Multi-physics Numerical Model and Code Development for Fuel Rod

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Abstract - *In this paper, a tightly coupled multi-physics numerical model for fuel rod has been proposed and employed in numerical fuel rod code YUAN, which integrates neutronics, thermal-hydraulics and mechanics, etc. based on unique floating finite element grids, so as to model the coupled fuel rod behavior of neutron transport, isotope depletion, thermal conduction, heat transfer and deformation of fuel pellet/cladding. The thermal conduction solver, mechanical solver and neutron transport solver of YUAN are verified by ABAQUS and MCNP. And YUAN's ability to capture multi-physics behavior of SFR fuel rod with metallic pellet is demonstrated through relevant calculation results.*

I. INTRODUCTION

During reactor operation, nuclear fuel is in an extreme environment of high temperature, high pressure and intense radiation, influenced by tightly coupled multi-physics behavior, such as thermal expansion, swelling, PCMI, etc. Traditional reactor design codes[1,2] generally solve the multi-physics problem by decoupling it under some particular assumptions which mainly aim at traditional PWR fuel, rather than taking full multi-physics-coupling effects into consideration. In the early time when computing capability was very limited, this method was of great significance for nuclear power industry. At the same time, it should be noted that the reduction of computation results from the simplification of physical model and the decrease of calculation precision. As a matter of fact, the method is limited by the related assumptions in some degree, and is not likely to adapt to some new-type fuels.

Among various kinds of new-type fuels, metal fuel stands out for its superior fissile density, neutron economy, thermal conductivity and the convenience in post treatment. It has been considered as the main candidate fuel for a number of advanced reactor concepts such as Traveling Wave Reactor (TWR) and In-situ Breed and Burn Reactor (ISBBR). However, the obvious irradiation swelling of metal fuel can be a serious challenge for two issues. One is to keep pellet/cladding out of hard contact before EOL, the other one is to consider deformation and calculate in real size, instead of nominal size.

Recently, some cutting-edge projects[3-7] have already begun to develop multi-physics codes, e.g. CASL. Inspired by the numerical reactor conception in CASL, in this paper, a tightly coupled multi-physics numerical model for fuel rod has been proposed and employed in the numerical fuel rod code YUAN. YUAN is able to handle multi-physics-coupling calculation of neutronics, thermal-hydraulics and mechanics, etc. Compared with traditional fuel codes, YUAN provides an innovative method to analyze and design metal fuel. As a preliminary exploration on nuclear fuel technology, this research will help to reveal some complex fuel behavior inside the reactor core.

In the following section, the concept and basic model of Numerical Fuel Rod code YUAN are introduced. Then the verification of major solvers of YUAN and the calculation results of SFR fuel cases are demonstrates, and the influences induced by multi-physics effects are analyzed.

II. NUMERICAL FUEL ROD CODE YUAN

The numerical fuel rod code YUAN, a fuel rod numerical simulation platform, is based on existing physical models and mathematical methods, aiming at predicting fuel behavior under the extreme in-reactor environment, and pursuing fuel performance optimization. The basic idea of numerical fuel rod is very similar to the numerical reactor concept in CASL project. The difference is that the YUAN's simulation object is only one fuel rod, so the total amount of data and computation is greatly reduced, and the application can be realized on personal computer. YUAN specializes in fuel rod multi-physics-coupling calculation and simulation. It innovatively integrates neutronics into thermo-mechanical coupling calculation. Thus thermal conduction, mechanical, neutron transport, isotopes depletion problems can be solved in a tightly coupled way. As a general purposed numerical simulation platform, YUAN can be applied to fuel rods with arbitrary sizes, shapes and materials. The geometry model and coupling strategy will be introduced in details as follows.

1. Geometry Model

Considering the amount of computations, "2+1" dimension (plane 2-D and axial 1-D) geometry is applied in the numerical fuel rod model instead of 3-D geometry. During the geometry processing, 3-D fuel rod is partitioned into a number of layers along axial direction, and each layer is then meshed into independent 2-D finite element grids.

Meshing is an important step in finite element modeling, as the quality of grids will directly determine the precision and accuracy of the calculation. An automatic quadrilateral mesh generation algorithm is adopted in YUAN. The size and density of the grids can be adjusted through input file. The generated grids have been tested in a variety of cases and the results are accurate enough to reveal the details in multi-physics behavior. The square and hexagonal fuel cell grids are shown in Fig. 1.

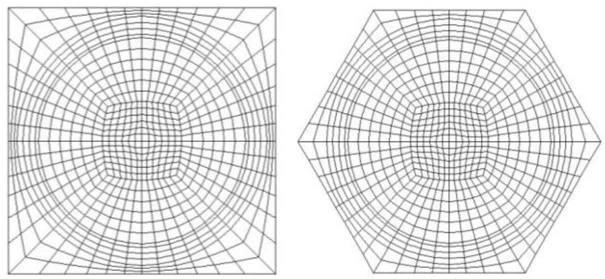


Fig. 1. 2-D Meshing for Square and Hexagonal Fuel Cells

YUAN is able to mesh asymmetric fuel cells as well, such as fuel rod containing a missing pellet surface (MPS), and fuel pellet off center position, as shown in Fig. 2.

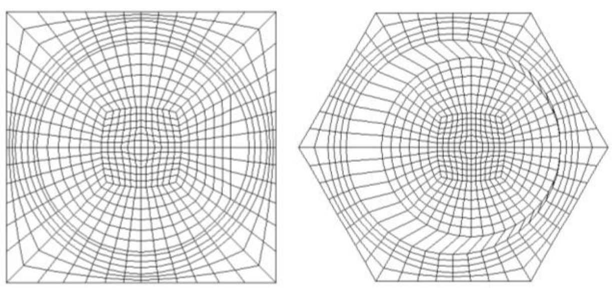


Fig. 2. MPS (Left) and Pellet off Center Position (Right) Fuel Cell Meshing

In YUAN, thermal conduction, mechanical and neutron transport calculation share the same grids. More details are discussed in the following section.

2. Coupling Strategy

In order to solve multi-physics problem, a thermal conduction solver, a mechanical solver (both based on finite element method) and a neutron transport solver (based on method of characteristics[8,9]) are developed. These solvers are so designed that they are able to work on arbitrary quadrilateral grids. During the calculation, there is only one set of grids for all three solvers. In other words, thermal conduction, mechanical and neutron transport calculation share the same grids.

In the iteration of multi-physics calculation, the three solvers are executed in turn, and temperature, deformation (displacement), neutron flux, etc. of every element are calculated and updated instantly. The multi-physics results are transferred among the solvers: after thermal conduction calculation, the element temperature are updated, then the material properties related to temperature like conductivity and cross section will also be updated in the following calculation; after mechanical calculation, the coordinates of grid nodes are updated according to node displacement, then the deformed grids will be used in the following calculation (deforming grids); after neutron transport calculation, the power distributions are updated, so are heat source distributions in the following thermal conduction calculation.

As a result, the multi-physics iteration is tightly coupled and the results after convergence will ultimately satisfy thermal conduction equation, mechanical equations and neutron transport equation at the same time. When the whole calculation is finished, the physical state of the fuel rod, such as temperature, displacement, density, stress, neutron flux, burnup, etc. will be output for post-processing.

Fig. 3 shows the main work flow of YUAN, which consists of an outer depletion loop and an inner multi-physics-coupling iteration. The inner iteration starts from axial 1-D neutron diffusion calculation, followed by thermal-mechanical and neutron transport calculation in each layer, and ends when axial offset converges.

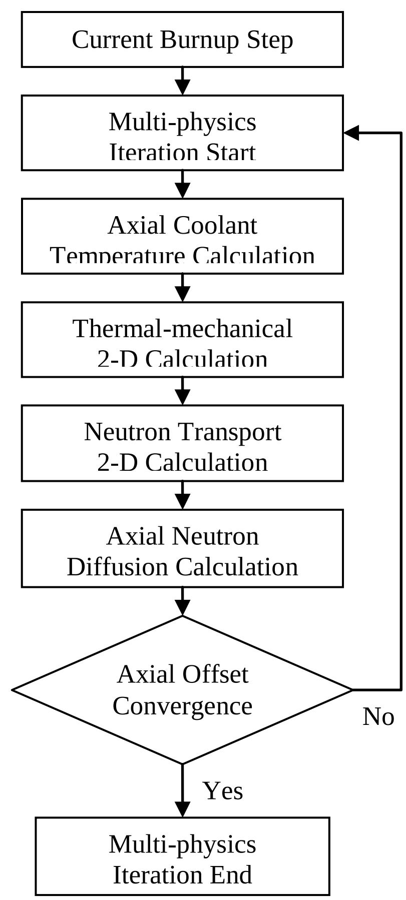


Fig. 3. Flow Chart of YUAN

3. Thermal Conduction Calculation

In 2-D solution domain Ω, The steady-state thermal conduction equation can be expressed as

$$\frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right)+\rho Q=0 \quad (1)$$

where, T - temperature field variable, *K*;

k_x, k_y - thermal conductivity along the two main directions of material, *W/m-K*;

ρ - material density, kg/m^3;

Q - internal heat source density, *W/kg*;

According to variation principle, original equation (1) is transformed into finite element equation:

$$K_T q_T = P_T \quad (2)$$

where, K_T is thermal conduction matrix, the expression is given as follows:

$$K_T = \int_\Omega \left[k_x \left(\frac{\partial N}{\partial x}\right)^T \left(\frac{\partial N}{\partial x}\right) + k_y \left(\frac{\partial N}{\partial y}\right)^T \left(\frac{\partial N}{\partial y}\right)\right] d\Omega + \int_{\Gamma_3} h N^T N d\Gamma \quad (3)$$

P_T is thermal conduction matrix, the expression is given as follows:

$$P_T = \int_\Omega \rho Q N^T d\Omega + \int_{\Gamma_2} q \cdot N^T d\Gamma + \int_{\Gamma_3} h T_\infty \cdot N^T d\Gamma \quad (4)$$

N in formula (3), (4) is interpolation function matrix, which is determined by finite element grid. Equation (2) is a system of linear equations, which can be easily solved by numerical method.

4. Mechanical Calculation

In YUAN, the gap element is treated as an imaginary elastic body for simplicity(extremely soft). In order to get gap deformation, thermal expansion, pellet swelling and fission gas release are considered in mechanical calculation.

In 2-D solution domain Ω, The 2-D (plane stress) elastic mechanical constitutive equations can be expressed as

$$\frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} = 0 \qquad \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} = 0 \quad (5)$$

$$\varepsilon_x = \frac{\partial u}{\partial x} \qquad \varepsilon_y = \frac{\partial u}{\partial y} \qquad \gamma_{xy} = \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \quad (6)$$

$$\varepsilon_x = \frac{1}{E}\left(\sigma_x - \nu\sigma_y\right) + \alpha_T \cdot \Delta T \quad (7)$$

$$\varepsilon_y = \frac{1}{E}\left(\sigma_y - \nu\sigma_x\right) + \alpha_T \cdot \Delta T \quad (8)$$

$$\gamma_{xy} = \frac{1}{G}\tau_{xy} \quad (9)$$

where, u, v - displacement along direction x, y, *m*;

σ, τ - normal stress and shear stress, *Pa*;

ε, γ - normal strain and shear strain;

E - Young's modulus, *Pa*;

ν - Poisson's ratio;

α_T - thermal expansion coefficient, $\alpha_T \cdot \Delta T$ is for thermal stress;

G - shear modulus, *Pa*;

According to variation principle, original equation (10) is transformed into finite element equation:

$$Kq = P \quad (10)$$

Where, K is stiffness matrix, the expression is given as follows:

$$K = \int_\Omega B^T D B d\Omega \quad (11)$$

P is nodal equivalent load matrix, the expression is given as follows:

$$P = \int_\Gamma N^T \bar{p} d\Gamma + \int_\Omega B^T D \varepsilon^0 d\Omega \quad (12)$$

B in formula (11), (12) is geometry matrix. N in formula (12) is interpolation function matrix, which is determined by finite element grid. D in formula (11), (12) is elastic coefficient matrix, which is determined by material elastic parameters. ε^0 in formula (12) is thermal strain matrix, which is determined by thermal stress prerequisite. Equation (10) is a system of linear equations, which can be easily solved by numerical method. And q is the displacement matrix to be solved.

5. Neutron Transport Calculation

The multi group characteristic line equation in the direction of discrete angle can be expressed as

$$\frac{d\varphi_g\left(s,\Omega_m\right)}{ds} + \Sigma_{t,g}\varphi_g\left(s,\Omega_m\right) = Q_g\left(s,\Omega_m\right) \quad (13)$$

where, φ_g - group *g* neutron angular flux;

s - spatial independent variables along the characteristic line, *m*;

Ω_m - discrete angular direction variable;

The equation (13) is generally processed by flat source approximation. That is, consider the source term $Q_g\left(s,\Omega_m\right)$ on the right as a constant in a certain region, and it can be replaced by the average source term $Q_{i,g}\left(\Omega_m\right)$ on characteristic line segment i:

$$Q_{i,g}\left(\Omega_m\right) = \frac{1}{4\pi}\left[\frac{\chi_g}{k_{eff}}\sum_{g'}\left(\nu\Sigma_f\right)_{g'}\varphi_{i,g'} + \sum_{g'}\Sigma_{s,i,g'\to g}\varphi_{i,g'}\right] \quad (14)$$

The characteristic line equations are calculated segment by segment along the characteristic line, which means that the neutron flux at the last line segment has been calculated when calculating the characteristic line equation of the current line segment. In this way, the solution of segment k's equation can be expressed as

$$\varphi_{i,k}\left(s,\Omega_m\right)=\varphi_{i,k}^{in}\left(\Omega_m\right)\exp\left(-\Sigma_{t,i}s\right)+\frac{Q_i\left(\Omega_m\right)}{\Sigma_{t,i}}\left[1-\exp\left(-\Sigma_{t,i}s\right)\right] \quad (15)$$

where, $\varphi_{i,k}^{in}\left(\Omega_m\right)$ - Angular flux at the entrance of current characteristic line segment, i.e. angle flux at the end of last line segment;

According to formula (15), the flux at the outlet of the characteristic line segment and the average angular flux can be obtained simultaneously:

$$\varphi_{i,k}^{out}\left(\Omega_m\right)=\varphi_{i,k}^{in}\left(\Omega_m\right)\exp\left(-\Sigma_{t,i}s_{i,k}\right)+\frac{Q_i\left(\Omega_m\right)}{\Sigma_{t,i}}\left[1-\exp\left(-\Sigma_{t,i}s_{i,k}\right)\right] \quad (16)$$

$$\bar{\varphi}_{i,k}\left(\Omega_m\right)=\frac{\varphi_{i,k}^{in}\left(\Omega_m\right)-\varphi_{i,k}^{out}\left(\Omega_m\right)}{\Sigma_{t,i}s_{i,k}}+\frac{Q_i\left(\Omega_m\right)}{\Sigma_{t,i}} \quad (17)$$

where, $s_{i,k}$ - length of characteristic segment k in region i, m;

In order to calculate the average scalar flux within the region, we need to sum up the angular flux of all the characteristic line segments in the region by its special and angular weight of polar angle and radial angle respectively. In this way, the average angular flux and average scalar flux in region i are

$$\bar{\varphi}_i\left(\Omega_m\right)=\frac{\sum_{k\in i,m}\bar{\varphi}_{i,k}\left(\Omega_m\right)s_{i,k}\delta A_{i,m}}{V_i} \quad (18)$$

$$\bar{\varphi}_i=\frac{\sum_m\bar{\varphi}_i\left(\Omega_m\right)\omega_m}{\sum_m\omega_m} \quad (19)$$

In order to guarantee the accuracy of the volume weight integral, volume correction for the length of the characteristic line segment in formula (18) is often required:

$$s'_{i,k}=V_i\Big/\sum_{k\in i,m}s_{i,k}\delta A_{i,m} \quad (20)$$

where, $\delta A_{i,m}$ - space between characteristic lines along direction m in region i, m;

Equation (13) for all the energy groups and all the characteristic lines can be solved by source iteration method.

III. SOLVER VERIFICATION

In this section, ABAQUS and MCNP are used to verify the thermal conduction solver, mechanics solver and neutron transport solver of the Numerical Fuel Rod code YUAN. The object is a 2-D square fuel cell model, as shown in Fig. 4. The size of pitch, cladding outer diameter, cladding inner diameter, pellet outer diameter are 1.5, 1.4, 1.2, 1.16 cm, respectively. The results given by YUAN are not only for verification, but will also a demonstration for the comprehensive simulation capability of the code.

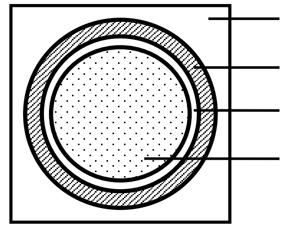


Fig. 4. Schematic Diagram of Fuel Cell

1. **Thermal Conduction Solver**

In this problem, the thermal conductivity of fuel pellet, gap space, cladding are respectively 3, 0.6, 18 W/m-K. An internal heat source of 4*108 W/m^3 distributes in the fuel pellet uniformly. The temperature at outer wall of cladding is 610 K.

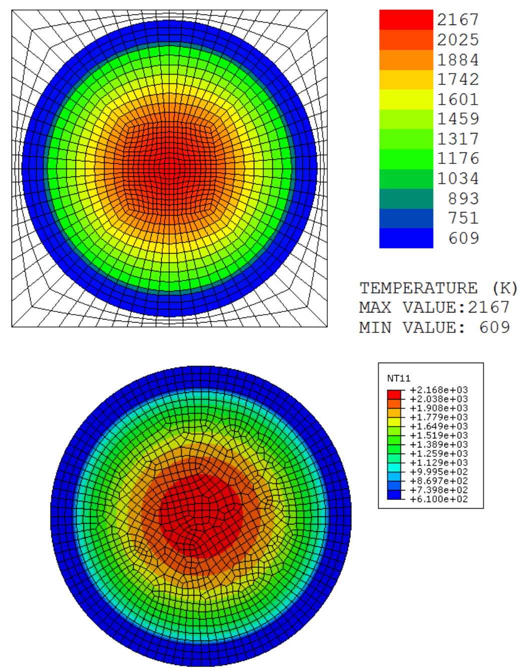


Fig. 5. Temperature Field Calculated by YUAN (Upper) and ABAQUS (Lower)

Under above conditions, the temperature field of the fuel rod is calculated by YUAN and ABAQUS respectively. Fig. 5 shows the temperature field distribution in the fuel cell. By comparison, the results of YUAN and ABAQUS are basically the same. From the center to the outer wall of cladding, the temperature is gradually reduced in both graphs. Table 1 shows the temperature at cladding inner surface, pellet outer surface and pellet center. The relative deviation is very small (less than 0.05%). Thus, the results of YUAN and ABAQUS are in good agreement.

Table 1. Temperature in the Fuel Rod

Temperature (K)	YUAN	ABAQUS	Relative Deviation
Clad Inner Surface	667.5	667.5	0.00%
Pellet Outer Surface	1046.9	1047.3	0.04%
Pellet Center	2167.4	2168.2	0.04%

2. Mechanics Solver

In this problem, material parameters of elastic mechanics used in the calculation are shown in Table 2. The initial temperature field of the fuel rod is assumed uniformly 293 K, and the current temperature field is just from the thermal conduction solver verification results for the sake of simplicity.

Table 2. Material Parameters of Elastic Mechanics

	Pellet	Gap	Cladding
Young's Modulus(Pa)	$1*10^{11}$	$1*10^{3}$	$7*10^{10}$
Poisson's ratio	0.33	0	0.37
thermal expansion coefficient (/K)	$2*10^{-5}$	0	$2*10^{-5}$

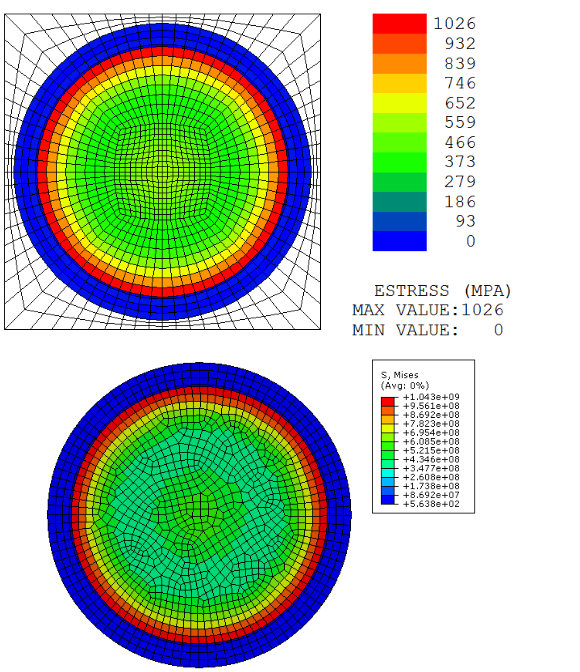


Fig. 6. Equivalent Stress Field Calculated by YUAN (Upper) and ABAQUS (Lower)

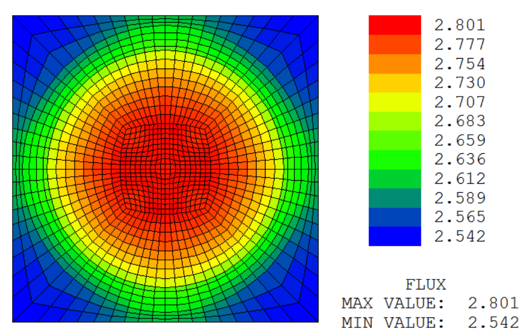
Under above conditions, the equivalent stress field generated by the thermal effect is calculated by YUAN and ABAQUS respectively. Fig. 6 shows the equivalent stress field distribution and table 3 shows the equivalent stress at cladding inner surface, pellet outer surface and pellet center. By comparison, it is found that the equivalent stress field distribution of YUAN is nearly the same as that of ABAQUS from the graphs. Then, the equivalent stress at cladding inner surface, pellet outer surface and pellet center was compared. The results of YUAN and ABAQUS are found to be slightly different, but the results are still in agreement. It should be noted that the larger equivalent stress distribution gradient is, the more sensitive result is to grids. So using different grids will inevitably produce a certain deviation.

Table 3. Equivalent Stress in the Fuel Rod

Equivalent Stress (MPa)	YUAN	ABAQUS	Relative Deviation
Clad Outer Surface	266	262	1.53%
Clad Inner Surface	269	273	-1.47%
Pellet Outer Surface	1026	1039	-1.25%
Pellet Center	560	559	0.18%

3. Neutron Transport Solver

In this problem, the material cross section used for neutron transport calculation is from C5G7 benchmark. All the boundary of the fuel cell are using total reflection boundary condition.



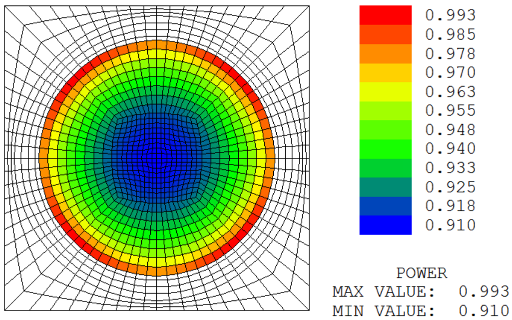


Fig. 7. 1st Group Neutron Flux Distribution (Upper) and Power Distribution (Lower)

Under above conditions, neutron flux distribution, power distribution and effective multiplication factor of the fuel cell are calculated by YUAN and MCNP. Fig. 7 shows the fast group neutron flux distribution and power distribution. Fig. 8 shows the 7 group of neutron energy spectrum. Table 4 shows the effective multiplication factor. There is no neutron flux distribution and power distribution for MCNP, because it is based on coarse mesh. So neutron flux distribution and power distribution are not compared here. The effective multiplication factor and the 7-group neutron energy spectra are compared. The results are very close and the relative deviation is less than 0.6%. Therefore, YUAN's results are in good agreement with MCNP's.

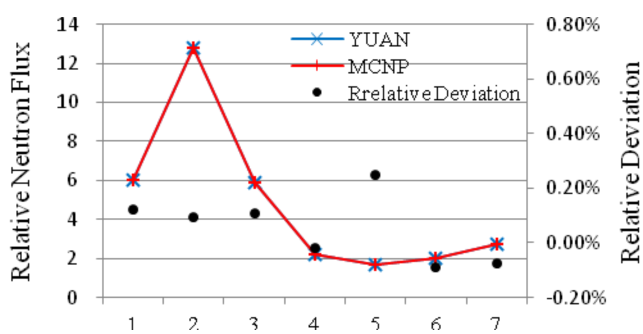


Fig. 8. 7-Group Neutron Energy Spectrum

Table 4. Effective Neutron Multiplication Factor

	YUAN	MCNP	Relative Deviation
K_{eff}	1.32917	1.32922	-0.004%

IV. SFR FUEL ROD SIMULATION RESULTS

In order to capture the multi-physical coupling effects of SFR fuel due to deformation, a typical SFR fuel rod is simulated by YUAN under the same conditions while considering deformation and not considering deformation. While considering deformation, thermal conduction, mechanics and neutronics calculation are all coupled. Otherwise only thermal conduction and neutronics calculation are coupled. By comparing the results, we can get a picture of the deformation multi-physical effects on both thermal conduction and neutronics.

The typical SFR fuel rod is based on hexagonal grid, consisting of U-Pu-Zr pellet, SiC cladding and liquid sodium filling in the gap. The pellet outer diameter, cladding inner diameter, cladding outer diameter and pitch are 0.8, 1.0, 1.1, 1.533 cm, respectively. The effective height of the fuel rod is 200 cm, which is divided into 10 segments uniformly along axial direction.

Deformation Coupling Effect on Thermal Conduction

The highest temperature versus burnup while considering deformation and not considering deformation is shown in Figure 9. The results have a small deviation at 0 GWd/tU (less than 1 K), then the deviation gradually increased and then stabilized (about 6 K).

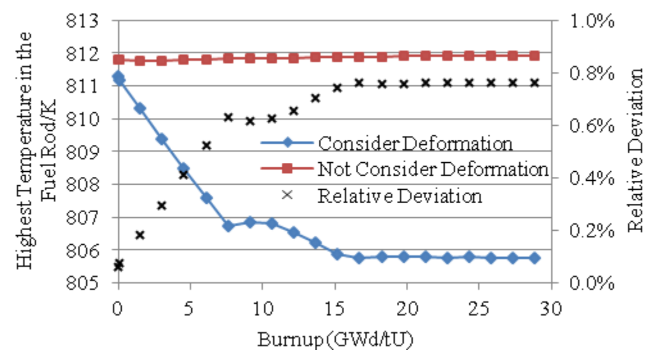


Fig. 9. Highest Temperature in Rod vs. Burnup While Considering Deformation and not Considering Deformation

Figure 10 shows the highest temperature versus different axial positions at 29 GWd/tU while considering deformation and not considering deformation. There is a slight deviation between the results, no more than 6 K.

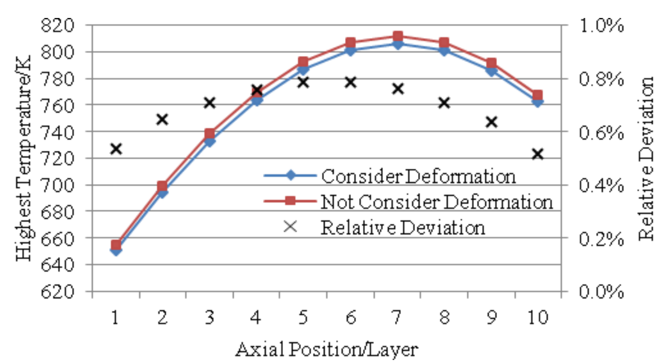


Fig. 10. Highest Temperature in different Axial Position at 29GWd/tU While Considering Deformation and not Considering Deformation

According to above results, deformation has a certain but slight effect on thermal conduction. The fact that the thermal conductance of SFR fuel is superior to traditional ceramic fuel can explain and that deformation has little direct impact on fuel temperature distribution.

Deformation Coupling Effect on Neutronics

The K_{eff} versus burnup is shown in Fig. 11. It can be seen that at 0 GWd/tU the K_{eff} curves are very close to each other, then the deviation grows as burnup goes deeper, and reach a maximum of approximately 600 pcm at 8 GWd/tU, which is quite notable from the viewpoint of neutronics.

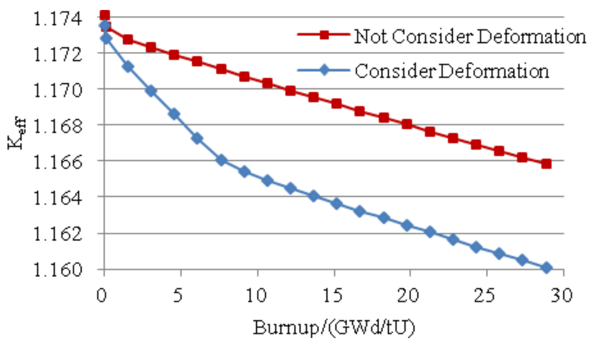


Fig. 11. K_{eff} vs. Burnup While Considering Deformation and not Considering Deformation

The results indicate that deformation multi-physical effect plays an important role in SFR fuel simulation, where the pellet deformation is significant. If deformation is not considered, the neutronics result can be inaccurate. Therefore, multi-physics-coupling calculation is necessary for SFR fuel with metal pellet.

V. CONCLUSIONS

In this paper, the concept of numerical fuel rod is put forward, and the numerical fuel rod code YUAN is developed. The main features of YUAN are given as follows:

- the multi-physics-coupling calculation capability;
- deforming grids which keep consistent with the deformation during the whole calculation process;
- powerful geometry modeling;
- feasible computation amount;
- a wide range of potential applications.

The verification of the thermal conduction solver, mechanics solver and neutron transport solver in YUAN has been completed, and multi-physics-coupling calculation has been realized. As the results show, for SFR fuel rod with metallic pellet, deformation has slight coupling effect on thermal conduction and notable coupling effect on neutronics. Therefore, multi-physics calculation with deformation coupled is necessary for SFR fuel.

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