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Multiphysics modeling of adhesive interface with damage

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Abstract :

In the context of fuel-cladding interaction modelling in fast nuclear reactors, a multiphysics cohesive zone model of an adhesive interface with damage is proposed in this work. For the moment, only traction/compression behaviour can be described with this model. The effects of temperature, mechanical state, damage and chemical reactions are incorporated in adhesive links modelling. Thermal conductivity is affected by damage. In traction, we model elastic-brittle behaviour which depends on temperature and adhesive links. In compression, we model solid-solid contact.

Keywords : Adhesive interface, Multiphysics, Damage

1 Introduction

In a fast reactor fuel element, cylindrical fuel pellets (mixed oxide $UPuO_2$) are nested inside their cladding (made of stainless steel) and pellets are initially separated from clad by a small radial gap of about $100 \mu\text{m}$ that can be closed during irradiation because of physical, mechanical and chemical phenomena activated by temperature profile imposed on pellets and cladding.

On one hand, an adhesive phenomenon can be observed at this interface after irradiation under specific conditions: a minimum contact time between pellet and cladding, a temperature gradient between 500 and $700 \text{ }^\circ\text{C}$, a closed gap with a low contact pressure (about 10 MPa), presence of fission products and a corrosion layer [1]. On the other hand, different power cycles imposed stresses at the interface can lead to an adhesive rupture (loss of contact), new adhesive interface (after a previous rupture) and damage (modify the interface physico-chemical state). Regarding the reactor safety, adhesive phenomenon modelling and his implementation in fast fuel performance code (GERMINAL) are critical.

We propose here a multiphysics approach to model this adhesive interface. We are particularly interested in mechanical damage and thermochemical effects. We take the hypothesis that adhesion is a chemical adhesion (ionic-covalent bonds) and adhesion is created by oxidation and phase change of stainless steel grains in contact with oxide fuel.

Thermo-chemico-mechanical solid models are particularly studied in concrete [2, 3, 4], biological, electrical batteries [5] and inelastic solids [6] domain. The coupling needs between physics can be justified by the diffusion phenomenon. Diffusion can change the microstructural state : swelling, phases change and create or repair

lacuna (crystal defect) that directly modify the mechanical and thermal behaviour. All these papers take into account the diffusion phenomenon.

In [5, 7] diffusion effect on heat generation and mechanical state (change stresses) are proposed. In [2, 5, 6] the stress/strain solution of the swelling created by diffusion are studied. In [2] damage created by phase change due to diffusion is considered.

In terms of adhesive and damage interface, some papers study the cohesive or adhesive failure with initial condition that adhesive energy is already at the maximum. They are not interested in modelling adhesive energy increase. Only papers on continuum damage-healing mechanics [8, 9] study both adhesive energy increase and damage at solid interface. In these papers, healing is always allowed by polymers' presence at the interface and movement capacity of polymer chains [10, 11]. [12] can be cited as a case where adhesive energy is activated by distance (Van der Waals theory).

In our approach, we model an adhesive interface with continuum mechanical damage, a theoretical adhesive energy higher than examples of the previously cited studies and an adhesive phenomenon activated by thermo-chemo-mechanical conditions. Mechanical behaviour depends on chemical reactions and temperature. On top of that, we propose to take oxidation and phase change models of steels to explain chemical bonds evolution.

2 Constitutive modeling

In consistency with [13, 14], we assume that the cohesive zone behaves like a standard generalized material. We first consider the case of a 1D interface i.e. an interface with only a traction/compression behaviour. We adopt a continuum point of view in the modeling of the finite-thickness interface. The normal displacement jump is denoted by U_n and the associated normal traction is denoted by t_n . To distinguish between traction and compression we assume that the normal displacement jump can be decomposed in a additive manner into extension, U_n^+ and compression, U_n^- .

To describe the oxidation phenomena and the creation of chemical adhesive bonds through the interface we introduce an internal variable, $\xi \in [0, 1]$, that corresponds to the relative percentage of chemical links ($\xi = 0$ means the absence of chemical bonds and $\xi = 1$ corresponds to 100% among all possible chemical bonds). The damage of the interface, i.e. the destruction of chemical bonds due to mechanical strain or stress, is described with the internal variable d that also varies in $[0, 1]$ ($d = 0$ means no damage).

The Helmholtz free energy, ψ , is assumed to be additively splitted into a mechanical part, a chemical part and a thermal part such that:

$$\psi(U_n, \Theta, \xi, d) = \psi_m^+(U_n^+, \Theta, \xi, d) + \psi_m^-(U_n^-, \Theta) + \psi_c(\xi, \Theta) \quad (1)$$

For the mechanical part we adopt a linear elastic behavior for the compression and traction but we assume that only the traction behavior is sensitive to damage and chemical evolution (initially the stiffness in traction is null and there is no damage and the compression stiffness is equal to the stiffness of the neighborhood of the interface):

$$\rho\psi_m^+(U_n^+, \Theta, \xi, d) = (1-d)^2 K^+(\xi, \Theta) \frac{(U_n^+)^2}{2} \quad (2)$$

$$\rho\psi_m^-(U_n^-, \Theta) = K^- \frac{(U_n^-)^2}{2} \quad (3)$$

where K^+ and K^- are the stiffness for traction and compression respectively. K^+ depends on temperature and chemical links such as :

$$K^+(\xi, \Theta) = K\xi \exp - \frac{\Theta - \Theta_0}{\Theta_0} \quad (4)$$

The last contribution is the chemical free energy. As we do not have a detailed knowledge of the reactive scheme we adopt a phenomenological point of view. The chemical reactions are simply modeled with the following energy:

$$\rho\psi_c = C \frac{(1 - \xi)^{n+1}}{n + 1} - \frac{C}{n + 1} \quad (5)$$

where n and C are chemical parameters.

With these thermodynamic potentials, we assume that the interface does not store thermal energy. The thermal energy is just used for making chemical reactions.

Knowing the expression of the free energy, we can write the total dissipation ϕ using the Clausius-Duhem inequality:

$$\phi = t_n \dot{U}_n - \rho \dot{\psi} - \rho s \dot{\Theta} - \frac{1}{\Theta} q_n \frac{\partial \Theta}{\partial x} \geq 0 \quad \forall q_n, \dot{U}_n, \dot{\Theta} \quad (6)$$

where ρ is the density of the interface, t_n is the normal stress, Θ is the absolute temperature, s is the local entropy and q_n is the normal thermal flux. The time derivative of the free energy is given by the following terms:

$$\rho \dot{\psi}_m^+ = (1 - d)^2 K^+ U_n^+ \dot{U}_n^+ - (1 - d) U_n^{+2} K^+ \dot{d} + (1 - d)^2 \frac{\partial K^+}{\partial \xi} \frac{(U_n^+)^2}{2} \dot{\xi} + (1 - d)^2 \frac{\partial K^+}{\partial \Theta} \frac{(U_n^+)^2}{2} \dot{\Theta} \quad (7)$$

$$\rho \dot{\psi}_m^- = K^- U_n^- \dot{U}_n^- \quad (8)$$

$$\rho \dot{\psi}_c = -C(1 - \xi)^n \dot{\xi} \quad (9)$$

Introducing eqs. (7)-(9) in eq. (6), one can obtain:

$$\begin{aligned} \phi = & (t_n^+ - (1 - d)^2 K^+ U_n^+) \dot{U}_n^+ + (t_n^- - K^- U_n^-) \dot{U}_n^- - \\ & \left((1 - d)^2 \frac{\partial K^+}{\partial \Theta} \frac{(U_n^+)^2}{2} + \rho s \right) \dot{\Theta} \\ & + \left((1 - d) U_n^{+2} K^+ \right) \dot{d} - \left((1 - d)^2 \frac{\partial K^+}{\partial \xi} \frac{(U_n^+)^2}{2} - C(1 - \xi)^n \right) \dot{\xi} - \\ & \frac{1}{\Theta} q_n \frac{\partial \Theta}{\partial x} \end{aligned} \quad (10)$$

The mechanical behavior is assumed to be elastic therefore we obtain the following constitutive equations for the stress:

$$t_n^+ = (1-d)^2 K^+ U_n^+ \quad (11)$$

$$t_n^- = K^- U_n^- \quad (12)$$

$$t_n = t_n^+ + t_n^- \quad (13)$$

From eq. (10) we also obtain a constitutive equation for the entropy:

$$s = -(1-d)^2 \frac{\partial K^+}{\partial \Theta} \frac{(U_n^+)^2}{2\rho} \quad (14)$$

For the normal thermal flux, we consider a standard Fourier law but affected by the damage: a fully damaged interface can not transfer heat by conduction mechanisms

$$q_n = -k_t(1-d) \frac{\partial \Theta}{\partial x} \quad (15)$$

It remains two terms in the total dissipation, one associated to damage and the other one associated to the creation of chemical bonds, eq. (10) becomes:

$$\overbrace{\left((1-d)U_n^{+2}K^+ \right)}^{A_d} \dot{d} + \overbrace{\left(-(1-d)^2 \frac{\partial K^+}{\partial \xi} \frac{(U_n^+)^2}{2} + C(1-\xi)^n \right)}^{A_\xi} \dot{\xi} \geq 0 \quad \forall \dot{d}, \dot{\xi} \quad (16)$$

The evolution of the damage is assumed to be of the following form:

$$\dot{d} = \frac{1}{\eta} \langle A_d - g_c d \rangle = \frac{1}{\eta} \left\langle (1-d)U_n^{+2}K^+ - g_c d \right\rangle \quad (17)$$

where η is a viscosity parameter and g_c is a critical fracture energy (MPa). For the chemical evolution we adopt the following form:

$$\dot{\xi} = a(\Theta)(1-d) \langle A_\xi \rangle = a(\Theta)(1-d) \left\langle -(1-d)^2 \frac{\partial K^+}{\partial \xi} \frac{(U_n^+)^2}{2} + C(1-\xi)^n \right\rangle \quad (18)$$

the term $a(\Theta) = A_m \exp(-E_a/(R\Theta))$ is an Arrhenius like term with E_a an activation energy, R the perfect gaz constant and A_m a kinetic factor. Introducing eqs. (17)-(18) into eq. (16) it can be seen that the Clausius-Duhem inequality is always satisfied. From eq. (18) it can be seen that the chemical affinity (thermodynamical force associated to a chemical evolution) can be negative in tension which leads to a null chemical evolution rate. The coupling between mechanical state and chemical reaction is controlled with the help of the parameter C .

3 Model behaviour under thermal and mechanical cycles

To study model behaviour we propose to impose thermal and displacement cycles as shown in figure 1 and 2. The model has been implemented in the open-source MFront code generator [15, 16] and we simulate the behaviour of a material point with MTest (a code delivered with MFront).

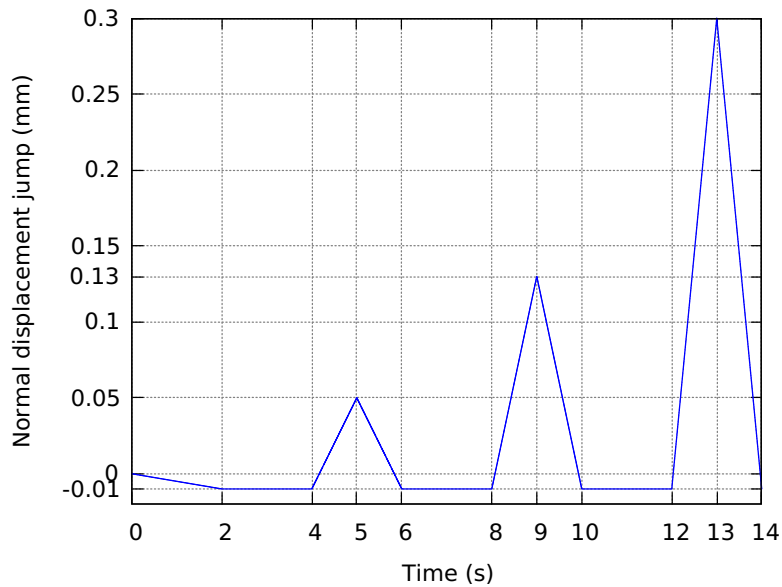


Figure 1: Normal opening displacement imposed versus times

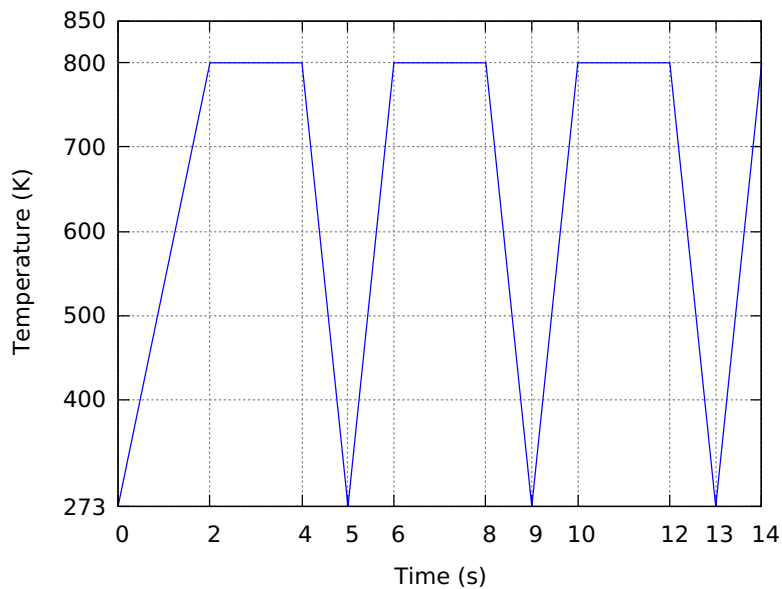


Figure 2: Temperature imposed versus times

Figure 3 shows that chemical links can't be created in traction and can increase over time in compression or null state. Temperature affects chemical links like threshold effect. Damage is similar to literature on continuum damage theory.

In figure 4 elastic-brittle behaviour is found with a stress response which depends on damage, temperature and chemical links.

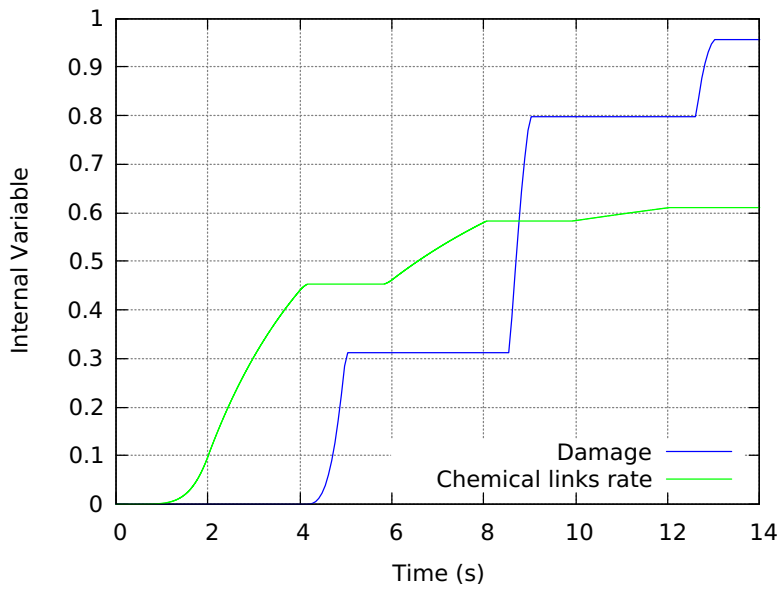


Figure 3: Internal variable evolution under cycles

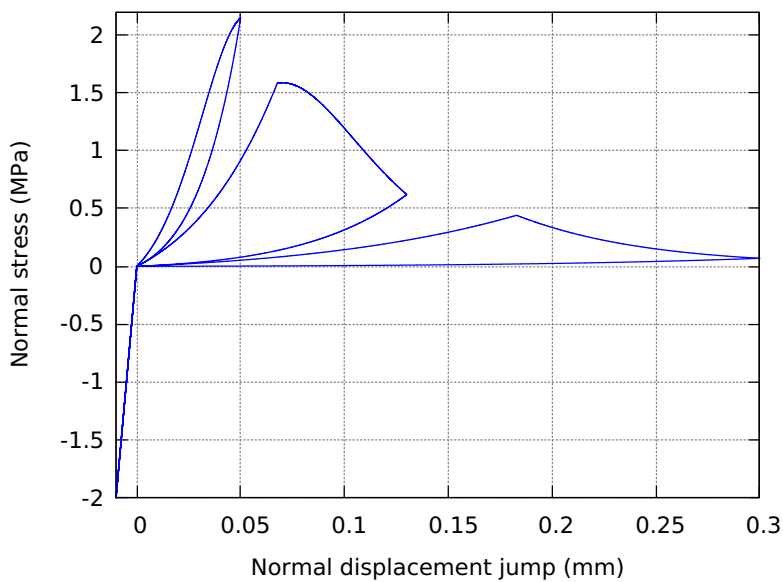


Figure 4: Model normal stress - normal displacement response under thermal and mechanical cycles

4 Adhesive contact finite elements simulation in 1, 2 or 3 dimensions

The model described in this work has been built to simulate an adhesive contact between the pellet and his cladding ,especially in 1 and 2 dimensions, with finite element method. To simulate pellet cladding adhesive interface, described in the introduction 1, we consider using an adhesive contact law with this multiphysics cohesive zone. We propose to add a cohesive zone to cladding mesh frontier as well as a cohesive contact law between cohesive zone and pellet mesh. The adhesive contact law only manages contact detection and links degree of freedom of cohesive zone and pellet mesh frontier. As for the cohesive zone, it links mechanically pellet and cladding , i.e it models solid-solid contact in closed gap and adhesive behaviour in opening gap.

5 Conclusion

This work presents a thermo-chemo-mechanical model of adhesive and damage interface based on an original approach that allow take into account the coupling between the three physics on traction/compression interface behaviour. Thermodynamic potential defines in this model seems to be easily adapted to model adhesive phenomenon that appears in solid-solid interface under temperature, contact pressure and corrosion. The perspective of this work is to reach a complete healing behaviour under cycles and to integrate the influence of compressive strain on chemical links evolution.

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