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Discrete Modeling of Early-Life Thermal Fracture in Ceramic Nuclear Fuel

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ABSTRACT: Fracturing of ceramic fuel pellets heavily influences performance of light water reactor (LWR) fuel, beginning with the initial ramp to power. Because of the important effects that fracture has on fuel performance, a realistic, physically based fracture modeling capability is essential to predict fuel behavior in a wide variety of normal and abnormal conditions. Modeling fracture within the context of the finite element method, which is based on continuous interpolations of solution variables, is challenging because fracture is an inherently discontinuous phenomenon. Two modeling techniques are being explored to model fracture as a discrete displacement discontinuity to nuclear fuel: the extended finite element method (XFEM), and the discrete element method (DEM). The XFEM is based on the standard finite element method, but with enhancements to represent discontinuous behavior. The DEM represents a solid as a network of particles connected by bonds, which can fail if a fracture criterion is reached. This paper presents initial results obtained by applying the aforementioned techniques to model fuel fracturing during the early life of ceramic LWR fuel. The results of this work will be used to inform behavior models in the BISON fuel performance code. It is expected that an improved physically-based representation of the effects of fracture will enhance predictivity in both normal and abnormal conditions.

KEYWORDS: *fuel fracture, discrete element method, extended finite element method*

I. INTRODUCTION

Fracturing of ceramic fuel pellets heavily influences performance of light water reactor (LWR) fuel[1,2]. Early in the life of fuel, starting with the initial power ramp, large thermal gradients cause high tensile hoop and axial stresses in the outer region of the fuel pellets, resulting in the formation of radial and axial cracks. Circumferential cracks form due to thermal gradients that occur when the power is ramped down. These thermal cracks cause the fuel to expand radially, closing the pellet/cladding gap and enhancing the thermal conductance across that gap, while decreasing the effective conductivity of the fuel in directions normal to the cracking. At lower length scales, formation of microcracks is an important contributor to the decrease in bulk thermal conductivity that occurs over the life of the fuel as the burnup increases. Fuel cracking also plays a significant role in cladding failure due to pellet-cad mechanical interaction (PCMI) because of stress concentrations that can occur in the cladding adjacent to cracked fuel.

Because of the important effects that fracture has on fuel performance, a realistic, physically based fracture modeling capability is essential to predict fuel behavior in a wide variety of normal and abnormal conditions. Current state-of-the-art fuel performance codes typically model fuel fracture using a combination of models for smeared cracking, which accounts for the loss of material strength, and relocation, which accounts for the outward radial movement of fuel fragments[3]. Modeling fracture within the context of the finite element method, which is based on continuous interpolations of solution variables, has always been challenging because fracture is an inherently discontinuous phenomenon. Smeared cracking models represent the displacement discontinuities that occur due to cracking as strains within the continuous finite element method. The shortcomings of the smeared cracking approach for modeling fracture are well-documented[4]. These assumptions lead to dependencies on the mesh size and orientation.

Fracturing nuclear fuel has been successfully modeled using cohesive zone models to represent discrete fracture[5]. A major shortcoming of this method, however, is that crack paths must be defined prior to running a simulation. Work is underway at Idaho National Laboratory to apply two modeling techniques to model fracture as a discrete displacement discontinuity to nuclear fuel: The extended finite element method (XFEM), and the discrete element method (DEM). Both of these methods permit arbitrary initiation and growth of discrete cracks, which is a significant advantage over the aforementioned alternatives. The XFEM is based on the standard finite element method, but with enhancements to represent discontinuous behavior. The DEM represents a solid as a network of particles connected by bonds, which can fail if a fracture criterion is reached.

This paper presents initial results applying the XFEM and DEM to model fuel fracturing. This work has initially focused on early life behavior of ceramic LWR fuel. A DEM model of coupled heat conduction and solid mechanics has been developed and used to simulate random initiation and propagation of thermally driven cracks during initial power cycles. This DEM model predicts the formation of realistic radial cracking patterns during power rise and circumferential cracks as power is ramped down. A coupled thermal-mechanical XFEM method that includes discontinuities in both temperature and displacement fields at crack locations has been developed and is being applied to thermal fracture of LWR fuel. These initial results are very encouraging, and these techniques are expected to provide improved understanding of fuel behavior in a wide variety of conditions.

II. DISCRETE ELEMENT METHOD

The discrete element method (DEM), was originally developed over 30 years ago[6], and has been widely used by the geotechnical engineering community to model mechanical deformation, fracturing, and flow of fragments of polycrystalline materials at a wide variety of scales. DEM represents a solid continuum as a network of nodes (also referred to as particles) connected by elastic beams. To model thermally induced fracture in ceramic nuclear fuel, a capability to model coupled heat conduction and mechanical deformation is needed. This capability has recently been developed and applied to nuclear fuel by the authors and described in detail[7]. A summary of the formulation and application of DEM to fracturing nuclear fuel is provided here.

1. Thermomechanical DEM Formulation

Each node in the DEM model exerts forces and moments on its neighbors. The bonds between neighboring nodes are represented as beams. The force $\boldsymbol{F}_{i,j}$ and moment $\boldsymbol{M}_{i,j}$ exerted on node i by its neighboring node, j are:

$$\boldsymbol{F}_{i,j} = k_n\left(d_{i,j} - d_{i,j}^0\right)\boldsymbol{n}_{i,j} + \frac{1}{2}k_s\left(\phi_{i,j} + \phi_{j,i}\right)\boldsymbol{s}_{i,j} \quad (1)$$

$$\boldsymbol{M}_{i,j} = k_s d_{i,j}\left[\frac{\phi}{12}\left(\phi_{i,j} - \phi_{j,i}\right) + \frac{1}{2}\left(\frac{2}{3}\phi_{i,j} + \frac{1}{3}\phi j, i\right)\right]. \quad (2)$$

In these equations, $d_{i,j}$ is the current distance between the centers of nodes i and j, and $d_{i,j}^0 = r_i + r_j$ is the initial equilibrium distance between those nodes, where r_i is the radius of particle i. $\boldsymbol{n}_{i,j}$ and $\boldsymbol{s}_{i,j}$ are unit vectors parallel and perpendicular, respectively, to the line connecting the two nodes. $\phi_{i,j}$ is the rotation angle of the beam connecting nodes i and j at node i. k_n and k_s are normal and shear force constants.

If a regular square or triangular lattice is used, the force constants are directly related to the macroscopic elastic moduli and geometric properties of the beam used to represent the bond. The normal force constant for each beam is calculated as $k_n = E_0 A/d$, where E_0 is the macroscopic Young's modulus, A is the cross-sectional area of the beam, and d is the length of the beam. The shear force constant is calculated as $k_s = 12E_0 I\left[d^2(1+\Phi)\right]$, where I is the geometric part of the moment of inertia, $\Phi = 12E_0 I/G_0 A d^2$, and G_0 is the shear modulus.

A random network is used in the present work to prevent lattice symmetry from affecting the simulated fracture pattern. In this case, the force constants must be calibrated to obtain the desired macroscopic elastic behavior.

The bonds in the DEM model are initially elastic, and behave that way until they reach a failure criterion:

$$\tau = \left(\frac{|\boldsymbol{F}_{i,j}|}{F_c}\right)^2 + \max\left(\frac{|\boldsymbol{M}_{i,j}|}{M_c}, \frac{|\boldsymbol{M}_{i,j}}{M_c}\right) > 1, \quad (3)$$

where F_c and M_c are the critical force and moment corresponding to a von Mises failure criterion for elastic beams. The critical force and moment are functions of the length of the beam and the critical tensile strain and rotation angle. Because of this strain-based criterion, tensile failure and shear failure under compression can be represented.

Heat conduction is based on the classical equation:

$$\rho C\frac{\partial T}{\partial t} = \nabla \cdot K\nabla T + Q, \quad (4)$$

where ρ is the density, C is the heat capacity, T is the temperature, K is the thermal conductivity, and Q is the volumetric heating. This equation is solved using the finite volume method. Finite volume cells are constructed using normal planes at the midpoints of the DEM bonds. Temperature-dependent models for the conductivity and heat capacity of UO_2 are used[8].

2. Nuclear Fuel Simulations with DEM

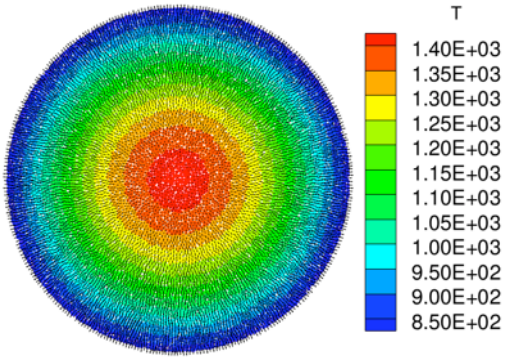
A 2D DEM model of a typical LWR fuel rod cross section was created to demonstrate the application this technique to ceramic nuclear fuel. This model employs a plane strain assumption, and includes only the fuel pellet, with no cladding. This is to simplify the model for this demonstration. To include the cladding, a bond model appropriate for ductile material and a model for heat transfer between the fuel/pellet would be required. Those additional features could be included in future versions of this model.

Because the cladding and pellet/cladding gap are not included in this model, it is necessary to use an alternative method to prescribe thermal boundary conditions on the fuel pellet surface. A 2D finite element model of the cross-section of a fuel rod including the fuel, cladding and gap was run in the BISON fuel performance code[9]. This model was run for the desired power histories, and time histories of the temperature at the pellet surface were output. These temperature histories are then used to prescribe Dirichlet boundary conditions at the nodes on the outer surface in the DEM model, in conjunction with compatible histories of volumetric heating in the pellet interior.

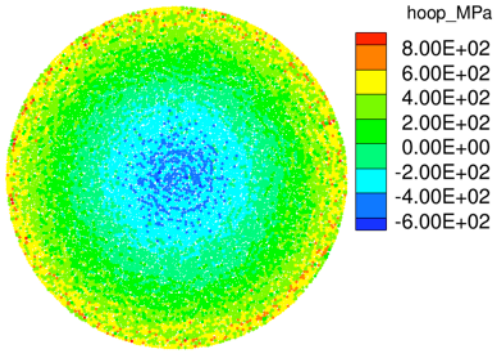
Prior to running the DEM model of the fuel pellet, it is necessary to calibrate both the elastic properties and the fracture properties of the bonds connecting particles. A rectangular block of UO_2 was modeled with DEM using mesh characteristics similar to those used in the fuel pellet model. This model was subjected to tensile loading, and

the critical strain criterion was adjusted until the material failed at a load close to the tensile strength of UO_2, assumed here to be 130 MPa.

Prior to using DEM to model fracturing fuel, the DEM fuel pellet model was run without allowing bonds to break to see how well the model predicted the thermal and mechanical response of un-fractured fuel. Figure 1 shows the temperature and hoop stress fields predicted by the DEM model without fracturing after a linearly increasing ramp from zero power to a full power of 25 kW/m over 10000 s. The randomness in the hoop stress field is due both to the fact that the DEM model uses a random packing of particles, and that the elastic moduli of the bonds are randomized to account for inhomogeneities in the material.



(a)

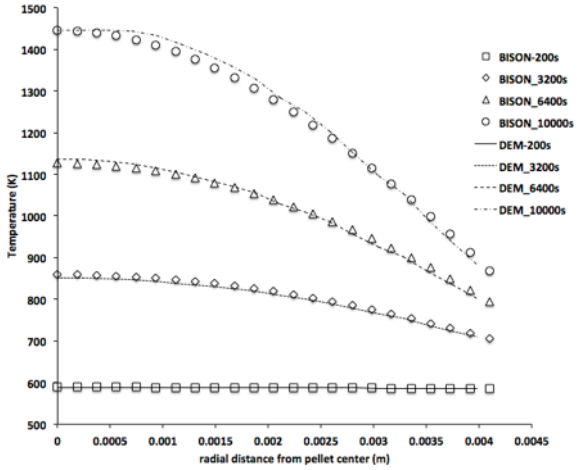


(b)

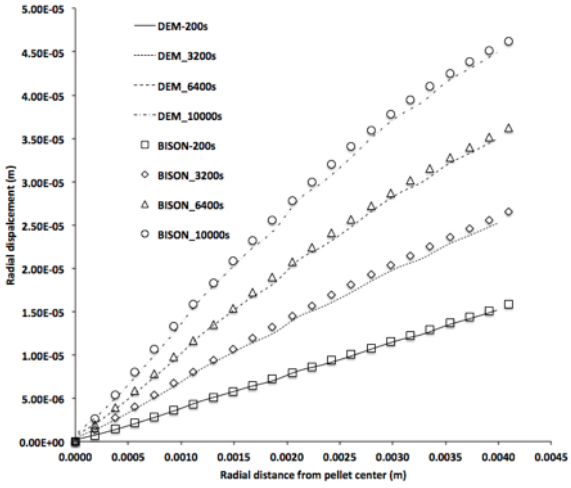
Figure 1: Results of DEM simulation of fuel pellet without fracturing following rise to 25kW/m power showing (a) Temperature field (K) (b) Hoop stress field (MPa).

To check the validity of these results, the temperature and displacements of the DEM model without fracturing were compared with the finite element model of the pellet that was used to obtain thermal boundary conditions. If the DEM model is functioning correctly, it should produce results very similar to those from the finite element model, which also treated the fuel as an unfractured continuous material, and used compatible thermal and mechanical material models. Figure 2 shows comparisons of the thermal and radial displacements obtained from these two models along radial lines from the fuel center to the exterior at various points in time along the 10000 s ramp to full power. It is evident that aside from some slight local deviations, which are to be expected, the DEM results match the benchmark finite element solutions very well.

Once the DEM model without fracture was demonstrated to reasonably capture the thermo-elastic response, the model was run again, but this time allowing for bonds to break between particles when the failure criterion calibrated on the tensile specimen was reached. Figure 3 shows the results of this simulation, including (a) the temperature, (b) the hoop stress, and (c) the crack aperture.



(a)



(b)

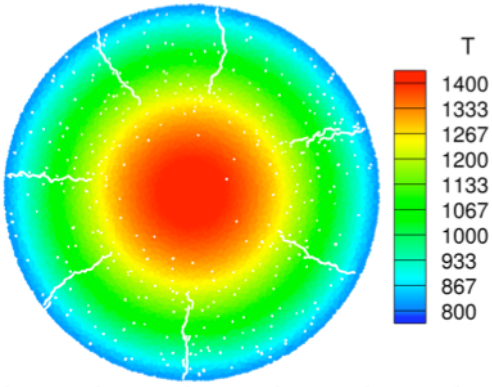
Figure 2: Comparison of simulation results from DEM and BISON finite element model at various times on ramp up to 25 kW/m power. (a) Temperatures (b) Radial displacements.

From these results, it can be seen that there are microcracks distributed throughout the pellet, and that microcracks coalesced to form seven major radial macroscopic cracks that started at the outer surface, and terminated when they reached the zone of compressive stress at the center of the pellet.

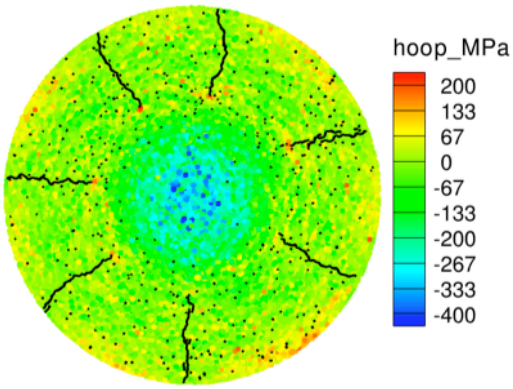
In this model, no heat conduction is permitted across broken bonds. It is important to include that in cases where there are significant temperature gradients across cracks, but in this case, where the cracking is primarily radial, heat flows parallel to the cracks, and the presence of the cracks has very little influence on the temperature field, as seen in Figure 3(a). Heat conduction across the gaps is important

when circumferential cracks form, and can be included in future work.

A comparison of the hoop stresses shown in Figure 3(b) for the cracked case and the hoop stresses in Figure 2(b) for the uncracked case clearly demonstrates how the high tensile stresses on the exterior are relieved by the cracking, and the compressive stresses in the core are also reduced.



(a)



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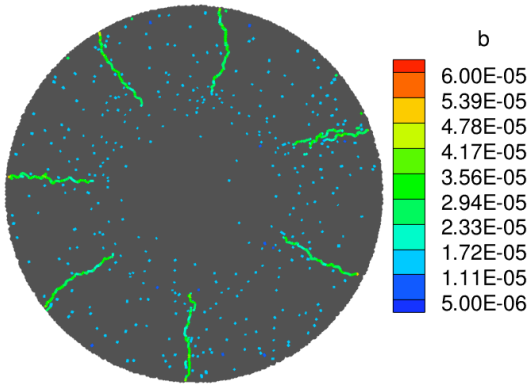


(c)

Figure 3: Results of DEM simulation with fracturing after rise to 25 kW/m power, showing (a) temperature (K), (b) hoop stress (MPa), and (c) cracks colored by aperture (m).

The pattern and number of cracks is consistent with expected behavior at this power level[1]. This model has been run under linear ramps to a variety of powers ranging from 10 kW/m to 40 kW/m, and crack patterns are consistent with expectations at those power levels.

The DEM fuel pellet model was also used to model fuel fracture during a ramp down from full power. The model was subjected to a linear ramp to 25 kW/m over 10000 s. The power was held at that level for 10000 s, and then linearly ramped down to zero power over 10000 s. During the power ramp-down, the radial cracks that formed during the ramp to power were able to extend through the pellet center as it went from a compressive state to a tensile state. In addition, the tensile stresses in the core permitted the formation of circumferential cracks that spanned between some of the radial cracks. Most of these circumferential cracks initiated at the locations of radial cracks and propagated to span adjacent radial cracks. Because the current model does not permit heat transfer across fractured material, and there are significant thermal gradients normal to these circumferential cracks, this model is not expected to accurately model heat transfer in a pellet with circumferential cracks. It does, however, demonstrate that the DEM model is capable of predicting the expected formation of circumferential cracks during power-down.

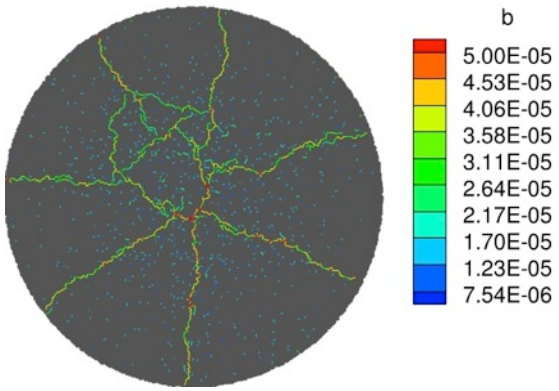


Figure 4: Results of DEM simulation with fracturing after rise to 25 kW/m power and ramp down to zero power, showing cracks colored by aperture (m).

III. EXTENDED FINITE ELEMENT METHOD

The XFEM is an extension of the standard finite element method that allows for discontinuities that pass through the domain at arbitrary locations[10,11]. The XFEM has been used with great success for modeling a variety of discontinuities, including fractures and interfaces between materials with dissimilar properties. The assumption of continuity of the solution fields in the finite element method, which has led to the success of that method for continuum mechanics applications, has been a significant weakness for the finite element method for modeling fracture. Efforts to model fracture by modifying stress-strain relationships in the standard finite element method lead to dependencies both on the mesh size and orientation due to the assumptions of continuity.

1. XFEM Formulation

The XFEM permits arbitrary discontinuities by enriching the basis functions used in the finite element method with discontinuous functions. In the standard finite

element method, the solution vector $\boldsymbol{u}$ at a given position, $\boldsymbol{x}$, and time, t, is interpolated from the nodal solution $\boldsymbol{u}_I$ using continuous shape functions N_I:

$$\boldsymbol{u}(\boldsymbol{x},t) = \sum_{I=1}^{n} N_I(\boldsymbol{x})\boldsymbol{u}_I(t) \quad (5)$$

The XFEM introduces a discontinuity in a continuous solution field using the Heaviside function H, which evaluates to 1 on one side of the discontinuity and 0 on the other. Additional degrees of freedom $\boldsymbol{e}_I$ corresponding to this enrichment are added to all nodes whose basis is intersected by the discontinuity. The enriched displacement field is then expressed as:

$$\boldsymbol{u}(\boldsymbol{x},t) = \sum_{I=1}^{n} N_I(\boldsymbol{x})(\boldsymbol{u}_I(t) + H(\boldsymbol{x})\boldsymbol{e}_I(t)) \quad (6)$$

The addition of the degrees of freedom corresponding to the discontinuity distinguishes the XFEM from other methods for representing embedded discontinuities. In addition to Heaviside-function enrichment, additional higher-order enrichment functions are often employed in the region near the crack tip in fracture mechanics applications to capture the effects of singularities in that region while still using a relatively coarse computational mesh.

Because the XFEM can be used to rigorously treat the effects of cracking as a strong discontinuity within the elements traversed by a crack, it overcomes the mesh dependencies inherent in smeared crack modeling approaches. The enhancement of the continuous field permits cracks to be modeled discretely, but allows them to propagate arbitrarily through the mesh without regard to the locations of finite element boundaries. The XFEM has a significant advantage over techniques that represent discrete cracks using interface elements at solid element boundaries, because the mesh does not need to conform to the crack path, and the crack path does not need to be defined prior to the analysis.

Following the initial development of the XFEM, an alternative method for representing Heaviside discontinuities has emerged. This technique, often referred to as the phantom node method[12], introduces a Heaviside discontinuity by replacing the finite element that contains the discontinuity with two overlapping elements that have the same topology as the original element. Each of these elements has a part that represents physical material, and a part that is outside the solution domain, and is thus non-physical. The nodes connected to the non-physical material are referred to as phantom nodes. The physical nodes are connected to the original nodes that are shared with neighboring elements, and non-physical nodes are connected to each other. The standard finite element interpolations are used across the physical and non-physical parts of the elements, but integrals are performed only on the physical parts of the domain. Following the introduction of this method, it was demonstrated[13] that it is equivalent to the original Heaviside-enriched XFEM. These methods result in the introduction of the same number of new degrees of freedom to the system, and continuous fields are interpolated across the domain in the same manner.

The phantom node method is often more straightforward to implement in an existing finite element code than the classical XFEM, particularly for the treatment of crack branching and coalescence. In the classical XFEM, a set of additional degrees of freedom is added to all finite element nodes whose basis is intersected by a discontinuity. If a node's basis is intersected by multiple discontinuities, an additional set of degrees of freedom is required for each discontinuity. Many finite element codes do not naturally permit an arbitrarily changing set of degrees of freedom at each node. Managing the degrees of freedom also becomes a challenge when nodes are affected by multiple discontinuities.

The primary challenge in the phantom node method is developing a general mesh-cutting algorithm that duplicates elements cut by discontinuities and connects the nodes of these newly-created partial elements in a way that ensures that the model correctly represents the topology of the fractured material. An effective algorithm to accomplish this task has been developed[14] and used in this work. In this algorithm, nodes of neighboring elements are merged if those elements both have physical portions adjacent to each other along the common edge shared by those elements.

A version of this mesh cutting algorithm has been developed within the BISON fuel performance code to permit using XFEM to model fractures in nuclear fuel. This implementation currently only supports 2D models, but the mesh-cutting algorithm is naturally extensible to support 3D models. The implementation of this algorithm in BISON currently supports multiple cracks in the mesh, but does not yet support cutting an element with multiple cracks. This is necessary to support crack branching, and will be developed in the future.

BISON is based on the MOOSE multiphysics finite element framework, which is a modular object-oriented code that facilitates the solution of arbitrary multiphysics problems. MOOSE uses the Jacobian-free Newton Krylov method to solve coupled systems of equations, which permits the use of Newton's method for solving nonlinear problems without forming the Jacobian. Because the XFEM was developed in this framework using the phantom node method, once the mesh is cut by a discontinuity, the discontinuity affects all of the coupled physics that are being solved in a model. For BISON problems, a coupled system of equations for stress equilibrium and heat conduction is solved. Stress equilibrium is enforced:

$$\nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{f} = 0, \quad (7)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, ρ is the density, and $\boldsymbol{f}$ is the applied body force per unit mass. The energy balance equation (Equation 4) is used to describe heat conduction. The same mesh is used to solve the equations of stress equilibrium and heat conduction. Because the phantom node method modifies that single, shared mesh to introduce discontinuities in the solution fields, those discontinuities are introduced to both the temperature and displacement fields at fracture locations.

The current implementation of XFEM in MOOSE/BISON does not yet support boundary conditions on the surfaces created by the cut plane. For thermomechanical fracture mechanics problems, this means that there is currently no capability for heat transfer across fracture planes, and there are no tractions due to cohesive

zone laws or contact constraints, so only brittle fracture is supported. Enforcement of boundary conditions on cut planes will be added in the near future.

2. Nuclear Fuel Simulation with XFEM

To demonstrate the applicability of the XFEM to modeling nuclear fuel fracture, a 2D plane strain finite element model of a fuel pellet with the same properties as the DEM model discussed earlier was created. For consistency with the DEM model, only the fuel was modeled, and the same temperature boundary conditions were applied to the pellet exterior. Figure 5 shows the finite element mesh used for the XFEM fuel pellet simulation.

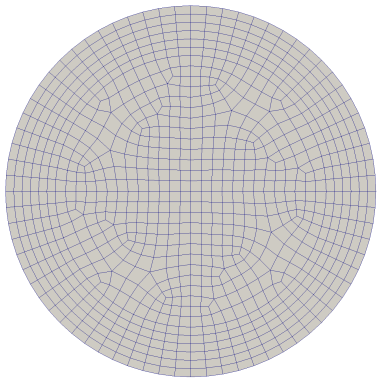
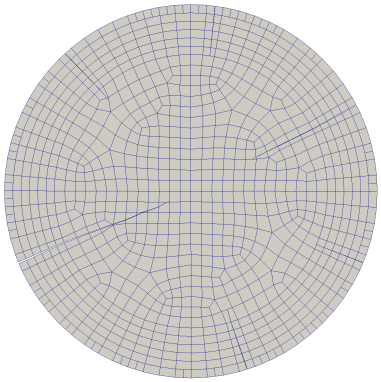


Figure 5: Mesh used for the XFEM fuel pellet simulation

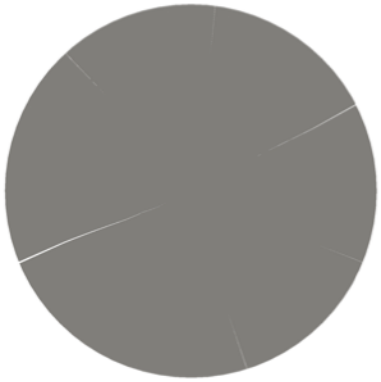
The fuel pellet model was ramped to the same power history as the DEM model was (linear ramp to 25 kW/m power over 10000 s). Cracks were permitted to initiate in elements adjacent to the exterior boundary of the fuel pellet, and extend from existing cracks in adjacent elements. The model is solved at each step, and elements are checked to see whether a condition for crack initiation or extension is met. Cracks are extended or initiated if the criterion is met, and the solution is repeated until no elements meet the cracking conditions. A wide variety of conditions for crack growth and crack orientation could be used. The intent of this analysis is to assess the ability of the model to represent radial cracks, so cracks are initiated or grown if the hoop stress exceeds the tensile strength of UO_2, assumed here to be 130 MPa. Cracks are oriented normal to the hoop direction. A more general criterion would be needed to capture circumferential cracking.

In a cylindrical fuel pellet, before any cracking occurs, the hoop stress is uniform in the circumferential direction. Because of this uniformity in the stress, cracks would simultaneously initiate at every element around the pellet exterior once the critical hoop stress criterion was met. In reality, there are slight nonuniformities in the pellet that cause elevated stress and fracture localization at some locations. To permit the model to capture fracture localization, the tensile strength was randomly varied spatially. This was accomplished by multiplying it by a randomly sampled parameter following a uniform distribution ranging from 0.95 to 1.05. Figure 6 shows the pattern of cracks that developed after the model had been ramped to full power. Figure 6(a) shows the finite element mesh with the cut plane boundaries, and Figure 6(b) shows a silhouette of the deformed mesh. Contour plots of the temperature and hoop stress predicted at full power by the XFEM model, with the crack patterns, are shown in Figure 7.

From Figures 6 and 7, it can be seen that numerous cracks initiated near the exterior boundary of the fuel pellet, but with increased power, fracture localized at 6 macroscopic cracks, which is consistent with the DEM model results presented earlier, and with expected results[1]. As expected, the radial cracks have little influence on the temperature solution because heat conduction occurs in the radial direction, tangential to the cracks. The cracks relieve the tensile hoop stresses on the exterior of the pellet as well as the compressive hoop stresses on the interior.

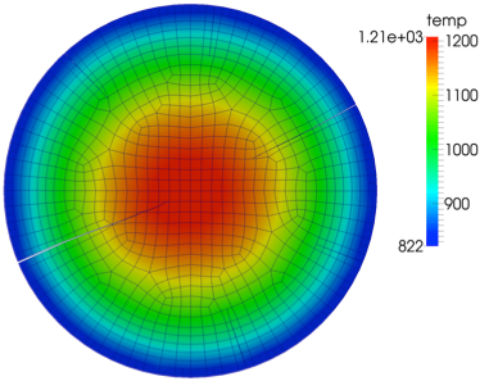


(a) Finite element mesh showing cut plane boundaries

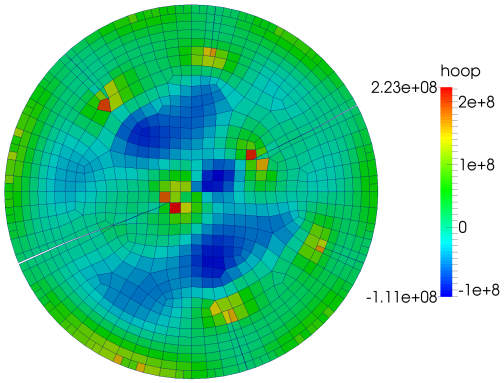


(b) Silhouette of deformed mesh

Figure 6: Fracture pattern in the XFEM model at 25 kW/m



(a) Temperature (K)



(b) Hoop stress (Pa)

Figure 7: Temperature and Hoop Stress contours in the XFEM model at 25 kW/m

III. REALTIVE MERITS OF DEM AND XFEM

The XFEM and DEM are very different modeling techniques, both with their own relative merits and challenges. As has been demonstrated here, both methods can reasonably predict the behavior of fracturing ceramic nuclear fuel pellets.

Because the XFEM is based on the finite element method, the continuum mechanics of the uncracked material is represented in a natural manner. The material models and modeling techniques currently in use will for the most part be directly applicable with the XFEM. The XFEM has been proven to be a highly effective tool for modeling discrete cracks that follow arbitrary paths through the mesh. The major drawback of the XFEM is that although cracks need not follow element boundaries, they are normally represented as being continuous across element boundaries. This is a manageable problem in 2D, but becomes increasingly challenging as the complexity of the crack pattern grows, especially in 3D.

Because the DEM is not based on assumptions of continuous fields, distributed fracture is handled naturally in this method, as in other particle methods. Once a bond between neighboring particles meets a prescribed failure criteria, the bond is broken and the connection between those two nodes is severed. There is no need to track cracks, and as a result, distributed fracture can occur naturally. This aspect of DEM makes it well suited to the fuel fracture problem, where fracture is very distributed in nature. A significant drawback to DEM, however, is that the constitutive material behavior is represented by the behavior of bonds and contact between particles, rather than by traditional continuum material constitutive models. The parameters controlling bond behavior must be calibrated for each application.

IV. CONCLUSIONS

Two very different methods for representing discrete fracture: the XFEM and the DEM, have been applied to model thermally-driven fracture of ceramic nuclear fuel during early life. Initial 2D simulations performed using these methods have demonstrated their ability to realistically predict the formation of crack patterns.

By more realistically modeling the physics driving fuel behavior, this work has the potential to improve the predictivity of fuel performance simulations, especially under abnormal conditions. The techniques demonstrated here could be directly used on a larger scale to simulate sections of a fuel rod under accident conditions. These models would likely require significant computational resources. Alternatively, these techniques could be used as a basis for the development of improved models that represent the effects of fracturing on fuel behavior, such as relocation models. These could then be incorporated into BISON for improved engineering simulations of fuel rods. In either case, the insights gained from modeling the physics of fuel fracture will improve predictivity under conditions outside the range of applicability of current engineering models.

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