Advanced Finite Element Modelling of a Horizontal Fuel Element using a Multiphysics Object-Oriented Simulation Environment

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Summary

The thermal and mechanical behavior of nuclear fuel is a complex and highly coupled system. Predictive capabilities of current computer models are limited because of the high computational requirements. The larger the model becomes the less physics that can be included. The purpose of this work is to use the Multiphysics Object-Oriented Simulation Environment (MOOSE) developed at Idaho National Laboratory (INL) to produce a software application capable of modeling a horizontal nuclear fuel element with the ability to change the fuel type from stoichiometric UO_2 to hyperstoichiometric UO_2 and thoria-based fuels.The preliminary results of the first phase of this project will be presented.

1. Introduction

The ability to model the thermo-mechanical behaviour of nuclear fuel is important from both operational and regulatory perspectives as it helps further refine the safety and operational limits. The issue with predictive modelling is as the amount of coupled physical phenomena increases the size of the model has to decrease from a bundle, to an element or to a pellet due to computational restraints. For example, Prudil et al. have developed a Fuel and Sheath modeling Tool (FAST) which includes complicated nuclear phenomena such a fission gas production and release, fuel swelling and densification, and sheath thermal and irradiation creep among others, but the model is only a 2D axisymmetric representation of half of a fuel pellet (i.e. a quarter of the pellet is modelled) [1]. In another example by Bell et al.the deformation of a full CANDU fuel bundle was modelled with several modeling assumptions, such as the contact model [2].References 1 and 2 illustrated that as thegeometry increases from a quarter fuel pellet to a full fuel bundle the complexity of the physics included decreases. The purpose of this work is to examine the feasibility of using Idaho National Laboratory's Multiphysics Object-Oriented Simulation Environment (MOOSE) to develop an application capable of modelling a full horizontal nuclear fuel element in three dimensions, as the first phase.It is anticipated that the use of MOOSE will facilitate the analysis of other fuel materials other than UO_2.

2. The Computational Framework

Idaho National Laboratory's MOOSE is a computational framework developed for solving complex fully coupled engineering problems. All the physics that MOOSE solves is included in other animals in the MOOSE herd. The Extended Library of Kernels (ELK) houses general physics that is applicable to a variety of research fields such as solid mechanics, Navier-Stokes and heat transfer. Built on top of ELK is FOX which is a more specialized library containing general nuclear performance equations. It

is upon FOX that the HORizontal nuclear fuel Simulation Environment (HORSE) developed within this work is built.

Current commercial software packages such as ANSYS and COMSOL use the Newton-Raphson method to solve the system of fully coupled nonlinear equations. The Newton-Raphson technique has fast convergence properties but requires the analytical computation of what is known as the Jacobian matrix. To avoid the large computational requirements to perform analytical derivatives and to store the Jacobian, MOOSE uses what is known as a Jacobian-Free Newton Krylov (JFNK) technique for solving the system of equations. [3] The details of the Jacobian-Free technique are given in the following subsection.

2.1 Jacobian-Free Newton Krylov

A Jacoabian-Free Newton Krylov method is a numerical technique used in conjunction with Finite Element Analysis to solve systems of fully coupled nonlinear equations. To better understand exactly how JFNK works, one needs to break it down into its two components, the Newton method and the Krylov method.

2.1.1 Newton's Method

Newton's method is a root finding method of solving nonlinear equations. For a nonlinear equation of a single variable Newton's method yields

$$x_{n+1} = x_n + \delta x_{n+1}, \tag{1}$$

wherex_n is the current value of the variable, x_{n+1} is the next iteration of the variable and

$$\delta x_{n+1} = -\frac{f(x_n)}{f'(x_n)}. \tag{2}$$

For a single variable it is quite simple to solve this equation, computational constraints can become a factor when solving a system of nonlinear equations as one obtains

$$\mathbf{J}(\mathbf{u}_n)\delta\mathbf{u}_{n+1} = -\mathbf{R}(\mathbf{u}_n), \tag{3}$$

where**R** is the residual vector given by the weak form of each nonlinear equation and **J** is the Jacobian matrix with its elements given by

$$J_{ij} = \frac{\partial R_i(\mathbf{u}_n)}{\partial u_j}. \tag{4}$$

It can be seen from equation 4 that the Jacobian matrix is a complex object to find. The elements of the Jacobian are given by taking the partial derivative of each nonlinear equation in the system with respect to each variable being solved for in the system. Derivative calculations can be difficult and error prone. Therefore, a method that eliminates the need to solve for the Jacobian explicitly is desired. Equation 3 is essentially a system of linear equations that need to be solved to obtain

$\delta\mathbf{u}_{n+1}$ which is then used to solve the nonlinear system as given by equation 1 but in vector form. The system of linear equations is solved using a Krylov solver.

2.1.2 Krylov Method

MOOSE employs the Generalized Minimized Residual (GMRES) Krylov method. In this method the representation of the solution to the linear system of equations is given by

$$\delta\mathbf{u}_{n+1,k} = a_0\mathbf{r}_0 + a_1\mathbf{J}\mathbf{r}_0 + a_2\mathbf{J}^2\mathbf{r}_0 + \ ... + a_k\mathbf{J}^k\mathbf{r}_0. \quad (5)$$

Using equation 5, the Krylov method is iterated until the right-hand side of equation 3 is within some specified tolerance of zero. Once that is achieved the nonlinear step has to have converged. By examining equation 5, it can be seen that only the action of the Jacobian on a vector is required which can be approximated by a finite difference of the form[4]

$$\mathbf{J}\mathbf{v} \approx \frac{\mathbf{R}(\mathbf{u}+\varepsilon\mathbf{v})-\mathbf{R}(\mathbf{u})}{\varepsilon}. \quad (6)$$

The advantage of using this approximation is that a large amount of computational time is saved as analytical derivatives are not required to compute **J** and no memory space is needed to store the potentially large **J** matrix.

3. Model Development

Now that an understanding of the mathematical method employed by MOOSE has been provided, an explanation of the development of a 3D thermo-mechanical model of a horizontal nuclear fuel element within HORSE discussed in this section. The model is developed in three phases, a smeared pellet model, discrete pellet model and an advanced nuclear phenomena model. Within these three phases are four submodels including the fuel, sheath, gap and coolant channel models. The details of the three phases are included in the subsequent subsections. In this work, the geometries and finite element meshes are constructed in the preprocessing software Trelis. An ExodusII file is output and used in the input file into HORSE where all the relevant physics, boundary conditions and material properties have been added. The simulation is run and an output ExodusII file is produced, which is opened in the postprocessing software Paraview to produce plots and animations of the fuel behaviour.

3.1 Phase 1 - Smeared Pellet Model

The first phase of the modelling process a monolithic fuel stack of natural UO_2 the length of one element is created including the Zircaloy sheath and end caps. Figure 1 shows the geometry created in Trelis for this analysis.

In the first phase the amount of physics included is kept to a minimum to ensure everything is working as expected. The fuel and sheath models contain only the thermal and mechanical properties such as density, specific heat, and thermal conductivity. The gap model is of utmost important for accurate predictions of heat transfer and is the primary focus of phase 1. The gap heat transfer, mechanical contact between the pellet and sheath, and gap pressure is developed in phase 1.

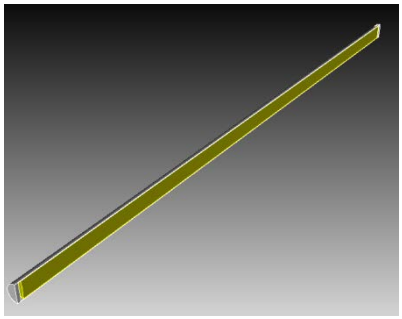


Figure 1: Geometry of the smeared pellet model used in phase 1.

The gap heat transfer, mechanical contact between the pellet and sheath, and gap pressure is developed in phase 1. The gap heat transfer requires two models, one for a closed gap and one for an open gap. Both of the models used in this work were developed by Olander [5]. For an open gap the heat transfer coefficient is given by

$$h_{gap} = \frac{k_g}{t_{gap}} + \frac{4\sigma T^3}{(1/\varepsilon_s)+(1/\varepsilon_f)-1}, \quad (7)$$

wherek_g is the thermal conductivity of the gas, t_{gap} is the thickness of the gap, σ is Boltzmann's constant, and ε_s and ε_f are the emmisivities of the sheath and fuel respectively. For a closed gap the conductance can be written as

$$h_{gap} = \frac{k_g}{\delta+g_s+g_f} + C\left(\frac{2k_f k_s}{k_f+k_s}\right)\frac{P_i}{\delta^{1/2}H}, \quad (8)$$

where δ is the gas film thickness, g_s and g_f are the jump distances of the sheath and fuel, C is a constant that is approximately unity, k_f and k_s is the thermal conductivities of the fuel and sheath , P_i is the interfacial pressure between the fuel and sheath, and H is the Meyer hardness of the softer material. For the coolant channel model only the coolant pressure and heat transfer coefficient is required. The pressure is set to 10 MPa whereas the heat transfer coefficient is calculated for normal operating conditions using the Dittus-Boelter correlation given by

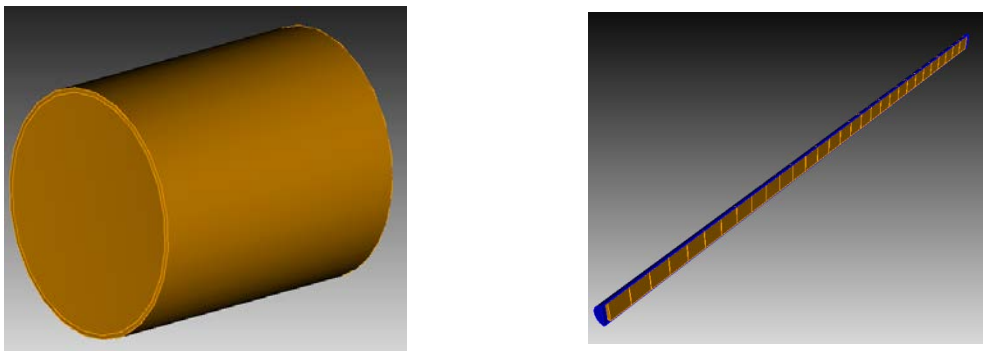
$$h = \frac{k_f}{D}0.023Re^{0.8}Pr^{0.4}, \quad (9)$$

wherek_f is the conductivity of the fluid, D is the outer diameter of the sheath, Re is the Reynolds number and Pr is the Prandtl number. Note that equation 9 is valid for 0.7<Pr<100, Re>10 000 and L/D>60. L/D is the length to diameter ratio of the nuclear fuel element.

3.2 Phase 2 - Discrete Pellet Model

In phase 2, two additional phenomena are added to the model developed in phase 1. The monolithic stack of fuel is divided into 30 discrete fuel elements and fission gas production and release is introduced. As the fuel is burned fission products and gas are released into the gap and affect the heat transfer properties. Since the prediction of the fuel centreline temperature is important to prevent

melting an accurate model of fission gas production and release is required. Figure 2 shows the geometry developed for a single pellet and the full discrete element.



(a) (b)

Figure 2: (a) Fuel pellet geometry, (b) fuel element with discrete pellets

3.3 Phase 3 - Advanced Phenomena Model

The final phase of the model is to add advanced nuclear phenomena as well as the ability to change the fuel type from UO_2 to hyperstoichiometric UO_2 and thoria-based fuels. The advanced phenomenon to be added are fuel swelling and densification, sheath plasticity and irradiation growth, and thermal and irradiation creep of both the fuel and sheath.

4. Conclusion

In conclusion, work has just begun on this project. Preliminary results from phase 1 will be presented and an analysis of the computational time saved using the JFNK will be given. The final goal of this work is to develop a complex fuel element model and potentially expand to a full fuel bundle.

5. References

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