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PUMA Development through a Multiphysics Approach

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1. Introduction

Nuclear fuel performance analysis codes are essential tools to simulate multiphysics in fuel. These have been mostly evolved based on their precursors developed in 1970s by uncoupling the multiphysical problem. Meanwhile advances of numerical methods make it possible for the multiphysics problem to be solved in a fully coupled way [1-2].

In addition to a multidimensional, multiphysical approach [2], a nuclear fuel performance analysis code, which is 1D code, should be improved by accommodating the state-of-the-art in the numerical analysis to support current fuel design and performance analysis. In particular, the coupling between the mechanical equilibrium equation and a set of numerically stiff kinetics equations for fission gas release is of great importance for a multiphysics simulation of nuclear fuel. Instead, coupling between temperature and fuel constituent was found to be made with a relative ease by employing an ordinary differential equations solver [3].

As an effort for a new SFR metal fuel performance analysis code, called PUMA (Performance of Uranium Metal fuel rod Analysis code), the deformation of U-Zr fuel for SFR in connection with a fission gas release model is analyzed. A finite element analyses for purely mechanical problems are performed using a backward differentiation formula, and are subjected to scrupulous verification with Abaqus. Then mechanical equilibrium equation and the equations for fission gas release are coupled with the same differential-algebraic equations (DAE) solver.

2. Fuel Deformation under Gaseous Swelling

In LWR fuel, pellet-cladding mechanical interaction is a typical example of why multiphysics simulation is needed. An Abaqus thermo-mechanical interaction simulation was performed with a loosely coupled method [4]. Similarly an external iteration process is required to couple the mechanical problem and the gaseous swelling problem [5]. In contrast, we introduce a fully coupled approach.

2.1 Definition of DAEs

A generalized plane strain condition is assumed. In a cylindrical coordinate system, three strain components are defined as

$$\boldsymbol{\varepsilon}_{\mathbf{t}} = \{\varepsilon_r, \varepsilon_\theta, \varepsilon_z\} \tag{1}$$

The vector of all independent variables $\mathbf{y}$ includes radial displacement, axial strain, stress components, creep strain, swelling strain, and fission gas concentrations for all radial elements.

$$\mathbf{y} = \{\mathbf{u}, \boldsymbol{\sigma}, \boldsymbol{\varepsilon}_{\mathbf{c}}, \boldsymbol{\varepsilon}_{\mathbf{s}}, \mathbf{N}_{\mathbf{b}}\} \tag{2}$$

where each vector consists of its components as follows
$\mathbf{u} = \{u_1, \cdots, u_i, \cdots, u_{n+1}, \varepsilon_z\}$, $\boldsymbol{\sigma} = \{\boldsymbol{\sigma}_1, \cdots, \boldsymbol{\sigma}_i, \cdots, \boldsymbol{\sigma}_n\}$,
$\boldsymbol{\sigma}_i = \{\sigma_r, \sigma_\theta, \sigma_z\}$, $\boldsymbol{\varepsilon}_{\mathbf{c}} = \{\varepsilon_{c1}, \cdots, \varepsilon_{ci}, \cdots, \varepsilon_{cn}\}$,
$\boldsymbol{\varepsilon}_{\mathbf{s}} = \{\varepsilon_{s1}, \cdots, \varepsilon_{si}, \cdots, \varepsilon_{sn}\}$, and $\mathbf{N}_{\mathbf{b}} = \{\mathbf{N}_{\mathbf{b1}}, \cdots, \mathbf{N}_{\mathbf{bi}}, \cdots, \mathbf{N}_{\mathbf{b}5}\}$
where $\mathbf{N}_{\mathbf{bi}} = \{C_{s0}, N_{b1}, N_{b2}, N_{b3}, N_{b4}, N_{b5}, N_{b6}\}$.

A finite element formulation of the mechanical equilibrium equation yields purely algebraic equations

$$\int_{\Omega_e} \mathbf{B}^T \boldsymbol{\sigma} d\Omega = \int_{\partial\Omega_e} \mathbf{N}^T \mathbf{t} ds \tag{3}$$

Stress components are related with total strain from displacement, creep strain and swelling strain as follows

$$\boldsymbol{\sigma} = \mathbf{D}\left(\boldsymbol{\varepsilon}_{\mathbf{t}} - \varepsilon_c \mathbf{n} - \frac{1}{3}\varepsilon_s \mathbf{m}\right) \tag{4}$$

where $\boldsymbol{\varepsilon}_{\mathbf{t}}$ is the total strain, $\mathbf{s}$ is the deviatoric stress, $\mathbf{n} = 3\mathbf{s}/2q$, $\mathbf{m} = \{1,1,1\}$, q is equivalent stress, and p is hydrostatic pressure.

The model for creep strain rate takes the form below

$$\frac{d\varepsilon_c}{dt} = f_c(\boldsymbol{\sigma}, \varepsilon_c) \tag{5}$$

The model for swelling strain rate includes the gaseous swelling due to fission gas

$$\frac{d\varepsilon_s}{dt} = \frac{4\pi}{3}\sum_{i=1}^{6} r_{bi}^3 \frac{dN_{bi}}{dt} \tag{6}$$

The GRSIS model [6] is used for the kinetics of fission gas behavior.

$$\begin{aligned}
\frac{dC_{s0}}{dt} &= Y \cdot \dot{F} - \sum_{i=1}^{6} J_m(i) - J_n \\
\frac{dN_{b1}}{dt} &= \frac{1}{\rho_1}\left(J_n + J_m(1) - \sum_{j=1}^{6} J_g^{1,j} - \sum_{i=2}^{3} J_g^{i,1} - N_{b1}\frac{d\rho_1}{dt}\right) \\
&\vdots \\
\frac{dN_{b6}}{dt} &= \frac{1}{\rho_3}\left(\sum_{i=1}^{3} J_g^{i,6} + J_m(6) - N_{b6}\frac{d\rho_3}{dt}\right)
\end{aligned} \tag{7}$$

where $C_{si} = \rho_i N_{bi}$, C_{si} gas concentration, ρ_i the number of gas atoms in a bubble, and N_{bi} bubble concentrations. ρ_i is given by a function of temperature and hydrostatic pressure. J_m, J_n and J_g are defined in [6].

For the number of radial elements $n = 5$, the number of variables is $67(=13n+2)$.

2.2 Example problem

A set of coupled equations given by Eqs. (3)-(7) is solved with IDA in Sundials [7] for a representative irradiation condition before the open bubble forms.

Fig. 1 and Fig. 2 plot the calculated results of the coupled equations for $n = 5$. Fig. 1 shows how the variation of displacement is caused by swelling increments. Fig. 2 shows that the number of bubbles is closely interrelated to hydrostatic pressure.

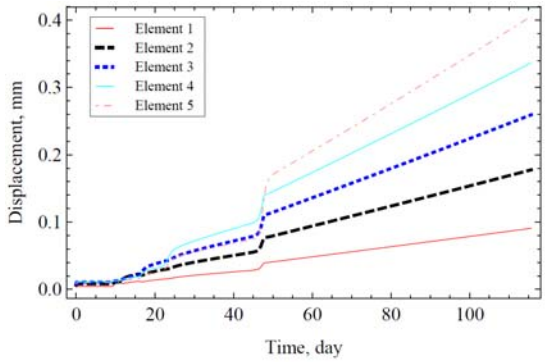

Fig. 1. Displacement as a function of time.

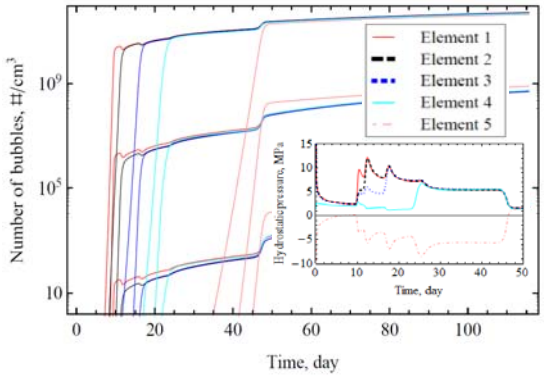

Fig. 2. Number of bubbles and hydrostatic pressure where each element has three class of closed bubbles in size which appears consecutively with time.

By examining the relative factor of run time for a various set of conditions with respect to $n = 5$, a code run is expected to take about 5 min under a condition of 10 radial elements and 10 axial segments, and a burnup of 20 at% if it is completed in such a coupled manner.

3. Verification Results

Verification has been made by putting time-varying solutions into the coupled equations. As for nodal displacements, error measure defined by L2 norm for whole FE equations is far less than 0.1%. As for variables other than nodal displacements, residuals of the equations relative to the variables or their derivatives are evaluated to check the quality of solutions. Maximum relative residual occurs as stresses become extremely small, which turns out not to have significant meaning. By excluding stress during the evaluation of maximum relative residual over time, however, the relative residual remains less than 0.5% ,which is shown in Fig. 3, and is also found to be dominated by a negligibly low gas concentration in the matrix.

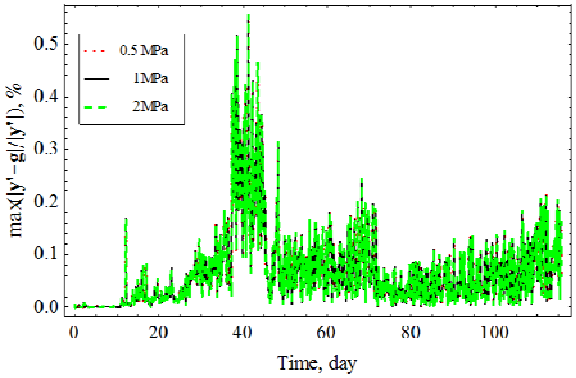

Fig. 3. Maximum of relative residual of governing equations under various cutoff stresses.

4. Summary

A multiphysics approach is applied to develop PUMA with our advanced numerical methods. As an example, the deformation of U-Zr fuel under gaseous swelling is analyzed with a one-level Newton scheme using a backward differentiation formula. Calculation results show that the present approach is viable and efficient. With a little effort this can be extended to model fuel-cladding mechanical interaction, and to attach additional physics for temperature and fuel constituent.

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