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Peridynamic modeling of fuel pellet cracking

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ABSTRACT

This study presents the peridynamic simulation of thermal cracking behavior in uranium dioxide, UO_2 fuel pellets that are used in light water reactors (LWR). The performance of the reactor is influenced by the thermo-mechanical behavior of the pellets. During the fission process, the pellets are subjected to high temperature gradients, and the oxygen diffusion significantly affects the temperature distribution. Therefore, a coupled analysis of temperature and oxygen diffusions and deformation is unavoidable in order to predict accurate cracking behavior in a fuel pellet. The accuracy of the predictions is verified qualitatively by comparing with the previous studies.

1. Introduction

Nuclear fuel pellets are used to generate heat for power generation as a result of fission process. Therefore, it is essential to understand its thermal transport for enhancing power output and preventing potential accidents. Uranium dioxide (UO_2) is the main component of the fuel pellet. Its composition can have both an excess and deficiency of oxygen relative to stoichiometric UO_2 [13]. Studies by show that in hyper-stoichiometric Urania ($UO_2 + x$), the oxygen ions tend to accumulate in the regions of high temperature gradient or the Soret effect (the transport of oxygen atoms due to a temperature gradient) [1,23]. It is experimentally found that the thermal conductivity of UO_2 decreases with temperature [15] and with increasing non-stoichiometry [2]. The fuel pellets are placed in a cladding and there exists a gap between fuel pellet and the cladding. The cooling water passing through the fuel elements extracts heat from the nuclear fuels [5]. However, significant microstructural changes and deterioration of the fuel pellet occur due to the fission process. As a result, the degraded physical state of the fuel becomes the limiting factor for long term and transient reactor performance [4].

As the fuel temperature increases, radial cracks occur and propagate towards the center of fuel pellet. Also, circumferential crack patterns develop during a steady-state operation. Cracking patterns significantly affect the fuel thermal conductivity and neutron diffusion coefficient. Therefore, it influences the overall pellet thermal expansion; thus, the gap closure occurs between the pellet and clad. Moreover, the oxygen diffusion affects the thermal conductivity which leads to an increase in temperature. Hence, the analysis of fuel pellet behavior requires a fully coupled consideration of thermal diffusion, oxygen diffusion, deformation and cracking process.

The Finite Element Method (FEM) has been extensively used by Ito et al. [9], Lassmann [14], Berna et al. [3] and Gates et al. [6] while disregarding the coupling of multi-physics modeling and crack propagation in fuel pellets. Also, they simulated the fuel rod behavior in the radial direction under axisymmetric assumptions. Furthermore, Ramirez et al. [23] performed finite element simulations to couple heat and oxygen diffusion for UO_2 fuel rods in one-dimensional (radial)

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configurations by using COMSOL Multiphysics, a commercially available software. Their study revealed the influence of oxygen on thermal conductivity which significantly increases the maximum temperature in a fuel rod. Newman et al. [19] coupled thermomechanics with heat and oxygen diffusion in UO_2 fuel rods. They coupled the governing equations through the material properties that are functions of density, temperature and oxygen concentration, and investigated the opening of a pre-determined crack in a fuel rod due to thermal expansion. Mihaila et al. [18] studied the coupling of thermomechanics with heat and oxygen diffusion in UO_2 fuel elements by using COMSOL Multiphysics. In their study, they presented one-dimensional simulations; thus, it did not include crack propagation in fuel pellets.

Williamson and Knoll [28] simulated the discrete dynamic fracturing of nuclear fuel by using cohesive zone elements under thermomechanical loads. The cohesive surfaces are placed along the potential crack paths, and the cohesive crack initiation is triggered at locations where the maximum principal stress reaches the fracture strength. Williamson [29] also tested smeared cracking approximation of pellets and compared with discrete fuel pellet analysis. This study revealed that smeared pellet simulation predicts slightly higher temperatures and delay in gap closure.

Rashid et al. [24] performed a two-dimensional finite element analysis to predict thermal, mechanical and chemical behavior of a fuel rod during irradiation by assuming a predetermined crack location. Williamson et al. [30] performed a multi-dimensional multi-physics finite element analysis of nuclear fuel pellets by including fracture via relocation and smeared crack models. Recently, Sercombe et al. [25] used FEM to simulate hydride blister cracking in fuel pellets. When a pre-determined hoop stress is exceeded at the clad outer surface, a radial cracking of the blister is introduced in the simulation by modifying the boundary conditions.

Majority of the aforementioned FE models introduced cracks at a priori known crack paths. However, such paths are not available prior to the analysis. The presence of stress singularity at the crack tips and material heterogeneity introduce additional challenges in predicting crack initiation sites. By using Discrete Element Method (DEM), Huang et al. [8] removed these challenges, and simulated thermally driven randomly initiated cracks in fuel pellets. They were able to predict radial and circumferential cracks in a fuel pellet.

Alternative to DEM is the peridynamic theory which is based on the integral-differential equations and free of spatial derivatives [26]. Although its governing equations are solved numerically through discretization, it is based on the assumptions of nonlocal continuum mechanics. Also, it enables crack nucleation and propagation without an external failure criteria. Mella and Wenman [16] predicted the fracture behavior of a pellet for specified (pre-computed) temperature profiles by using peridynamics. The present study also employs peridynamics to predict cracking in a fuel pellet while considering the fully coupled field equations of heat and oxygen diffusion and mechanical deformations. The material properties are dependent on temperature and oxygen concentration. The accuracy of the predictions is verified both quantitatively and qualitatively by comparing with the previous studies and finite element analysis prediction.

2. Pellet thermomechanical model

The peridynamic equation of motion was introduced by Silling [26] as

$$\rho(C,\Theta)\ddot{\mathbf{u}}(\mathbf{x},t)=\int_H \mathbf{f}(\mathbf{x}'-\mathbf{x},\mathbf{u}'-\mathbf{u})dV'+\mathbf{b}(\mathbf{x},t) \tag{1}$$

where $\mathbf{u}(\mathbf{x},t)$ and $\mathbf{b}(\mathbf{x},t)$ represent the displacement and body force density vectors at material point, $\mathbf{x}$. The force density vector including the thermal effects is suggested by Kilic and Madenci [11] as

$$\mathbf{f}=c(C,\Theta)[s-\alpha(\Theta)T_{avg}(\Theta)]\frac{(\mathbf{x}'+\mathbf{u}')-(\mathbf{x}+\mathbf{u})}{|(\mathbf{x}'+\mathbf{u}')-(\mathbf{x}+\mathbf{u})|} \tag{2}$$

where Θ and C represent temperature and oxygen concentration, respectively. The stretch between two material points $\mathbf{x}$ and $\mathbf{x}'$ is defined as

$$s=\frac{|(\mathbf{x}'+\mathbf{u}')-(\mathbf{x}+\mathbf{u})|-|\mathbf{x}'-\mathbf{x}|}{|\mathbf{x}'-\mathbf{x}|} \tag{3}$$

The material parameter c is derived by Gerstle et al. [7] as a function of elastic modulus, E, thickness, h and horizon size, δ as $c=\frac{9E}{\pi h\delta^3}$ for 2D and $c=\frac{12E}{\pi\delta^4}$ for 3D, and α is the coefficient of thermal expansion. The mean value of the change in temperatures, T_{avg} at material points $\mathbf{x}$ and $\mathbf{x}'$, is defined as

$$T_{avg}=\frac{(\Theta-\Theta_0)+(\Theta'-\Theta_0)}{2} \tag{4}$$

in which Θ and Θ' represent the temperature at material points $\mathbf{x}$ and $\mathbf{x}'$, Θ_0 represents the reference temperature.Failure process begins when the stretch between the two material points, $\mathbf{x}$ and $\mathbf{x}'$ exceeds a critical stretch value, s_{cr}. The critical stretch value can be obtained from the critical energy release rate of the material, G_c as [27]

$$s_{cr}=\sqrt{\frac{\pi G_c}{3\kappa\delta}}\ \text{for 2D and}\ s_{cr}=\sqrt{\frac{5G_c}{9\kappa\delta}}\ \ \text{for 3D} \tag{5}$$