3D FE simulation of PCMI (Pellet-Cladding Mechanical Interaction) considering frictionless contact

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1. Introduction

When the heat generation increases the temperature of the nuclear rod, the pellet could contact the cladding. This phenomenon is called pellet to cladding interaction (PCI), which was discovered in 1970s. In order to understand this phenomenon, a large number of the simulation tools interpreting PCI have been developed. METEOR [1] and TOUTATIS [2] have been developed at the CEA. METEOR is one-dimensional axisymmetric PCI simulation code that has been made from TRANSURANUS [3]. The goal of this code is coupling every aspect of physical phenomenon. Monodimensional FE model [4] has been made for METEOR. It is good to evaluate the global behavior in high burn up levels. However, the multi-dimensional PCI analysis code is necessary to precisely analyze the stress distribution especially in case of the crack analysis. CAST3M [5] 3D finite element code has been developed considering thermo-mechanical interaction in detail for TOUTATIS code. The advanced multidimensional code called ALCYONE [6] has been developed considering chemical-physics and thermomechanical aspects. Although there are many codes that analyze pellet and cladding interaction, it is difficult to consider every physical aspect. In this paper, pellet to cladding mechanical interaction in 3D has been simulated with frictionless contact using the developed module, which is written in FORTRANN90.

2. General model of PCMI

2.1 The mechanical analysis

When nuclear rods burn up, the gap between the pellet and the cladding tube narrows due to thermal expansion leading to the contact between the pellet and the cladding. This paper suggests a scheme of a frictionless contact to describe the contact condition. The contact method used in this paper is the node to node method which is one of the simple typical methods in the contact analysis [7].

Before contact, each stiffness matrix of the pellet and the cladding is assembled independently. During the mechanical analysis, nodes are checked by penetration function to determine that the contact has occurred. In order to check penetration, normal direction of the pellet surface's nodes should be defined. In the PCMI contact case, the normal direction is defined using circular geometric properties.

The penetration function which is the change in the gap width upon fuel and cladding expansion is given by

$$\mathbf{g}_{\mathrm{N}} = (\mathbf{u}^{\mathrm{c}} + \mathbf{X}^{\mathrm{c}}) \cdot \mathbf{n}^{\mathrm{p}} - (\mathbf{u}^{\mathrm{p}} + \mathbf{X}^{\mathrm{p}}) \cdot \mathbf{n}^{\mathrm{p}} \qquad (1)$$

where \mathbf{u}^{p} and \mathbf{u}^{c} are respectively the displacement of the pellet and the cladding, \mathbf{X}^{p} and \mathbf{X}^{c} are respectively the initial coordinate of the pellet and the cladding and \mathbf{n}^{p} is the normal direction of the pellet's node.

In the frictionless contact analysis, the penalty method is generally used. When penetrated nodes are detected, penalty stiffness matrix and penalty residual vector have been made. Then, the pellet and the cladding interact on each other. Using this interaction, penalty matrix and residual vector have been constructed and these are embedded to the stiffness matrix before the contact.

The penalty residual vector in the frictionless contact problem is given by

$$\mathbf{G}_{i}^{cP} = \varepsilon_{N} \mathbf{g}_{Ni} \, \mathbf{C}_{i} \tag{2}$$

where C_i is the normal direction of the pellet nodes and

 $\boldsymbol{\epsilon}_N$ is a normal penalty parameter.

The penalty stiffness matrix is given by

$$\mathbf{K}_{i}^{cP} = \varepsilon_{N} \mathbf{C}_{i} \mathbf{C}_{i}^{T}$$
(3)

In FE frictionless contact analysis, normal reaction force could be calculated by the penetration function. Penalty parameter has a physical meaning of the spring that has to be used to get the reaction force with the penetrated displacement to the normal direction.



Fig.1 Physical meaning of the penalty parameter

2.2 The thermal analysis

Ross and Stoute [8] introduced that the gap conductance between the pellet and the cladding in 1962. Gap conductance is divided into three parameters which are gas, solid and radiation.

$$h_{gap} = h_{gas} + h_{solid} + h_{radiation} \tag{4}$$

In the PCMI analysis, the radiation gap conductance is not considered because its effect is small. Before the contact between the pellet and the cladding tube, the gas conductance is only considered as the gap conductance.

$$h_{gas} = \frac{k_g(T_g)}{d_g + C_r(r_p + r_c) + g_p + g_c}$$
(5)

where k_g is the conductivity of the gas in the gap, d_g is the gap width (computed in the mechanics solution), C_r is a roughness coefficient with r_1 and r_2 the roughness of the two surface, and g_1 and g_2 are respectively jump distance at the two surface.

After contacts between the cladding and the pellet, the gap conductance has been considered with the gas and solid conductance. The solid conductance is given by

$$h_{\text{solid}} = 1.45 \frac{1}{\sqrt{\Delta R_{p} + \Delta R_{c}}} \left(\frac{P_{i}}{H}\right)^{n} \left(\frac{2k_{p}k_{c}}{k_{p} + k_{c}}\right) (6)$$

where H is Meyer hardness, ΔR_p and ΔR_c are respectively the roughness of the pellet and cladding surface, P_i is a interfacial pressure, k_p and k_c are respectively the conductivity of the pellet and cladding. In case of elastic deformation, n is 0.5 and in plastic deformation case, n is 1. The interfacial pressure is a main factor in the solid heat coefficient. When the fuel pellet contacts the cladding inner wall, the pressure on the contact region has been calculated by using the reaction force.

3. 3D FE Simulation using frictionless contact

Thermal FE analysis and deformation module with frictionless contact are weakly coupled. This calculation has been continued until the temperature is converged. The frictionless contact module is verified by the interference cylinder problem [9].





Fig. 2 (a) Boundary condition of the pellet and the cladding (b) FE Model of the pellet and cladding

Fig.2 represents one of the eight cracked pieces of the pellet and the symmetric cladding with respect to the 22.5 degree on the x-y plane. In Fig.2 (a), gap conductance is applied on the space between the pellet and the cladding(\overline{CD} and \overline{EF}). It is assumed that the temperature of the water that surrounds the cladding is 513K and the heat convection coefficient of the coolant is 1000mW / mm² · K . It is also supposed that other surfaces are adiabatic.

Table I: Properties of pellet and cladding

	Conductivity (mW/mm-K)	Thermal expansion (mm/mm)	Elastic modulus (GPa)	Poisson's ratio
Pellet	3.54	12	191	0.316
Cladding	15.29	6.7	84	0.349

Michel et al. [10] uses the heat generation rate under the accident conditions to describe the PCI using ALCYON. For the heat generation rate to simulate the behavior of the pellet and the cladding under the contact, we use 40kW/m, which is equivalent to a linear power level. It is supposed that the initial gap distance is 0.05mm. The FE model uses a second order element (Pellet : 114 elements and 686 nodes, Cladding tube : 84 elements and 571 nodes).



Fig. 3 Open gap region and closed gap region between pellet and cladding

The pellet deformation looks like a bamboo because the top region of the gap is closed but the bottom is open as shown in Fig. 3.



Fig. 4 (a) Von-Mises stress of the cladding and (b) Temperature distribution of the fuel rod

Fig. 4 represents the contour of the von-mises stress and temperature distribution. Using obtained displacement, strain has been obtained.

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$
(7)

Then stress also has been calculated by elastic modulus and strain components.

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}, \ C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + 2\mu \delta_{ik} \delta_{jl} \ (8)$$

where λ and μ are lame constant. The von-mises stress, which is generally used in bulk metal, on the contact region is more concentrated than the stress on the open gap area. The most concentrated von-mises stress is about 12 times higher than the lowest von-mises stress on the cladding. The highest temperature on outer surface of the pellet has been found to be 684K because of the gas on the open gap region. The lowest temperature has been found to be 625K on the outer pellet surface due to the contact. The difference of temperature occurs because the gap conductance on the contact region and the open gap region are different.

4. Conclusion

In this paper, 3D PCMI FE model is simulated with frictionless contact and elastic deformation. From the frictionless contact analysis, the interfacial pressure has been calculated and then this is used to obtain the solid heat coefficient which is a main factor to analyze the thermal distribution. The Von-Mises stress is very important information to predict the failure of the cladding for the fuel safety. Further works should include the elasto-plastic analysis for a more accurate simulation of the nuclear fuel rod.

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