

The development of a computer code for predicting fast reactor oxide fuel element thermal and mechanical behaviour (FIBER-Oxide)

Fuhai GAO¹ Qidong CHEN¹ Lubo WANG¹

¹China Institute of Atomic Energy (CIAE), Beijing, China

E-mail contact of main author: golfhigh@163.com

Abstract. The in-core behaviors of fast reactor oxide fuel element are highly complicated and coupled due to the overall irradiation, thermal and mechanical effects. The structural integrity of fuel cladding in steady and transient conditions is important for the safe operation of reactors. A computer code FIBER-Oxide is developed to simulate fuel element behavior and further to predict life. First, based on international open literatures, the main adopted material property models are presented. Second, according to solid heat transfer equation and mechanical equilibrium equation, numerical resolving equations for fuel pellet and cladding are derived and established. Finally, the general computation procedures are given and a sample is tested. The successful operation demonstrates the feasibility of adopted modeling methods. The future further development priorities for the code are also proposed. The development of FIBER-Oxide lays the foundation for the independent design of China fast reactor fuel element.

Key Words: fuel behavior; fuel; MOX; FIBER.

1. Introduction

FIBER-Oxide is developed to evaluate the mixed oxide (MOX) fuel performance under steady, transient conditions of sodium fast reactors. The characteristics for fast reactor fuel are fuel restructuring and high gas release ratio due to fuel use under high temperature. In order to treat these phenomena, fuel restructuring models were developed to determine centre void formation. For the gas release model, empirical relations are employed. This paper describes the models in FIBER-Oxide and the results of fuel pin performance analysis under steady state.

2. Physical models of FIBER-Oxide

2.1. Outline of FIBER-Oxide

The computer code for predicting fuel element thermal-mechanical behavior (FIBER) is a first Chinese independent-developed code for predicting fast reactor fuel element performance, which has thermal computation models for fuel and cladding, gap conductance models for fuel-cladding gap, fission gas release models and mechanical models for fuel and cladding. Main characteristics of FIBER are as follows: 6at.% burn-up, MOX fuel element with PuO₂ content ranges from 10 to 30% or UO₂ fuel, and two cladding materials : 316(Ti)SS and 15-15Ti.

The computation model for fuel element is usually divided into several segments in the axial direction. Each axial segment will be divided into some rings in radial direction. Axis-symmetry is assumed for thermal and mechanical analysis. For the analysis flow at each time

step, the fuel temperature calculation is conducted by considering heat generation, thermal conductivity. Following the temperature calculation, fission products swelling, fission gas release from pellet, the gas pressure in the fuel pin and fuel restructuring are evaluated. Figure 1 shows the analysis flow of the FIBER-Oxide code.

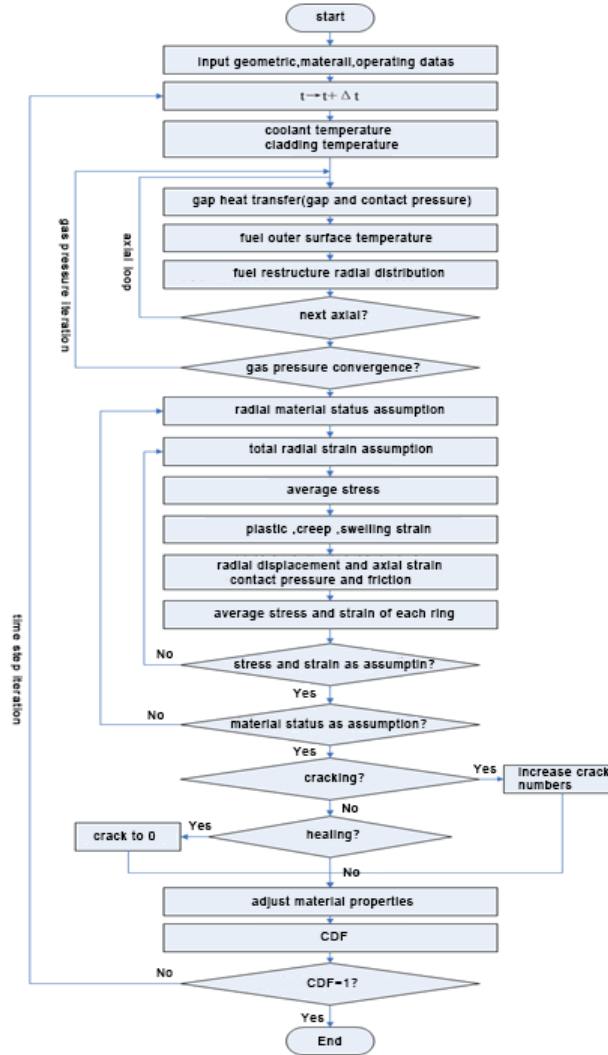


Figure. 1. Analysis flow

2.2. Thermal analysis model

2.2.1. Fuel thermal conductance model

The fuel thermal conductivity depends on the fuel temperature, composition, porosity and burnup^[1].

$$\lambda = K_{1d}K_{1p}K_{2p}K_{3x}K_{4r}\lambda_0$$

$$\lambda_0 = \frac{1}{0.06059 + 0.2754\sqrt{|2 - OM|} + 2.011 \times 10^{-4}T} + \frac{4.715 \times 10^9}{T^2} \exp\left(-\frac{16361}{T}\right)$$

$$K_{1d} = \left(\frac{1.09}{Bu^{3.265}} + \frac{0.0643}{\sqrt{Bu}} \sqrt{T} \right) \arctan \left(\frac{1}{\frac{1.09}{Bu^{3.265}} + \frac{0.0643}{\sqrt{Bu}} \sqrt{T}} \right)$$

$$K_{1p} = 1 + \frac{0.019Bu}{3 - 0.019Bu} \cdot \frac{1}{1 + \exp\left(-\frac{(T - 1200)}{100}\right)}$$

$$K_{2p} = 1 - \alpha_p \times P$$

$$K_{3x} = 1$$

$$K_{4r} = 1 - \frac{0.2}{1 + \exp\left(\frac{T - 900}{80}\right)}$$

Where OM : oxygen to metal ratio, Bu : burnup, α_p : porosity correction factor, P : porosity.

The modelling of oxygen radial redistribution and actinides radial redistribution is still in development.

2.2.2 Gap conductance model

A model applied in IAMBUS code^[2] is adopted in FIBER-Oxide. This model consists of three components: gas conductance; solid contact conduction through the cladding and pellet surface; radiation between cladding and pellet surface. It can evaluate the gap conductance under a gap width change with burnup during the steady state and with a contact force change during a transient.

$$h_g = \frac{k_{mix}}{\delta + l_{mix} + FRR(Ra_c + Ra_f)} + 0.85 \times 10^4 \tanh\left(\frac{P_c}{8.5 \times 10^6}\right)$$

$$+ \sigma \left(\frac{1}{\varepsilon_f} + \frac{r_f^2}{r_c^2} \left(\frac{1}{\varepsilon_c} - 1 \right) \right)^{-1} \frac{T_f^4 - T_c^4}{T_f - T_c}$$

Where k_{mix} : thermal conductivity of a gas mixture; δ : gap width; Ra_f, Ra_c : fuel and cladding surface roughness; FRR: correction factor for roughness values; P_c : contact pressure; σ : Stephan-Bolzman constant; r : radius; ε : emissivity; T: temperature.

The first term on the right of the equation is gas conductance in the gap, the second term is solid contact conductivity and the third term is the radiation contribution.

$$l_{mix} = \frac{15}{4} \times \frac{2 - 0.827 \times \alpha_{mix}}{\alpha_{mix}} \times L_m$$

$$L_m = \left(\sum_{s=1}^N C(s) \times L_0(s) \right) \times \frac{10^5}{P_{gas}} \times \frac{1 + \frac{S_{mix}}{273}}{1 + \frac{S_{mix}}{T}} \times \left(\frac{T}{273} \right)$$

Where L_0 : mean free path of gas at 0 °C and 1 bar, P_{gas} : gas pressure, C : molar fraction of gas.

$$\alpha_{mix} = \frac{\sum_{s=1}^N (C(s) \times \alpha(s) / \sqrt{M(s)})}{\sum_{i=1}^N (C(s) / \sqrt{M(s)})}$$

$$S_{mix} = \sum_{s=1}^N C(s) \times S(s)$$

Where α : harmonic mean taken from the accommodation coefficients of both surfaces, S: Sutherland's constant, M: molecular weight of gas.

2.2.3 Fuel material migration model

A central hole is formed by pore migration and pores are transported by vapor transportation from high temperature region to a cold region^[3].

$$\frac{\partial P}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (rv_p P)$$

$$P(r, 0) = P_0$$

$$\frac{P_i^{n+1} - P_i^n}{\Delta t} = \frac{1}{r_i} \frac{(rv_p P)_{i+1 \rightarrow i} - (rv_p P)_{i \rightarrow i-1}}{2\Delta r}$$

Where P: porosity; r: radius; v_p : pore migration velocity;

2.2.4 Swelling models and Fission gas release models

As for gas swelling model and gas release models, the empirical correlations are adopted in FIBER-OXIDE.

Fission product swelling:

$$S = 7.435 \times 10^{-13} f_{dens} \times \Delta Bu$$

Where f_{dens} : fuel initial density; Bu : Burnup.

Fission gas swelling^[4]:

$$S_g = 2.617 \times 10^{-39} \times f_{dens} \times \Delta Bu \times (2800 - T)^{11.73} e^{-0.0162(2800-T) - 2.4 \times 10^{-10} Bu \times f_{dens}}$$

Fission gas release ratio^[2]:

$$FGR = \begin{cases} \frac{1}{2} \times \frac{Bu}{Bu_K}, & Bu \leq Bu_K \\ 1 - \frac{1}{2} \times \frac{Bu_K}{Bu}, & Bu > Bu_K \end{cases}$$

$$Bu_K = \begin{cases} 8.0 \times \exp \left[7500 \times \left(\frac{1}{T} - \frac{1}{1273} \right) \right], & T > 1273 \\ 8.0, & T \leq 1273 \end{cases}$$

Where Bu_K : burn-up at which the fission gas incorporated within the fuel is dynamically saturated;

2.3. Mechanical model

2.3.1. Relocation

Fuel pellet cracking and relocation^[5] significantly influences the fuel pin performance particularly at the beginning of life. The following empirical correlation is adopted in FIBER-OXIDE.

$$\Delta = \frac{0.444 \times 10^3 R_{ci} \delta - 45 \times 10^{-6}}{2}$$

Where R_{ci} : the inner radius of cladding(m); δ : gap width in hot state(m). Δ : relocation radial displacement in considered slice(m).

2.3.2. Cladding Swelling model

$$\frac{\Delta V}{V} = \begin{cases} 0, & DPA < D_0(T) \\ \frac{A(T)}{100} \times [DPA - D_0(T)], & DPA \geq D_0(T) \end{cases}$$

Where DPA: neutron damage dpa; T: temperature; A(T) and $D_0(T)$: swelling rate (dpa^{-1}) and incubation dose for swelling (dpa). $A(T)=0.4$, $D_0(T) = 54$. The swelling strain:

$$\varepsilon^S = \frac{1}{3} \times \left(\frac{\Delta V}{V} \right)$$

2.3.3. Creep model

$$\frac{\Delta \varepsilon_{eq}^{irr}}{\sigma_{eq}} = 1.1 \cdot 10^{-6} \cdot \Delta D + 1.2 \cdot 10^{-2} \cdot \Delta \varepsilon^S$$

Where σ_{eq} : equivalent stress(MPa); $\Delta \varepsilon_{eq}^{irr}$: equivalent strain increment; ΔD : DPA increment; $\Delta \varepsilon^S$: swelling strain increment.

2.3.4. Cladding thermal expansion model

$$\varepsilon^T = (T - 20)(1.68 \cdot 10^{-5} + 3.36 \cdot 10^{-9}(T - 20))$$

3 Numerical methods for thermal and mechanical analysis

3.1 Numerical methods for thermal module

Energy balance principle is used to construct steady state equations. It's also assumed that all the fission heat is deposited in the fuel. Figure 2 shows the generic radial nodes for the fuel, gap and cladding regions.

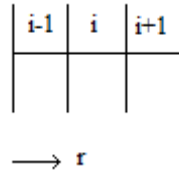


Figure. 2. Radial discretization nodes

$$\frac{T_{i-1} - T_i}{\frac{1}{2\pi k_{i-1,i}} \ln \frac{r_i}{r_{i-1}}} + \frac{T_{i+1} - T_i}{\frac{1}{2\pi k_{i,i+1}} \ln \frac{r_{i+1}}{r_i}} + q_i'' A_i = 0$$

T_i : Temperature of node-i

T_{i-1} : Temperature of node-(i-1)

$k_{i-1,i}$: Thermal conductivity between node-(i-1) and node-i

q_i''' : Heat generation rate

A_i : Cross-sectional area of the radial node-i

3.2 Numerical methods for mechanical module

The mechanical analysis module of FIBER-Oxide adopts the LIFE algorithm with a 1.5D models. It is assumed that the thermal, swelling and permanent strains are constant within each ring. The radial displacement “u” is acquired by integrating from the inner boundary of the i-th radial zone (r_{ai}) to radial position “r” within the ring.

$$u(r) = \frac{C_{1i}}{r} + C_{2i}r + \left(\frac{1+\nu}{1-\nu} \right) \left[\alpha_i (T - T_o)_i + (\varepsilon^s)_i \right] \frac{r^2 - r_{ai}^2}{2r} \\ + \frac{1}{2} \left(\frac{1-2\nu}{1-\nu} \right) \left\{ \left[(\varepsilon_r^c)_i + (\varepsilon_\theta^c)_i \right] \frac{r^2 - r_{ai}^2}{2r} + \left[(\varepsilon_r^c)_i - (\varepsilon_\theta^c)_i \right] r \ln \frac{r}{r_{ai}} \right\}$$

Where C_{1i} and C_{2i} are constants of integration for the i-th ring which remain to be determined, α the linear thermal-expansion coefficient, ν Poisson’s ratio, ε^s the swelling strains and ε^c creep/plastic strains.

The stresses are expressed in terms of the radial displacement,

$$\sigma_r = \frac{E}{1+\nu} \left[\frac{du}{dr} + \frac{\nu}{1-2\nu} \left(\frac{du}{dr} + \frac{u}{r} + \varepsilon_z - 3\alpha(T - T_o) - 3\varepsilon^s \right) - (\alpha(T - T_o) + \varepsilon^s + \varepsilon_r^c) \right] \\ \sigma_\theta = \frac{E}{1+\nu} \left[\frac{u}{r} + \frac{\nu}{1-2\nu} \left(\frac{du}{dr} + \frac{u}{r} + \varepsilon_z - 3\alpha(T - T_o) - 3\varepsilon^s \right) - (\alpha(T - T_o) + \varepsilon^s + \varepsilon_\theta^c) \right] \\ \sigma_z = \frac{E}{1+\nu} \left[\varepsilon_z + \frac{\nu}{1-2\nu} \left(\frac{du}{dr} + \frac{u}{r} + \varepsilon_z - 3\alpha(T - T_o) - 3\varepsilon^s \right) - (\alpha(T - T_o) + \varepsilon^s + \varepsilon_z^c) \right]$$

Combining the boundary conditions and axial force balance, the displacement u(r) can be determined.

3. Analysis results by FIBER-Oxide

3.1 Outline of CEFR MOX

The structure design of CEFR MOX element is showed in Table 1 and Figure 3.

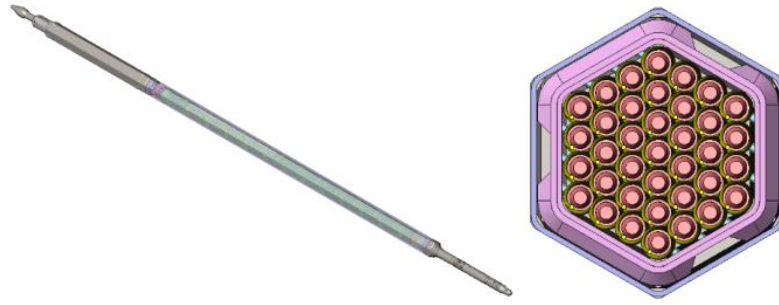


Figure. 3. CEFR MOX Assembly

Table. 1. structure design of MOX fuel element

Design parameters	Value
Outer and inner diameters of fuel pin $D_o \times D_i$, mm	6.0×5.24
Diameter of spacer wire, mm	0.95
Outer diameter (D_o) of fuel pellet, mm	4.86
Center hole diameter (D_i) of fuel pellet, mm	1.6
Pellet diameter of blanket, mm	4.86
Gap between pellet and cladding, mm	0.190
Height of plenum (down), mm	450
Overall length of pin, mm	1345

3.2 Analysis conditions

We have used FIBER to do some analytical evaluations of MOX fuel elements. The input parameters of other information are showed in Table 2.

Table. 2. Input parameters

Input parameters	Value
Inlet temperature , °C	360
Peak linear power , W/cm	430
Flow speed , m/s	4.3
Peak burnup	6at%
DPA	30dpa

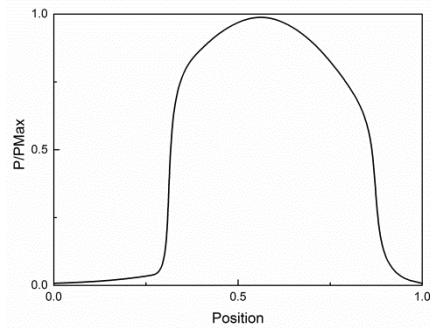


Figure 4. Axial Power Distribution

3.3 Analysis of steady state performance

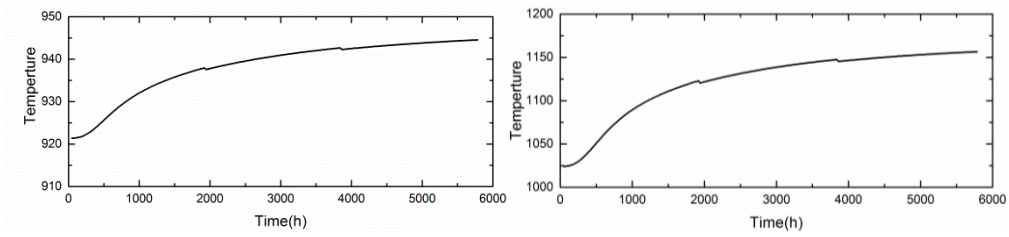


Figure 5 Upper Breeder Zone Center Temperature

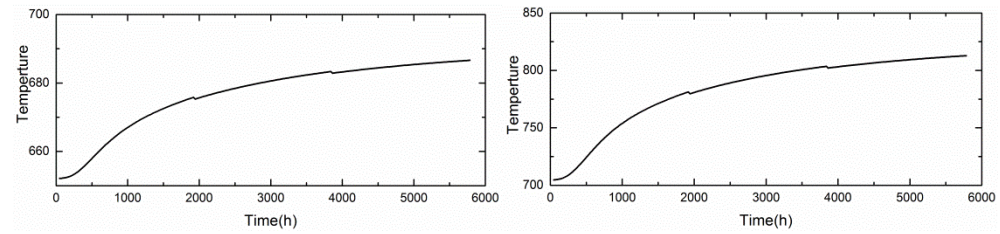


Figure 6. Low Breeder Zone Center Temperature

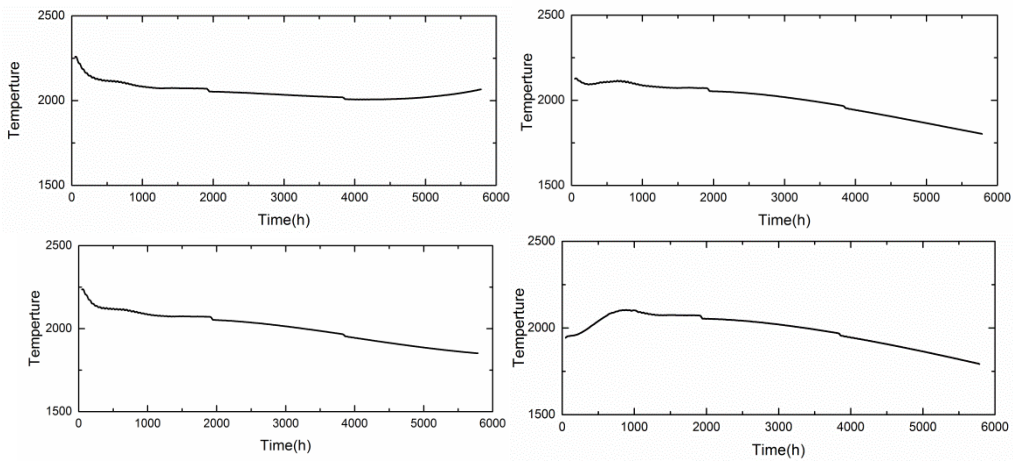


Figure 7. Active Zone Center temperature

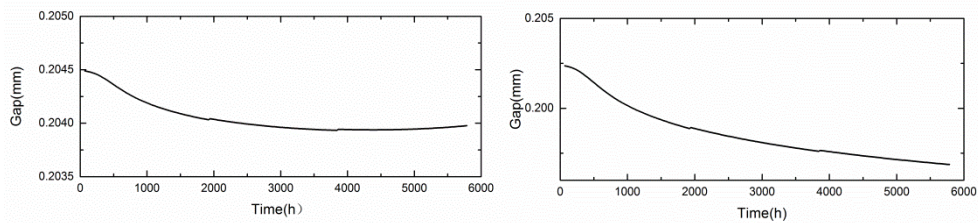


Figure 8. Upper Breeder Zone Gap

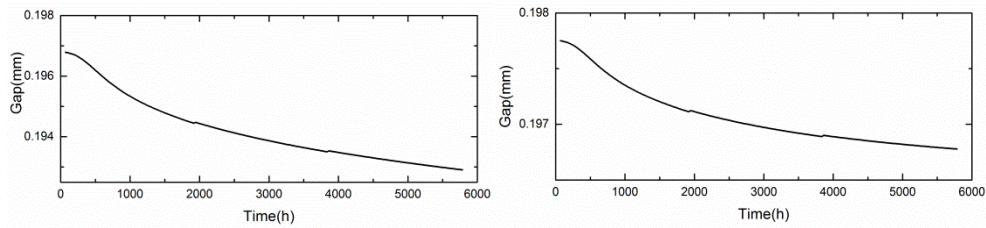


Figure 9. Low Breeder Zone Gap

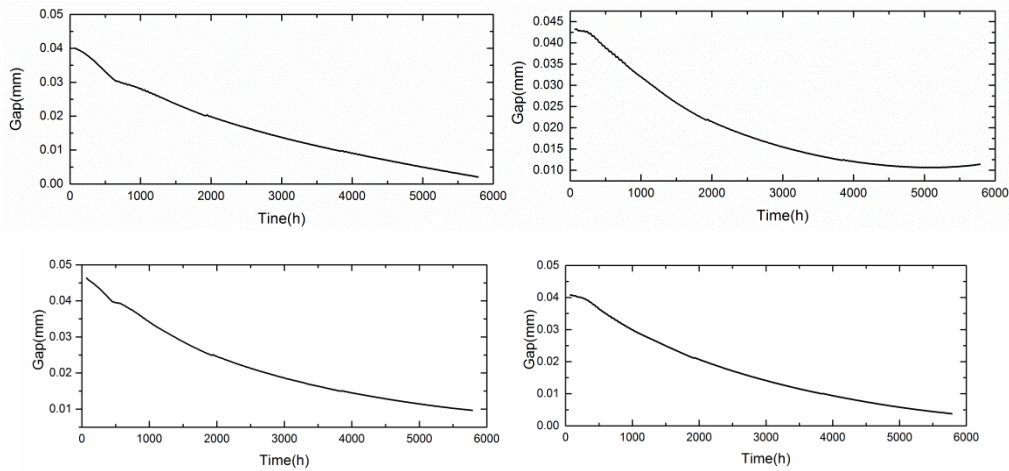


Figure 10. Active Zone Gap

Figure 5 to 7 shows the history of center temperature during irradiation in upper breeder zone low breeder zone and active zone. The pairs of curves in upper breeder zone and low breeder zone correspond to the extremities of each zone. The four curves in active zone correspond to the four axial sections near the center position. The maximum temperature occurred at the center keep increasing as the burn-up rises in breeder zone. The center temperature in active zone decreases with increasing burn-up. The evolutions of the center temperature in active zone at the beginning are affected by the pore migration. The different temperature history of breeder and active zone is due to the relocation and higher swelling ratio in active zone.

Figure 8 to 10 shows gap size(mm) during steady state. Gaps decrease with increasing burn-up due to relocation, thermal expansion, swelling of pellet.

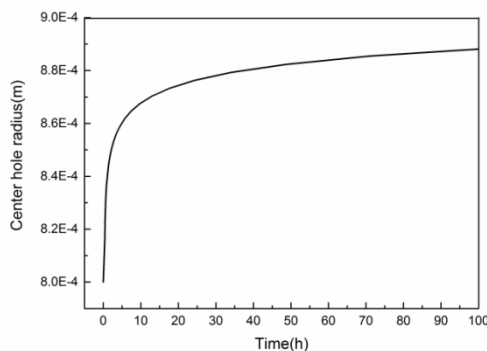


Figure 11. Central void radius

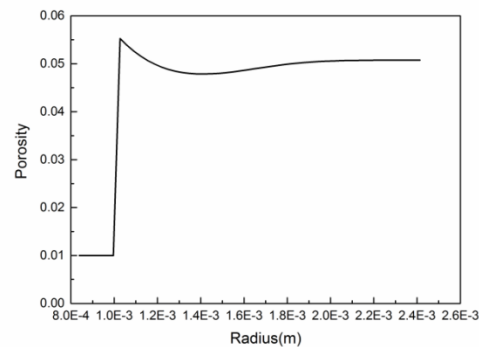


Figure 12. Porosity

Figure 11 shows the evolution of central void radius near the center position in the first 100 hours irradiation. Figure 12 show the radial distribution of porosity after irradiation for one hour. The correctness of pore migration still needs to be verified in the future work.

4. Conclusion

FIBER-oxide has capabilities for evaluating the fuel performance under steady conditions. FIBER-oxide can model the performances of central void formation, fuel restructuring caused by the high temperature gradient, the stress-strain state for fuel and cladding.

For future development, further verification and test validation are needed to conduct to improve the accuracy of FIBER-oxide.

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