A method for 3D simulation of internal gas effects on thermal-mechanical behaviors in nuclear fuel elements

JIANG Yijie CUI Yi HUO Yongzhong DING Shurong*

Department of Mechanics and Engineering Science, Fudan University, Shanghai 200433, China

Abstract A new method for three-dimensional simulation of the interaction between the gas and the solid around is developed. The effects of the gas on the thermal-mechanical behaviors within the surrounded solid are performed by replacing the internal gas with an equivalent solid in the modeling, which can make it convenient to simulate the thermal-mechanical coupling effects in the solid research objects with gases in them. The applied thermal expansion coefficient, Young's modulus and Poisson's ratio of the equivalent solid material are derived. A series of tests have been conducted; and the proposed equivalent solid method to simulate the gas effects is validated.

Key words Gas conductivity, Gas pressure, Equivalent solid method, Numerical simulation, Nuclear fuel elements, Thermal-mechanical behaviors, Fission gas release

1 Introduction

Nuclear fuel rods consist of UO_2 pellets and Zircaloy cladding, with the fuel-cladding gap being filled with a thin layer of helium gas to improve heat conduction. The cladding is the first containment barrier for fission products, but the pellet-cladding interaction (PCI) may induce large stresses in the fuel pellets and cladding, hence the fuel rod failure of bamboo effect[1-4] (Fig.1). It is therefore necessary to have a better understanding of the thermal-mechanical behaviors and to increase burnup of the nuclear fuel, so as to prevent PCI failure.

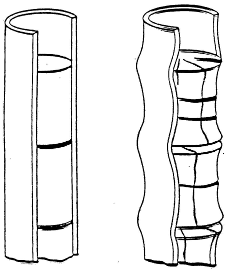

Fig.1 Bamboo effect.

While an irradiation test costs much time and money, the finite element method has been widely used for design optimization and analysis of the damage mechanism, with one-dimensional model[5], two-dimensional axisymmetric model[2,3] (Fig.2) and two-dimensional plane strain model[1,6] (Fig.3). And 3D finite element modeling has recently appeared, with improved simulation precision[7,8].

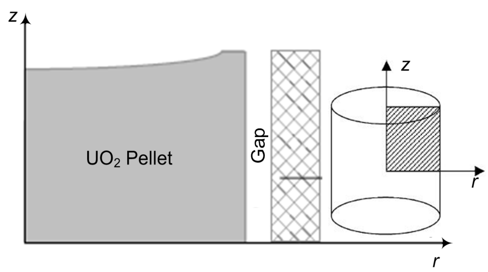

Fig.2 2D axisymmetric model.

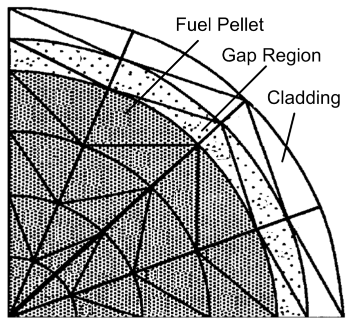

Fig.3 2D plane strain model.

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* Corresponding author. *E-mail address:* dsr1971@163.com

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With increasing burnup of the UO_2 fuel, the gaseous fission products may well be released into the fuel-cladding gap, hence considerable changes happen in thermal conductivities and gas pressure within the gap. The temperature and mechanical changes can affect the fuel pellet and cladding. The gas effects can be studied with constraint equations[2], which connect the pellet outer surface temperatures with temperatures of the cladding inner surface, and the mechanical impact on the materials can be studied by applying uniformly distributed pressures. Feltus M A[6] investigated the gas gap problem by assuming it as a conductive solid material. Recently, in studying thermal-mechanical behaviors in the monolithic nuclear fuel element, the interfacial flaw with gas in it was modeled as the filled solid material with negligible structural stiffness and with the same thermal conductivity as the gas[9]. This is a convenient way to simulate thermal properties of the gas. However, it is necessary to consider the effect of increased gas pressure, as gaseous fission products release continuously into the gap. The method of simulating the gas pressure shall be developed using the conductive solid material.

In this paper, based on precise elastic theory, a new equivalent solid method to model both the thermal and mechanical effects of the gas is proposed. The adopted material coefficients of the equivalent solid are deduced and effectiveness of this method is confirmed. It is used in 3D simulation of the thermal-mechanical behaviors in the nuclear fuel rod; and the results agree with those obtained with a usual method.

2 Equivalent solid simulation of gas effects

With the release of gaseous fission products, pellet deformations and cracks will appear. The phenomena make it difficult to calculate and analyze the gas effects on thermal-mechanical behaviors in the pellets and cladding. Using the equivalent solid of the same conductivity as the filled gas to replace the gas volume, it becomes convenient to model the temperature field. Then, how to consider the gas pressure with the equivalent solid becomes a critical problem.

We developed an equivalent solid simulation method based on the following thoughts. A typical solid material, of the same thermal conductivity coefficient as the gas, can employ certain thermal expansion deformations within it to exert the mechanical interaction with the other materials around. The Young's modulus, Poisson's ratio and thermal expansion coefficient were obtained for this method.

2.1 The parameters of equivalent solid

Due to the uniform gas pressure in the gap, stresses in the equivalent solid material satisfies $\sigma_{ij}=-p\delta_{ij}$, where p is the gas pressure and δ_{ij} is Kronecker delta. Based on the elastic theory for axisymmetric plane problem[10], the solution of radial displacement to the plane strain problem of a hollow cylinder under uniform gas pressure can be obtained as follows:

$$u_r(x)=\frac{1+v_s}{E_s}\left[\frac{1-2v_s}{b^2-a^2}a^2px+\frac{a^2b^2p}{b^2-a^2}\frac{1}{x}\right] \tag{1}$$

where, a and b is the inner and outer radius of the hollow cylinder, E_s is the cylinder's Young's modulus, and v_s is the Poisson's ratio.

This is the solid material of equivalent thermal expansion to simulate the gas pressure. The equivalent solid shall satisfy the following relations,

$$\begin{cases}\varepsilon_{ij}^{e}=\dfrac{1+v}{E}\sigma_{ij}-\dfrac{v}{E}\sigma_{kk}\delta_{ij}\\ \sigma_{ij}=-p\delta_{ij}\\ \varepsilon_{ij}^{T}=\alpha\Delta T\delta_{ij}\end{cases} \tag{2}$$

where ε_{ij}^{e} and ε_{ij}^{T} are the elastic strain and thermal strain components respectively.

The radial strain in the internal equivalent solid is independent of the point locations and is given as

$$\varepsilon_r=\varepsilon^e+\varepsilon^T \tag{3}$$

According to the continuous conditions of the radial displacement at the interface between the inner equivalent solid and the outer cylinder, we have

$$a\varepsilon_\gamma=u_\gamma(a)_{\text{cylinder}} \tag{4}$$

Substituting Eqs. (1), (2) and (3) into (4) yields

$$\alpha\Delta T=\frac{u_r(a)}{a}+\frac{1-2v}{E}p=\beta p+\frac{1-2v}{E}p \tag{5}$$

where $\beta=[(1+v_s)/E_s]\,[(1-2v_s)a^2+b^2]/(b^2-a^2)$.

The equivalent thermal expansion of the inner equivalent solid is related to the material properties and the cylinder wall thickness. For obtaining a more independent equivalent thermal expansion which can be applied in common conditions, a simplification of the expression is necessary. This can be achieved by selecting suitable material parameters.

2.2 The Young's modulus and Poisson's ratio

For a plane strain problem, the equation $\sigma_z=v(\sigma_x+\sigma_y)$ shall be satisfied at the equivalent solid. For obtaining the stress components in Eq.(2), v=0.5 shall be used, though such a Poisson's ratio is impracticable for any kind of solid material. Thus, the v tends to be 0.5.

The coefficient β in Eq.(5) is dependent on properties of the pellets and cladding, and β shall be as low as possible to obtain an equivalent thermal expansion strain independent of the outer material, hence the approximation of β:$(1-2v)/E\to 0$.

With the above ideas of $v\to 0.5$ and $(1-2v)/E$ being a large value, v=0.49 and $E=1\times10^{-4}$ MPa are suggested. Thus, the thermal expansion strain for a certain pressure in Eq. (5) can be expressed as

$$\alpha\Delta T=(1-2v)p/E \tag{6}$$

Except for extreme cases, e.g. the cylinder wall being extremely thin or the Young's modulus of the outer material being too low, these values are suitable and practicable. These selected coefficients will be validated in Section 3.

2.3 The equivalent thermal expansion coefficient

For the gap at different temperatures, the equivalent thermal expansion can be realized by applying the corresponding equivalent thermal expansion efficient.

Based on the state equation for ideal gases, and considering that the gap deformation is small, we have $pv/T=p_0v_0/T_0$ and $V\approx V_0$, and $p=Tp_0/T_0$. Thus the equivalent thermal expansion coefficient at gas pressure p can be obtained as,

$$\alpha(T)=\frac{Tp_0}{T_0(T-T_0)}\cdot\frac{1-2v}{E} \tag{7}$$

where T_0 is the initial temperature, T is the current temperature, and p_0 is initial inner gas pressure.

3 Validation of the equivalent solid method

Effectiveness of the solid simulation method is tested in this section. The results obtained from this method are compared with analytical solutions and those from a common method using gas pressure for simulating the mechanical gas effect. For the tests below, material properties of the cylinder are $E_s=2\times10^5$ MPa, v_s=0.3.

3.1 For different cylinder wall thicknesses.

The inner pressures of p=2, 2.67 and 3.33 MPa are chosen regardless of the variation of the cylinder wall thickness. The inner and outer radii are 0.5 and 1.0 mm, and 0.5 and 1.5 mm. The simulations are conducted by replacing the gas pressure with the equivalent thermal expansion of the inner equivalent solid. The simulated radial displacements are compared with the analytical solution using Eq.(1) and the inner gas pressure.

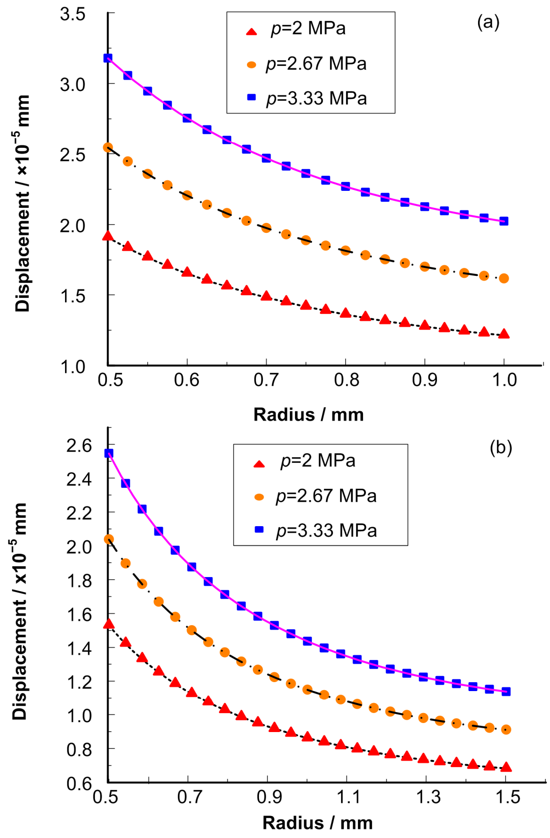

Fig.4 Comparison of numerical and analytical solutions for thin wall cylinder (a) and thick wall cylinder (b).

Figure 4 shows that the results obtained from the thermal expansion of the equivalent solid method (▲, ● and ■) fit well with the analysis results (the lines) for different gas pressures. This indicates that the selected material parameters and the thermal expansion strain given by Eq.(6) is effective, and this method is not sensible to the sizes of the outer solid.

3.2 The case for the square gas space shape

For studying the sensitivity of shape changes, a 1 mm×1 mm square traverse section of the pellet, and outer radius of the cylinder of 1.5 mm, is used, with the pressure p being 2, 2.67 and 3.33 MPa. The contour plot of the total displacement is shown in Fig.5, where the output path is shown. The numerical results in Fig.6 for different inner gas pressures are obtained from two methods: (1) the equivalent thermal expansion of the inner solid; (2) applying the pressures to the outer solids. They agree well with each other, indicating that the proposed equivalent solid method is independent of the gap shapes.

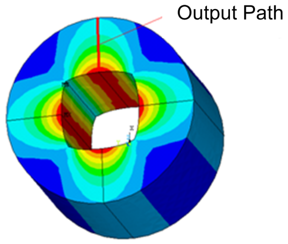

Fig.5 Total displacement of the cylinder.

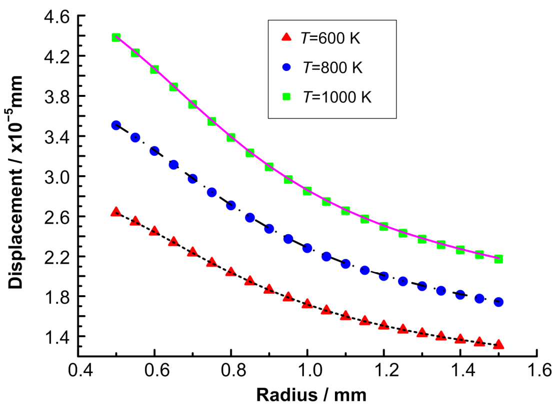

Fig.6 Comparison of the results from new method and those from usual method.

3.3 The case for the outer elasto-plastic solid

By increasing the inner gas pressure, the plastic strains emerge at the outer solid. It is necessary to investigate the applicability of the equivalent solid method for the elastic-plasticity materials. At the pressure of 150 and 200 MPa, the contour plot of the equivalent plastic strains is given in Fig.7, and the results along the radial output path from different methods are given in Fig.8. It can be seen from Fig.8 that the equivalent solid method is effective under the circumstances that even the plastic strains occur in the outer solid.

From the validation tests, one sees that the equivalent solid method is effective in simulating the mechanical performances of the gas. For fuel rods in nuclear reactors at various temperatures, the thermal expansion can be reflected with thermal expansion coefficient calculated by Eq.(7) to simulate the gas pressure. In Section 4, 3D simulations of the thermal-mechanical behaviors in the nuclear fuel rod from different methods are given.

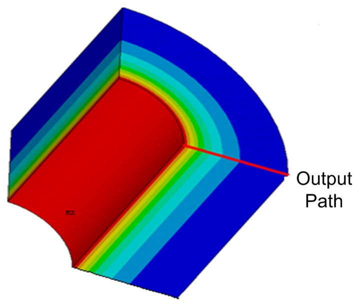

Fig.7 Equivalent plastic strain distribution at p=200 MPa.

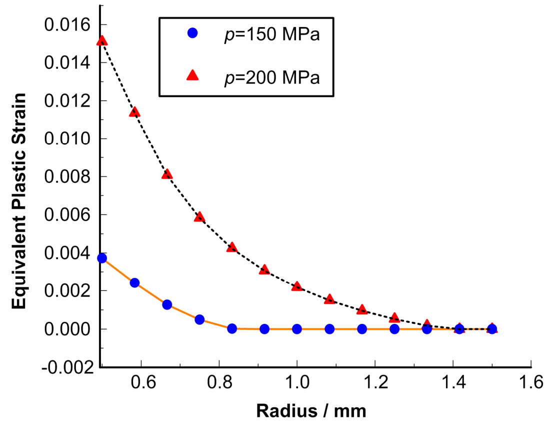

Fig.8 Equivalent plastic strain.

4 Simulation of thermal-mechanical behaviors in the nuclear fuel rod

4.1 Three-dimensional finite element models

At the initial stage of burnup, the thermal-mechanical behaviors in the fuel rod are mainly induced by the large temperature differences between the steady and initial temperatures. The steady temperature field and induced mechanical field are numerically simulated to further validate the equivalent solid method.

The finite element model is shown in Fig.9. It is 1/8 of a full length fuel rod. The pellet is 8.6 mm in diameter, the cladding is 0.5 mm thick and the initial gap width is 0.03 mm.

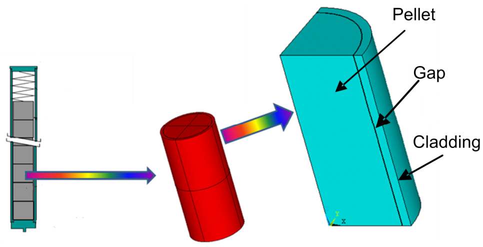

Fig.9 Geometrical model.

In this paper, the traditional method to simulate the thermal and mechanical effects of gas on nearby materials is called M1, and the equivalent solid simulation method is called M2. Their boundary conditions are shown in Fig.10.

M1 considers the external surface of the cladding as a convection one because of the coolant flow: $-k\cdot\partial T/\partial n= h(T-T_f)$, where k is the conductivity coefficient and h is the heat transfer coefficient. The thermal connection between the pellet and cladding can be calculated by the constraint function[2]: $h_g[T(r_{ef})-T(r_{ic})]=P(z)/(2\pi r_{ef})$, where h_g is the heat exchange coefficient of the gas, r_{ef}, is the pellet radius, r_{ic} is internal radius of the cladding, and $P(z)$ is the linear heat generation rate.

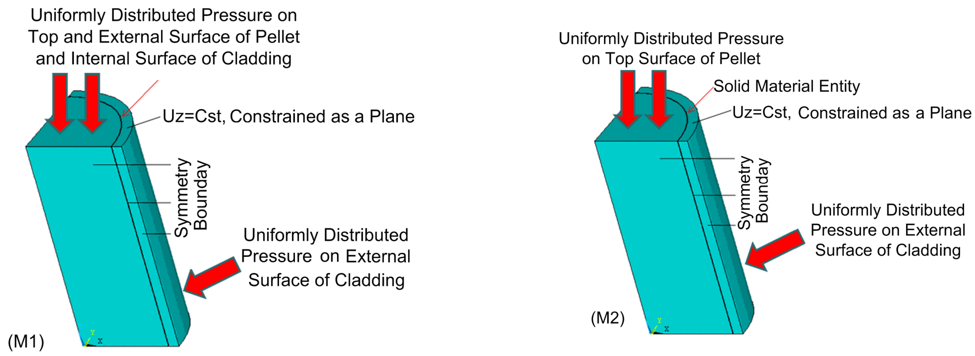

Fig.10 Boundary conditions for simulating the thermal and mechanical effects of gas with the traditional method (M1) and the equivalent solid simulation method (M2).

For M2, the boundary condition at the external surface of the cladding is the same as M1. In the gas gap between the pellet and cladding, an equivalent solid is used to replace the gas space.

Owing to the large temperature differences within the fuel elements at the initial stage of burnup, the temperature-dependent material parameters of UO_2 pellet and Zircalloy cladding are used[11-15].

4.2 Mesh grid and convergence

ANSYS element type SOLID90 and SOLID186 are applied in the thermal and mechanical computation of the finite element model respectively. The mesh grid is listed in Table 1 and the elements are shown in Fig.11.

Convergence of the mesh grids is indicated in Fig.12 by trend of the calculation data. Figs.12a and 12b show convergence of the temperatures and the Mises stresses for M1. Figs.12c and 12d show that the obtained temperatures and Mises stresses are converged for M2. Thus, the results obtained from Mesh 2 for both M1 and M2 can be testified to have enough precision.

Table 1 Mesh grid

Number		Element number	Node number
M1	Mesh 1	950	4991
	Mesh 2	3840	18296
	Mesh 3	6958	33598
M2	Mesh 1	1050	5112
	Mesh 2	4096	18585
	Mesh 3	7680	34125

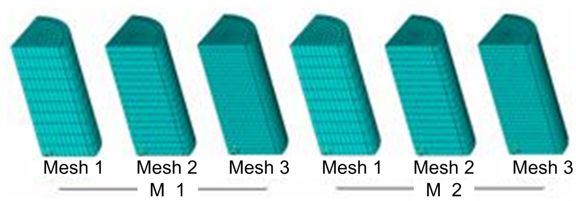

Fig.11 Finite element model of M1 and M2.

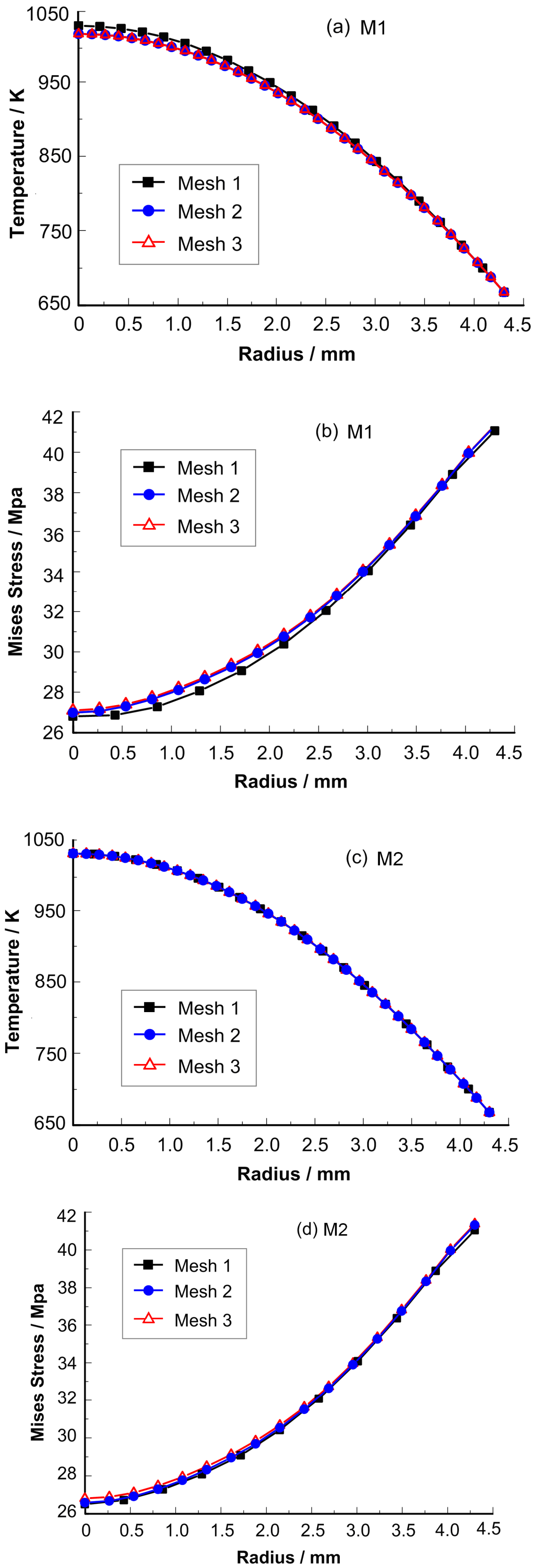

Fig.12 Calculated results along radius on top surface for different meshes.

5 Results and discussion

The computed thermal and the mechanical solutions at the beginning of burnup are obtained with M1 and M2 by using the 3D finite element models. According to contour plots of the temperature field and mechanical fields, four output paths are selected as showed in Fig.13.

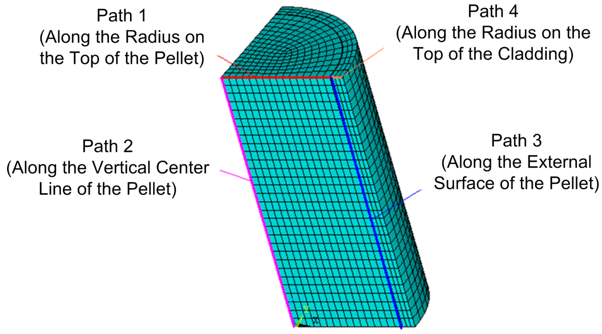

Fig.13 Selection of export pathes.

The obtained temperatures, the displacements, the Mises stresses and the first principle stresses at the four paths from M1 and M2 are shown in Figs.14, 15, 16, 17 and 18. It can be seen from these figures that the two methods differ slightly. And it confirms that the equivalent solid simulation method can be effectively applied in the 3D numerical simulation of the thermal- mechanical behaviors at the beginning of burnup.

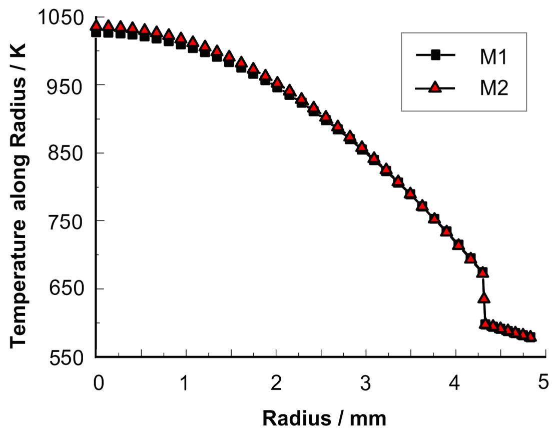

Fig.14 Contrast of M1 and M2's temperature along radius.

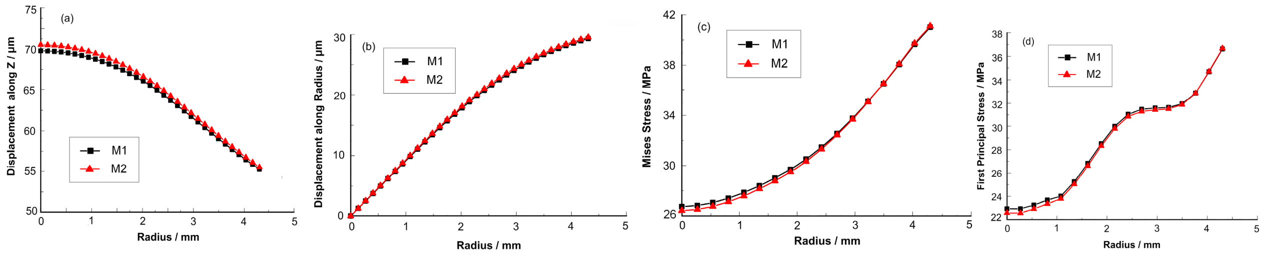

Fig.15 Axial displacement (a), the radial displacement (b), the Mises stress (c) and the first principal stress (d) along Path 1.

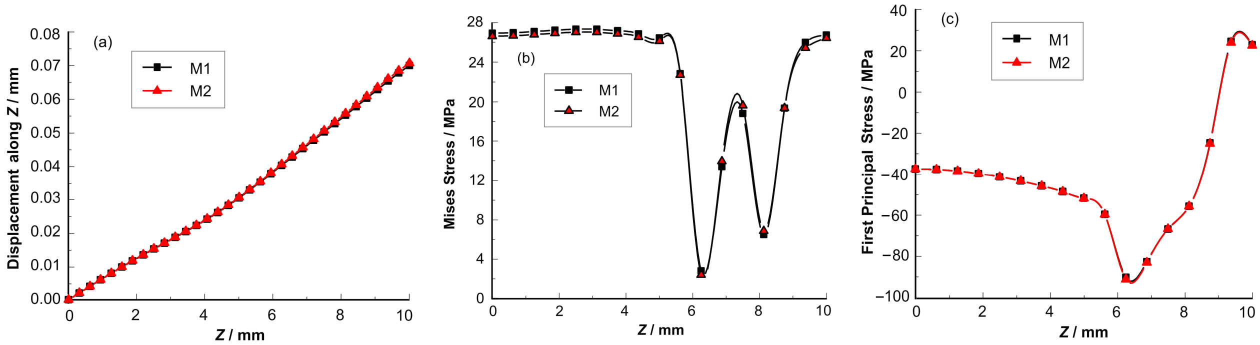

Fig.16 Axial displacement (a), the Mises stress (b) and the first principal stress (c) along Path 2.

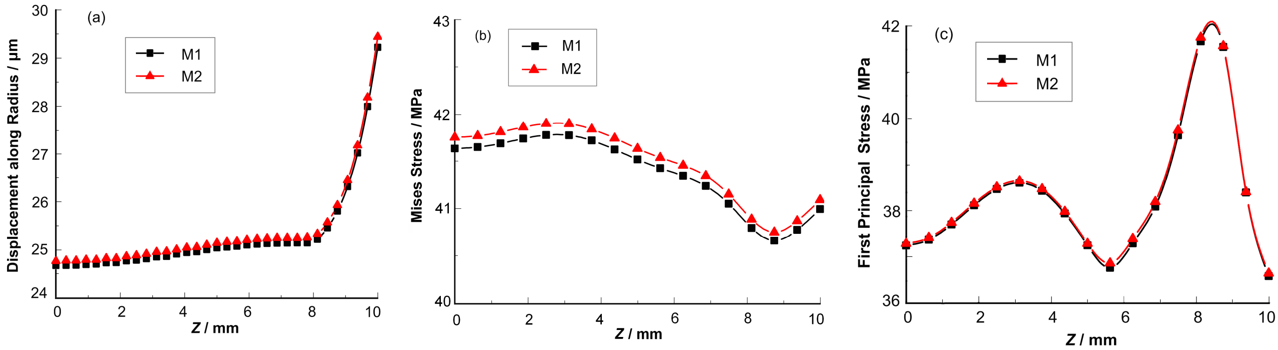

Fig.17 Radial displacement (a), the Mises stress (b) and the first principal stress (c) along Path 3.

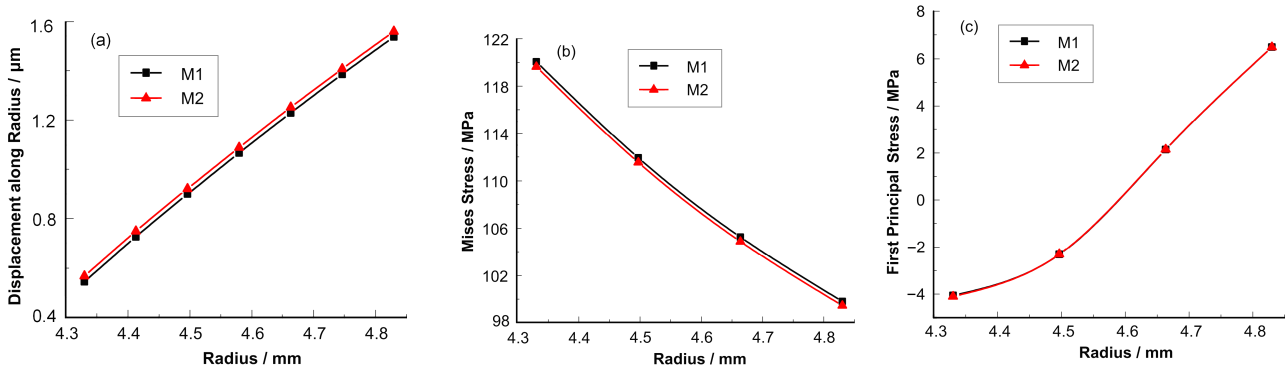

Fig.18 Radial displacement (a), the Mises stress (b) and the first principal stress (c) along Path 4.

6 Conclusion

In order to simplify the simulation of the complex thermal-mechanical coupling interactions between the gas filled in the gap and solid materials of the pellets and cladding of a nuclear fuel rod, a convenient equivalent solid method for finite element modeling is developed, which replaces the gas space with the equivalent solid to reflect the thermal and mechanical effects of the gas.

The expression of the equivalent thermal expansion coefficient is derived and the appropriate values of the material parameters, such as Young's modulus and Poisson's ratio of the equivalent solid material, are selected. Validations of this method are conducted by studing effects of the outer solid size, gas space and material performance.

Simulation of thermal-mechanical behaviors in the nuclear fuel rod at the beginning of burnup is carried out, using the common method and equivalent solid method. The results obtained from both methods are in consistency with each other. The current study provides a basis for further research on the thermal-mechanical coupling behaviors in nuclear fuel rods.

With increasing burnup, the fission gas will release into the free volume such as the initial flaws, the cracks, etc., which induces complex thermal-mechanical coupling behaviors in the nuclear fuel rods. The equivalent solid simulation method shows its advantages in these simulations, while this method should be improved if the gas volume changes greatly.

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