distribution comes from power oscillations and proves, that averaged impact of instabilities does no necessarily provide acceptable isotopic evolution.

In order to investigate the factors that impact the fluctuations, the parametrical studies were performed for similar system for different length of time steps, number of simulated neutrons and length of assembly. The results of such calculations is presented in the Table 4 below, the presence of oscillatory behavior is depicted.

<table>
<thead>
<tr>
<th>Step length</th>
<th>200 inactive/ 300 active neut. cycles</th>
<th>400 inactive/ 1600 active neut. cycles</th>
<th>Assembly height $h_0=3.66m$</th>
<th>Stability of burnup, 30days step</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 day</td>
<td>stable</td>
<td>stable</td>
<td>0.9$h_0$</td>
<td>oscillations</td>
</tr>
<tr>
<td>2 days</td>
<td>oscillations</td>
<td>oscillations</td>
<td>0.8$h_0$</td>
<td>oscillations</td>
</tr>
<tr>
<td>5 days</td>
<td>oscillations</td>
<td>oscillations</td>
<td>0.7$h_0$</td>
<td>oscillations</td>
</tr>
<tr>
<td>10 days</td>
<td>oscillations</td>
<td>oscillations</td>
<td>0.6$h_0$</td>
<td>stable</td>
</tr>
<tr>
<td>30 days</td>
<td>oscillations</td>
<td>oscillations</td>
<td>0.5$h_0$</td>
<td>stable</td>
</tr>
</tbody>
</table>

It seems, that for time steps longer than 1 day, the intensity of oscillations increases very quickly. Also the higher simulation precision does not bring visible reduction of oscillations (5000 particles/batch). Finally the occurrence of oscillations seems to be strongly correlated with the size of the system. Two shorter assemblies shows almost no oscillatory behavior for depletion steps of 30 days.

Similar simulation was performed for horizontal system 2) defined as slice of the square lattice of assemblies (Reflective Z and void XY boundaries). In this case, the oscillations were visible as well. The example of the unstable behavior can be found on the plots below (Fig. 5, Fig. 6, calculations refer to system of 15x15 assemblies, step length reaches 30 days).
The simulation was run for time steps of various length and number of fuel assemblies in square lattice. The examination of oscillation presence was done visually. The results are given in the following Table 5.

Table 5. Parametrical studies of burnup instabilities (system 2). “+” stays for stable and “-“ for unstable burnup

<table>
<thead>
<tr>
<th>simulation: 10000 neutrons per cycles, 300 inactive cycles, 700 active cycles</th>
<th>15x15 assemblies, different steps</th>
<th>30 days step, different size</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 day</td>
<td>5 days</td>
<td>10 days</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Source: Own work

The result of this parametrical study reveals, that 2D system is prone to instabilities just like 1D vertical single assembly. The obtained results are not final classification of stable and unstable systems, because Monte-Carlo approach bases on stochastic fluctuations, that are seed to begin oscillations and basically cannot be strictly predicted.

It is important to point out, that analogical instabilities were already observed even for full 3D core depletion calculations [5] with usage of staircase algorithm.
New Algorithm

In this chapter, the work and efficiency of the predictor-corrector model will be presented. The computation was performed for 1-st type of geometry: separate assembly.

Fig. 7 shows the comparison of burnup stability performance of staircase vs. SIEM model for 1-st system. The statistic of 5000 neutron per particle generation was applied. Staircase calculation used 200 inactive and 1000 active cycles per step, the SIEM model calculation used 200 inactive and 200 active cycles per iteration, 5 iterations per step were chosen. Time step increasing up to 60 days was adjusted for depletion.

Fig. 7. The power in zones at time steps (system 1, staircase-left and SIEM model-right)  
*Source: Own work*

The reduction of oscillations of power profile is visible on Fig. 7. As a result the oscillations of Xe135 profile were eliminated and isotopic content is depleted in correct way.

The impact of the predictor-corrector with EOS approach is clear and what is more the result was obtained with same amount of active neutron cycles.

Conclusions

The beginning-of-step constant flux approximation is not sufficient for modern point depletion calculations of nuclear fuel in reactor system. Spatial instability of burnup procedure exclude this method for large systems and simulations of fuel cycle with long time steps. The calculations confirm the existence of the problem for PWR geometry.

The *Stochastic Implicit Euler Method* was picked up as new step model and implemented in our Continuous Energy Monte-Carlo burnup code MCB5. The tests performed on the systems revealed, that such methodology provides stability of burnup procedure. The calculations for spatially large systems can be successfully performed.

The analyzed methodology is useful for the full core burnup calculation, that is helpful for a logistic planning of the reactor fuel cycle. Precise estimations of produced and consumed mass of isotopes is crucial for the transport and security issues in nuclear industry.

Abstract

In the paper we describe problems related to steady-state Monte-Carlo burnup calculations of nuclear fuel. The existence of power profile oscillations coupled with Xe$^{135}$ instabilities in LWR system was shown using code MCB5. The problem comes from instability of staircase point depletion algorithm applied to exponential solution of Bateman equations. The new methodology suggested in literature was implemented and tested. The results of calculations and efficiency of new model are important from
the point of view of fuel cycle analysis and nuclear fuel logistics. Precise information about production and consumption of mass of isotopes is desired for planning transport of radioactive materials.

**Keywords:** fuel logistics, material content, burnup simulation, step model, stability, nuclear reactor

**STABILNOŚĆ I DOKŁADNOŚĆ MODELI KROKU CZASOWEGO DLA OBLICZEŃ PRZEPAŁOWYCH JAKO ULEPSZENIE PRECYZJI I LOGISTYKI CYKLU PALIWA JĄDROWE-GO**

**Streszczenie**

W niniejszej pracy opisujemy problem związane z równowagowymi obliczeniami przepałowymi typu Monte-Carlo. Obecność oscylacji profilu mocy sprzężonych z niestabilnością $\text{Xe}^{135}$ w systemach lekko-wodnych została pokazana z użyciem kodu MCB5. Problem pochodzi z niestabilności schodkowego modelu kroku w użyciu do rozwiązań równań Batemana. Nowa metodologia sugerowana w literaturze została zaimplementowana i przetestowana. Wyniki obliczeń i efektywność nowego modelu są istotne z punktu widzenia analizy cyklu paliwowego i logistyki paliw jądrowych. Dokładna informacja o produkcji i konsumpcji izotopów jest cenna przy planowaniu transportu materialów promieniotwórczych.

**Słowa kluczowe:** logistyka paliw, schodkowy modelu kroku, stabilność, reaktor jądrowy, stabilność, obliczenia przepałowe

**References**


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