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Multidimensional multiphysics simulation of nuclear fuel behavior

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ABSTRACT

Nuclear fuel operates in an environment that induces complex multiphysics phenomena, occurring over distances ranging from inter-atomic spacing to meters, and times scales ranging from microseconds to years. This multiphysics behavior is often tightly coupled and many important aspects are inherently multidimensional. Most current fuel modeling codes employ loose multiphysics coupling and are restricted to 2D axisymmetric or 1.5D approximations. This paper describes a new modeling tool able to simulate coupled multiphysics and multiscale fuel behavior, for either 2D axisymmetric or 3D geometries. Specific fuel analysis capabilities currently implemented in this tool are described, followed by a set of demonstration problems which include a 10-pellet light water reactor fuel rodlet, three-dimensional analysis of pellet clad mechanical interaction in the vicinity of a defective fuel pellet, coupled heat transfer and fission product diffusion in a TRISO-coated fuel particle, a demonstration of the ability to couple to lower-length scale models to account for material property variation with microstructural evolution, and a demonstration of the tool's ability to efficiently solve very large and complex problems using massively-parallel computing. A final section describes an early validation exercise, comparing simulation results to a light water reactor fuel rod experiment.

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1. Introduction

Nuclear fuel operates in an extreme environment that induces complex multiphysics phenomena, occurring over distances ranging from inter-atomic spacing to meters, and times scales ranging from microseconds to years. This multiphysics behavior is often tightly coupled, a well known example being the thermomechanical behavior during final gap closure in light water reactor (LWR) fuel rods. Adding to this complexity, important aspects of fuel behavior are inherently multidimensional, examples include pellet–clad mechanical interaction (PCMI), fuel fracture, oxide formation, non-axisymmetric neutronics and cooling, and coupling to lower length scale models.

Current fuel rod simulation codes typically approximate this complex behavior using an axisymmetric, axially-stacked, one-dimensional radial representation (often referred to as 1.5D) [1–3] and, often, separate codes are used for steady and transient (or accident) conditions. Notable exceptions are the EPRI proprietary code FALCON [4] which is 2D and can be applied to steady or transient operation, and the French codes TOUTATIS [5] and ALCYONE [6,7] which are 3D, and typically used to investigate localized behavior. Current nuclear fuel simulation codes also rely heavily on correlational models derived from experimental data, limiting application to materials, geometries, and burnups where data are available. The need for improved modeling of PCMI [8] and, particularly, the importance of multidimensional capability for accurate fuel performance simulation [9] has been identified. A recent review article [10] clearly outlines the need for improved multiphysics, multidimensional, multiscale capability for nuclear fuel simulation.

Since 2008, the Idaho National Laboratory (INL) has been developing next-generation capabilities to model nuclear fuel behavior. Parallel efforts have included adapting the ABAQUS [11] commercial thermomechanics code to model fuel behavior, and the development of a new multidimensional finite element fuels code called BISON. The ABAQUS effort was designed to provide guidance and a prototyping environment for code development, plus provide the INL with near-term multidimensional fuel modeling capability; results and conclusions from that work were published recently [12]. The BISON fuel behavior code, first described in [13], is the subject of this paper. Significant new capability has been included in BISON since that early paper, including application of the code to a variety of nuclear fuel problems.

We begin with a brief description of the computational framework used for BISON, and describe the governing equations used to solve 2D axisymmetric and 3D nuclear fuel performance prob-

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lems. We outline the models currently implemented to simulate fuel and cladding material behavior and describe the approach used to simulate thermal and mechanical behavior in a fuel–clad gap and plenum. We then discuss results for a set of applications which demonstrate the variety and complexity of problems that can be solved, as well as the need for multidimensional analysis in many cases.

The first application considers a traditional LWR fuel rodlet, modeled assuming 2D axisymmetric behavior. In contrast to typical analyses, the fuel is modeled as discrete pellets rather than a smeared column. This problem employed the full set of multiphysics capabilities available in BISON, which run concurrently in each nonlinear solve. That is, all unknowns (displacements, stresses, temperature, fission gas released, plenum pressure, etc.) are solved concurrently at each time. No operator splitting, staggered, or predictor–corrector approach is required. This solution approach is used in all BISON analyses.

We next consider PCMI analysis of a section of a LWR fuel rod containing a missing pellet surface (MPS). In contrast to typical MPS analyses, which involve a series of coupled 2D simulations, we solve the problem in 3D beginning with fresh fuel, follow a typical irradiation history, and complete the simulation with a power ramp.

Although much of the early BISON development has focused on LWR fuel, the code is designed to be a general tool, applicable to a variety of fuel forms. We demonstrate this with a third application, where we consider coupled heat transfer and fission product diffusion in a spherical TRISO-coated fuel particle containing defects in the silicon carbide containment layer. This problem is a further example where a multidimensional treatment is important.

A fourth application demonstrates BISON's ability to couple to lower-length scale models to account for material property variation with microstructural evolution. This problem exemplifies our underlying modeling approach, to replace highly empirical material behavior models with mechanistic models to produce a more predictive tool for nuclear fuel simulation.

The last application considers BISON's ability to efficiently solve very large and complex problems using massively-parallel computing. Parallel scaling is studied using a high-fidelity, three-dimensional LWR fuel rod model, containing up to 320 discrete fuel pellets.

A final section describes an early validation exercise, comparing predicted fuel centerline temperatures to measured values from a LWR integral fuel rod experiment. We close with a discussion of future work.

2. BISON description

2.1. Multiphysics computational framework

BISON is built using the INL Multiphysics Object-Oriented Simulation Environment, or MOOSE [14]. MOOSE is a massively parallel, finite element-based framework to solve systems of coupled non-linear partial differential equations using the Jacobian-Free Newton Krylov (JFNK) method [15]. MOOSE supports the use of complex two and three-dimensional meshes and uses implicit time integration, important for the widely varied time scales in nuclear fuel simulation. An object-oriented architecture is employed which minimizes the programming required to add new material and behavior models.

2.2. Governing equations

The BISON governing relations currently consist of fully-coupled partial differential equations for energy, species, and momentum conservation. The energy balance is given in terms of the heat conduction equation

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} - E_f \dot{F} = 0, \tag{1}$$

where T, ρ and C_p are the temperature, density and specific heat, respectively, E_f is the energy released in a single fission event, and $\dot{F}$ is the volumetric fission rate. $\dot{F}$ can be prescribed as a function of time and space, input from a separate neutronics calculation, or computed based on input rod average power and axial profile data. The heat flux is given as

$$\mathbf{q} = -k\nabla T, \tag{2}$$

where k denotes the thermal conductivity of the material.

Species conservation is given by

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{J} + \lambda C - S = 0, \tag{3}$$

where C, λ, and S are the concentration, radioactive decay constant, and source rate of a given species, respectively. The mass flux $\mathbf{J}$ can be specified as

$$\mathbf{J} = -D\nabla C, \tag{4}$$

where D is the diffusion coefficient; this definition has been used to simulate fission product transport within the fuel. Also implemented in BISON is a hyperstoichiometric model for oxygen diffusion in UO_2 fuel as described in [13]. In this case $\mathbf{J}$ denotes the oxygen flux in the hyperstoichiometric regime with,

$$\mathbf{J} = -D\left(\nabla C + \frac{CQ^*}{HRT^2}\nabla T\right), \tag{5}$$

where D is diffusivity, Q^* is the heat of transport of oxygen, H is the thermodynamic factor of oxygen, and R is the universal gas constant.

Momentum conservation is prescribed assuming static equilibrium at each time increment using Cauchy's equation,

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f} = 0, \tag{6}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\mathbf{f}$ is the body force per unit mass (e.g. gravity). The displacement vector $\mathbf{u}$, which is the primary solution variable, is connected to the stress field via the strain, through kinematic and constitutive relations.

2.3. Kinematic and general constitutive behavior

For geometrically linear analysis, the strain $\underline{\varepsilon}$ is defined as $1/2[\nabla\mathbf{u} + \nabla\mathbf{u}^T]$ and, with a linear elastic constitutive model, the stress is simply $\underline{\underline{C}}\,\underline{\varepsilon}$ where $\underline{\underline{C}}$ is the material matrix.

Nonlinear kinematics is included following the approach in [16] and the software package FMA-3D [17]. Beginning with a complete set of data for step n, displacements and stresses are sought at step $n+1$. This is done by first computing an incremental deformation gradient,

$$\widehat{\mathbf{F}} = \frac{\partial x^{n+1}}{\partial x^n}. \tag{7}$$

Having $\widehat{\mathbf{F}}$, the next step is to compute a strain increment that represents the rotation-free deformation from the configuration at n to the configuration at $n+1$. Following [16], the stretching rate $\mathbf{D}$ is given by:

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