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Abstract. The paper concerns a transmutation of UO_2, MOX and ThO_2 fuels in the typical PWR geometry. The problem is solved by the linear chain method implemented in the MCB code. In the study, it was applied the novel trajectories period folding method which allows for tracking nuclide formation process for a whole fuel cycle. This approach aims to identify pathways for isotopes build-up during entire fuel evolution. The simulated system can be represented by a linear tree graph of all possible transmutation chains. The positions in a graph represent transmutation chain history while its values define the assigned transitions and passages. This model allows us to represent the evolution of nuclide field as a series of physically occurring nuclide transitions over the entire fuel irradiation time. It was used the tree graph approach together with the concept of network entropy as a characteristic measure of network topology. The Shannon entropy applied to the considered numerical problem is a measure of uncertainty and it was compared with the numerical uncertainties of nuclide field. The numerical uncertainties were obtained using the independent replica calculations, which allowed assessment of statistical error propagation in the considered model of the PWR fuel element.

1. Introduction

The depletion problem describes the evolution of the nuclide composition over time. The formation of new isotopes can take place due to a natural radioactive decay or due to nuclear reactions induced by neutrons (or other particles). The depletion problem is described by the first-order differential equations known as the Bateman equations. This problem can be solved by using the linear chain approach where linear chains represent series of physically occurring nuclide transitions. Transition chains preserve entire quantitative information about transmutation process. This solution allows us to represent the transmutations in physical meaning. In this work, it was used version of the linear chain approach obtained through the Transmutation Trajectory Analysis (TTA) method [1] and implemented in the MCB code [2]. The method develops an algorithm, which automatically forms analytical linear chains set with control of the chain extension process.

2. Motivation

One of the goals in fuel cycle design is to model nuclear reactor in a better description in uncertainties. For this consideration, reasonable identification and qualification of potential uncertainties derived from the experiment are of the same importance as the reliability of the model. Proper identification of uncertainties in computational calculations can be useful in qualification and experimental verification of neutronic calculations. Motivation behind introducing Shannon entropy [3] is performance preliminary step towards developing higher-order or hybrid uncertainty measure, which would be

beneficial in uncertainty measure of the Monte Carlo burnup calculation [4]. Therefore, the primary comparison between the function of uncertainty which is entropy [5] and uncertainties obtained directly from the comparison was examined.

3. The period folding methodology

Reaction rates in the depletion problem are time depended. However, the Bateman solution assumes constant reaction rates through the calculated period. Therefore, the only stepping solution allows us to find time-dependent behavior and enables us the quantitative interpretation of nuclides evolution. In this type of solution, the transmutation rates calculated in particular time step are used for calculation of the new material composition and then transmutation rates are not used any longer, yet they are overwritten by values of the next step. In doing so, there are no means of transmutation rate interpretation over analyzed fuel cycle. The transmutation vectors are calculated stepwise only.

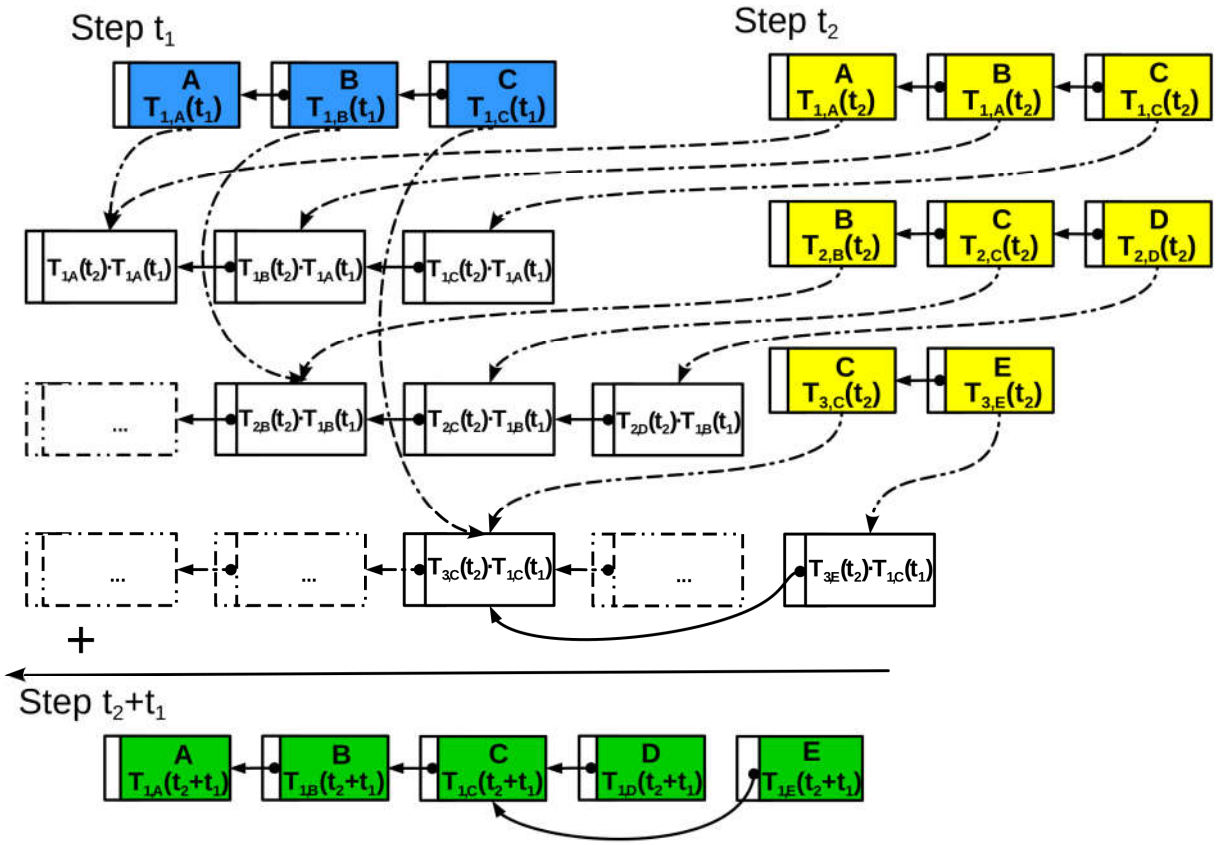

Figure 1. The graphical representation of the trajectory folding for the N-ary data structure.

The new method, the transmutation chain period folding allows for tracking nuclear trajectories, fold them in the time domain and then identifying physical pathways for isotopes buildup during entire fuel evolution [6]. The process of composed joint trajectory distribution is recursively repeated for each last step in the previously defined trajectory.

Linear chain approach together with the novel transmutation chain period folding is implemented and performed by the MCB code [2]. MCB store information of trajectory set in the implementation of the parent pointer tree data structure. Each initial nuclide chain family is attributed to one N-ary tree in which each node has a pointer to its parent node, but no pointers to child nodes. The structure stores nuclide index, transition and passage values of each chain. Moreover, the structures also contain information about generation number (i.e. length of the current chain or the tree level in the computer science nomenclature) or special position containing information about fission or particle emission.

The parent pointer tree structure is regarded as singly linked lists that each element is a tail of next chain represented by the last nuclide with its transition and passage value of the chain. The parent pointer tree data structure are used to implement the developed methodology for the trajectory folding procedure. The procedure is proceeds recursively in two steps approach (Figure 1).

4. Shannon entropy

Shannon entropy was introduced in the paper [7]. Entropy refers to disorder or uncertainty. There are many relationships established on the basis of the properties of entropy. In this work, it was used the assumption, that entropy is a measure of unpredictability of the state. Thanks to the period folding procedure, we exactly know how each share of initial nuclide transmutes in each trajectory. Therefore, we can treat this as model basing on informational theory holding transmitter (ancestor nuclides), channel (trajectories) and receiver (distribution at the end of computational step).

Entropy is zero when outcome is certain. This is starting position for calculation where all ancestor are defined well. With time new nuclides are produced and entropy increases with occurrences of more and more resulted nuclides. Shannon entropy quantifies disorder resulted from the increased number of trajectories. Growing value tells us about a large number of possibilities that initial nuclide can transmute. In Monte Carlo burnup calculations are connected with an increased chance of slightly different statistical distribution resulted from neutrons source convergence miscalculations. Every single run should have slightly different nuclide composition, which can be measured by standard deviation obtained from *n* independent runs. We guess that disorder is high when there is more possible different states and uncertainties grow. For a long computational time, more trajectories become resulted in fission event, which is no longer extended. The distribution of states and their probabilities is finite, thus entropy function with time should asymptotically approach to some value.

It was assumed, that the transition value describing each trajectory represent a stochastic process which defines the probability in which each ancestor nuclide transmute to the resulted nuclide $T_{i,j} = p_{i,j}$. It describes the transition rate from nuclide $i \to j$ through unique trajectory where $p_{i,j} \geq 0$ and $\sum_j p_{i,j} = 1$. For simplicity, we do not consider weighted entropy of the nuclide distribution. Each nuclide ancestor is treated separately. Therefore, the dynamical entropy of the distribution $[p_{i,1},\ldots,p_{i,N}]$ of each ancestor $H_i(t)$ is defined as follows:

$$H_i = -\sum_j p_{i,j} log\, p_{i,j}$$

where i is the ancestor index.

5. Description of the model

In this study, the popular model of the PWR fuel assembly based on the elementary PWR fuel derived from the standard Westinghouse PWR fuel assembly was used [8]. The model comprising the lattice of 17 x 17 rods and 25 rods replaced by guide tubes. Such model is sufficient for observing eventual systematic discrepancies of burnup procedure. Main physical properties of the model are presented in Table 1.

Table 1. Characteristics of the fuel assembly chosen for burnup calculations.

Physical feature of assembly	**Value and unit**
Radius of fuel pellet	0.41 cm
Density of fuel	10.4 g/cm^3
Density of helium in cladding gap	0.00222 g/cm^3
Inner radius of cladding	0.418 cm
Outer radius of cladding	0.475 cm
Inner radius of guide tube	0.555 cm
Outer radius of guide tube	0.616 cm
Density of cladding (Natural Zr)	6.57 g/cm^3
Density of moderator (H_2O)	0.712 g/cm^3
Lattice pitch	1.262 cm
Temperature of fuel (average)	900 K
Temperature of cladding (average)	600 K
Temperature of moderator (average)	600 K
Height of fuel pin	366 cm

The calculation considers three types of oxide ceramic fuel: UO_2, MOX and ThO_2. The fuel compositions are presented in Table 2.

Table 2. Characteristics of the initial fuel chosen for considered case.

UO_2	MOX	ThO_2
^{238}U - 96.5% ^{235}U - 3.5%	^{238}U - 92.0% ^{238}Pu - 0.2% ^{239}Pu - 4.36% ^{240}Pu - 2.016% ^{241}Pu - 0.792% ^{242}Pu - 0.632%	^{232}Th - 96.5% ^{233}U - 3.5%

The three-dimensional continuous-energy Monte Carlo reactor physics burn-up calculation code MCB is used for this study [2]. It includes state-of-the-art neutronics software and a point depletion module. It keeps track of the nuclide mixture for the user-defined depletion zones. In order to simplify analysis and avoidance nonlinear effect from neutron transport and burnup coupling, only single burnup zone is considered which set power density to 274.36 W/cm^3. A periodic boundary condition is used, setting up an infinite lattice of fuel elements for all three fuel cases. All necessary data are read from the JEFF-3.2 general purpose neutron data library. Each calculation uses 5,000 source neutron per batch, 20 inactive cycles and 200 active cycles. Time step length is 50 days. The calculation considers up to 1600 Full Power Days (FPD) in each case.

6. Results

The implementation of the MCB code is performed on the PROMETHEUS cluster [9]. The implementation of the transmutation chain period folding is performed by the parent pointer tree data structure. The offered method uses a transmutation calculation system that potentially involves hundredths of nuclides which can create even millions of different transmutation transitions. Presented examples follow each ancestor nuclide and develop its transmutation tree after each computational step. The calculation multiplication neutron factor was investigated first. It drops below one after: 950 FPD for UO_2; 1156 FPD for MOX; 1156 FPD for ThO_2. Results which exceed this period should be treated with greater attention as not physical.

6.1. Shannon entropy

The entropy was automatically calculated for each step based on trajectory's transitions obtained from the period folded methodology. Three cases using different initial fuel are presented in the Figure 2-4. Results from calculated entropy shows which nuclides lead to larger diversity of the resulted nuclides. Observations agree with the common knowledge, that fissile material faster than fertile material undergo fission and further transmutation. Also, plutonium fuel shows higher transmutation dynamic then ^{235}U or ^{233}U. ^{235}U and ^{233}U reach maximum, and after that, the value drops. This can be explained as follows: before maximum disorder grows, new trajectories are produced, survival of the ancestor also is decreased. After a certain point of maximum entropy, more transmutation trajectories results in fission, which value grows at the expense of remain trajectories in the transmutation chain. The same observation we can observe in the simplified case presenting decay of nuclide which consists of two following decay. At the beginning, all concentration is in the base state (the entropy is zero), after certain time period part of the nuclide decay into the intermediate state and following final state (the entropy grows and reach its maximum). In the next step, whole nuclide concentration will decay into its base state and entropy again will be zero (the probability to find nuclide will be maximum).

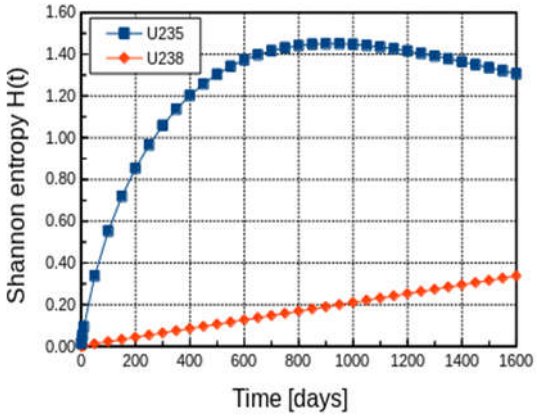

Figure 2. Shannon entropy change in function of time for UO_2 fuel.

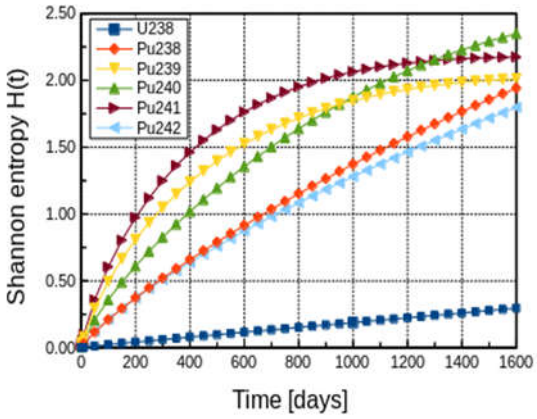

Figure 3. Shannon entropy change in function of time for MOX fuel.

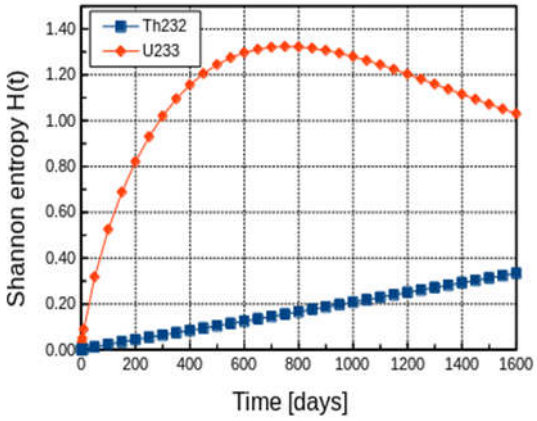

Figure 4. Shannon entropy change in function of time for ThO_2 fuel

6.2. Replica calculations

The Monte Carlo statistical uncertainties were obtained by using 50 independent replica calculations, which are used to assess statistical error propagation in the considered model of the PWR fuel element. Two cases were presented for UO_2 and MOX. Their results are presented in Figure 5 and Figure 6.

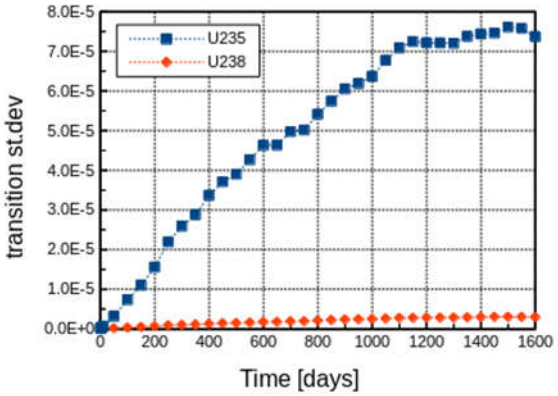

Figure 5. Uncertainty of total amount of trajectories ended with fission in function of time for UO_2 fuel.

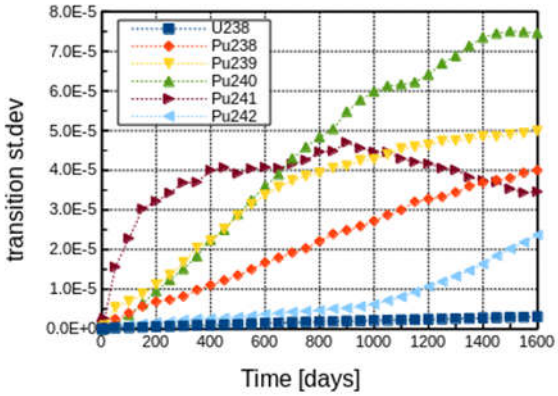

Figure 6. Uncertainty of total amount of trajectories ended with fission in function of time for MOX fuel.

The propagation of the statistical error is obtained by using total value of trajectories which undergo fission. Results were obtained separately for each ancestor nuclide. Similar results were observed for trajectories producing Minor Actinide nuclides. The numerical results provide interesting information: Presented trend lines show that uncertainties grow with time and stabilize dependent on the ancestor nuclide. The behavior of obtained standard deviation is strongly dependent on the considered ancestor nuclide.

7. Conclusions

Presented in this paper preliminary results are promising. They show the positive correlation between the Shannon Entropy and statistical uncertainties of the modeled system. The assumption that each slightly independent case obtained from replica calculation may differ, when disorder is growing is confirmed. However, obtained results, so far have not answered, if the Shannon entropy can be a quantification of uncertainty. Rather, we agree with the statement [5] that, Shannon entropy is a function of uncertainty. In this work, we addressed a novel application of entropy in research. Using period folded trajectories allows us to analyze burnup system with the tools originating from system analysis. This has to lead us to two questions: the first, whether burnup systems can be described in terms of probabilistic networks and the second question of how entropy can quantitatively describe uncertainties. Seeking answers to the above questions will be continued in future research taking into account spatial effects and usage a pathway heatmap.

Acknowledgments

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