Monte Carlo Study on Radial Burnup and Isotope Distribution

Cenxi Yuan, Shengli Chen and Xuming Wang

Abstract The radial distribution of the power, the isotope distributions, and other properties of the UO_2 and MOX fuel in the PWR are investigated with the increasing average burnup through the continuous-energy Monte Carlo code TRIPOLI-4. The local burnup phenomena mainly come from the high (n, γ) reaction rates of ^{238}U and ^{240}Pu near the surface of the fuel rod because of the self-shielding mechanism. The present Monte Carlo study shows that the local burnup and cumulative ^{239}Pu near the surface are much larger compared with those at the center of the fuel rod. The local burnup and the isotope distributions are investigated up to 45 MWd/kgU in UO_2 fuel and 84 MWd/kgU in MOX fuel.

Keywords Monte Carlo simulation · Burnup · Isotope distribution · UO_2 fuel · MOX fuel

1 Introduction

In a thermal reactor, the local burnup near the surface of the fuel rod is much higher than that at the center. The mechanical structure of the high burnup region near the surface of the fuel rod can be very different from that at the center. Many investigations are performed to understand the structure of the high burnup region [1–3]. The bubbles in the high burnup region, which are highly overpressurized [4], are formed by the fission fragments depending on the reaction rate [5]. It is important to study the radial burnup and the isotope distribution when the increment of average burnup is considered.

The theoretical calculations and simulations are very important in nuclear science. In the fundamental research, the binding energies, levels, electromagnetic moments and transitions, Gamow–Teller transitions, and other properties of the

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stable, extreme neutron- and proton-rich nuclei can be well described through the nuclear shell model, as shown in our previous works [6–8]. Because of the safety reason, the calculations and simulations are even more important in the nuclear reactor. Several of the models can be used to solve the present problem on the local burnup and the isotope distribution.

The most important origin of the high burnup near the surface is the (n, γ) reaction of the ^{238}U and ^{240}Pu. At the resonance region, the (n, γ) reaction rates of the ^{238}U and ^{240}Pu have certain large peaks [9], resulting in strong absorption of neutrons at certain energies. The moderator in the thermal reactor slows down the neutrons. If the slowed neutrons enter the fuel rods with those energies, they are almost all absorbed by the fuel near the surface, resulting in large production rate of ^{239}Pu and ^{241}Pu. The cumulated ^{239}Pu and ^{241}Pu near the surface correspond to the large local fission reaction rates and the burnup. In general, the other reactions induced by the slowed neutron have larger reaction rates near the surface, such as those of the (n, f) reactions of ^{235}U and ^{239}Pu, but not as obvious as the (n, γ) reaction of ^{238}U and ^{240}Pu.

Based on the origin of the local burnup, various models are suggested to obtain the numerical results on the local burnup and the isotope distributions, such as the TRANSURANUS [10–12], RAPID [13], and DIONISIO [14–16]. Our recent work suggested a simple formula based on approximately constant of the relative reaction rate [17].

In the present work, the single fuel rod with UO_2 and MOX fuel is simulated through the Monte Carlo (MC) code, TRIPOLI-4 [18]. After obtaining the reaction rates, the Bateman equation is solved by assuming the reaction rates do not change during a burnup step. The concentrations of next burnup level are thus got to be used as the next round simulation. Through such procedures, the local burnup and the isotope distributions are simulated up to certain burnup levels.

2   Description of Model

The present used MC code, TRIPOLI-4 developed by CEA, is a three-dimensional, continuous-energy code solving the Boltzmann equation based on the MC methods. The continuous-energy cross sections of the code are in ENDF format, from several evaluations, such as JEFF-3.1.1, ENDF/B-VII.0, JENDL4, and FENDL2.1.

The MC code simulates the reaction rates when the geometry sizes and the concentration of each isotope are given. The Bateman equation for each isotope can be solved by assuming the reaction rates do not change during time T:

$$\Delta N_i(r) = \left[-R_{a,i}(r) + R_{c,i+1}(r) \right] \Delta T,$$

where i is one kind of the nuclide and $i + 1$ is the nuclide which finally transforms to i in the reactor. If the nuclide i does not transform from other nuclei in the

reactor, there is no the term $R_{c,i+1}$ (r). $R_a(r)$ and $R_c(r)$ are the absorption and the captured reaction rates per unit volume at the radius r, respectively. $\Delta N(r)$ is the change in the concentration at the radius r during the time ΔT. The link between change in the average burnup ΔBU and the time duration ΔT is:

$$\Delta BU = Q\Delta T\Sigma R_{f,i}(r)/\rho,$$

where Q is the energy released per fission, $R_f(r)$ is the fission reaction rate per unit volume at the radius r, and ρ is the density of the fuel.

Through the MC simulations and the above equations, the local burnup and the isotope distributions can be obtained.

3   Calculation and Discussion

In the following discussion, one fuel rod model is used for the MC simulation. The size of the fuel rod is shown in the following figure.
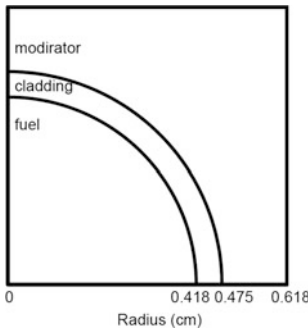

The simulations are based on three types of the fuel, UO_2, MOX with low and high Pu concentration. The enrichment of each isotope in the fuel is listed in the following table.

	UO_2	MOX_Low	MOX_High
^{235}U	3.3	0.24	0.226
^{238}U	96.7	95.562	89.975
^{238}Pu	0	0.063	0.147
^{239}Pu	0	2.528	5.9
^{240}PU	0	1.029	2.401
^{241}Pu	0	0.37	0.862
^{242}Pu	0	0.21	0.49

The MC simulations are based on the above geometry sizes and enrichment.

The local burnup of the UO_2 fuel is shown in the following figure. It is seen that the local burnup near the surface is around two times of that at the center, when the average burnup is 45 MWd/kgU. The phenomenon of the local burnup becomes obvious when the average burnup reaches 15 MWd/kgU.
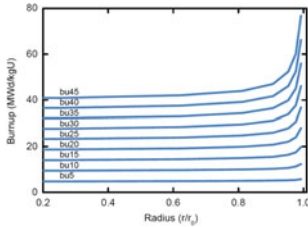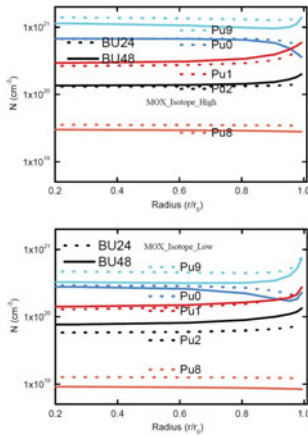

The following figure presents the isotope distribution of $^{235,236}U$, ^{237}Np, and $^{238,239,240,241,242}Pu$ at the average burnup 20 and 40 MWd/kgU. It is found that the concentration of ^{239}Pu is almost the same from 20 to 40 MWd/kgU burnup, which means that the production and cost of ^{239}Pu obtain a balance.
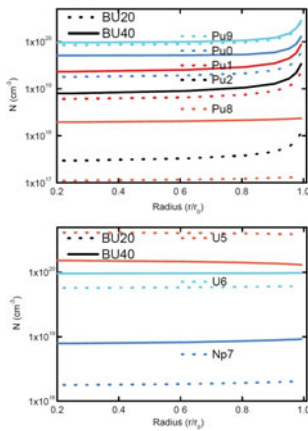

The local burnup of high and low concentration of MOX fuel is shown in the following figure. Generally speaking, the shape of the local burnup is more flat in the MOX fuel than that in the UO_2 fuel. The local burnup of the high-concentration MOX fuel has similar local burnup to that of the UO_2 fuel near the surface, two times of that at the center. The low-concentration MOX fuel has the larger local burnup near the surface, more than two times of that at the center.
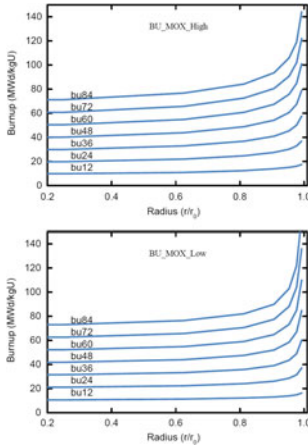
The Pu isotope distributions of the MOX fuel at the average burnup 24 and 48 MWd/kgU are presented in the following figure. The shapes of the isotope distributions of the MOX fuel are similar to those of the UO_2 fuel, except that of the ^{240}Pu. In the UO_2 fuel, all ^{240}Pu comes from ^{239}Pu. The shapes of their distributions are also similar to each other. But in the MOX fuel, the ^{240}Pu originally exists in the fuel rod, and the cost is larger than the production near the surface.

The *U* and *Np* isotope distributions of the MOX fuel at the average burnup 24 and 48 MWd/kgU are presented in the following figure. The shapes of the distribution of these isotopes are more or less the same between the UO_2 fuel and high- and low-concentration MOX fuel, but much smaller in the latter.
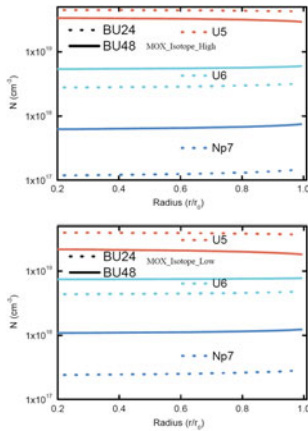
4   Conclusions

In summary, the local burnup and the isotope distribution of three types of the fuel are investigated through the MC simulation using TRIPOLI-4. The different results between the UO_2 and MOX fuel are shown, originated from the existence of Pu isotopes at the beginning in the latter.

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