COMSOL Simulations for Steady State Thermal Hydraulics Analyses of ORNL's High Flux Isotope Reactor

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Abstract: Simulation models for steady state thermal hydraulics analyses of Oak Ridge National Laboratory's High Flux Isotope Reactor (HFIR) have been developed using the COMSOL Multiphysics simulation software. A single fuel plate and coolant channel of each type of HFIR fuel element was modeled in three dimensions; coupling to adjacent plates and channels was accounted for by using periodic boundary conditions. The standard k-ε turbulence model was used in simulating turbulent flow with conjugate heat transfer. The COMSOL models were developed to be fully parameterized to allow assessing impacts of fuel fabrication tolerances and uncertainties related to low enriched uranium (LEU) fuel design and reactor operating parameters. Heat source input for the simulations was obtained from separate Monte Carlo N-Particle calculations for the axially non-contoured LEU fuel designs at the beginning of the reactor cycle. Mesh refinement studies have been performed to calibrate the models against the pressure drop measured across the HFIR core.[†]

Keywords: CFD, HFIR, LEU conversion, conjugate heat transfer, turbulent flow, thermal safety, COMSOL Multiphysics.

1. Introduction

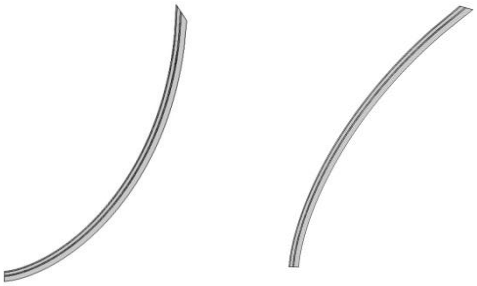
The High Flux Isotope Reactor (HFIR) is a beryllium-reflected, light water cooled, highly enriched uranium (HEU)-fueled research reactor operating at 85 MW_{th} at Oak Ridge National Laboratory (ORNL). HFIR is the highest flux reactor-based source of neutrons for research in the United States. Thermal and cold neutrons produced by HFIR are used to study physics, chemistry, material science, engineering, and biology. The HFIR core resides in an 8 ft diameter pressure vessel located in a pool of water. The core has two fuel elements, the inner fuel element (IFE) and the outer fuel element (OFE), consisting of 171 and 369 involute fuel plates, respectively, for a total of 540 fuel plates. These involute-shaped fuel plates are uniformly spaced in order to provide an equal coolant flow area for each plate within each element [1]. To remove the core heat, a highly turbulent water flow passes through involute-shaped coolant channels from the top to the bottom of the core. A total of 13,000 gal of water passes through the HFIR core every minute. Several physical phenomena including turbulent flow, conjugate heat transfer, thermal-structure interaction, and fluid-structure interaction are of significant interest when analyzing the thermal safety of the HFIR core.

The US Department of Energy's National Nuclear Security Administration (NNSA) is conducting the Global Threat Reduction Initiative [2] to reduce and protect vulnerable nuclear and radiological materials located at civilian sites worldwide. As an integral part of one of NNSA's subprograms, Reduced Enrichment for Research and Test Reactors [3], a research project is being carried out to investigate the conversion of HFIR from the present HEU core to a low enriched uranium (LEU) core with less than 20% ^{235}U by weight. Cost and availability considerations suggest making only minimal changes to the overall HFIR facility. Therefore, the primary goal of this conversion program is to substitute LEU for the fuel type in the existing fuel plate design, retaining the same number of fuel plates, with the same physical dimensions, as in the current HFIR HEU core. Because LEU-specific testing and experiments will be limited, COMSOL Multiphysics was chosen to provide the needed simulation capability to validate against the HEU design data and previous calculations, and predict the performance of the proposed LEU fuel for design and safety analyses [4]. Advanced

COMSOL Multiphysics simulations, including computational fluid dynamics (CFD) models, are now being developed to capture the turbulent flows and associated heat transfer in fine detail and to improve predictive accuracy.

2. 1P1C Models for IFE and OFE

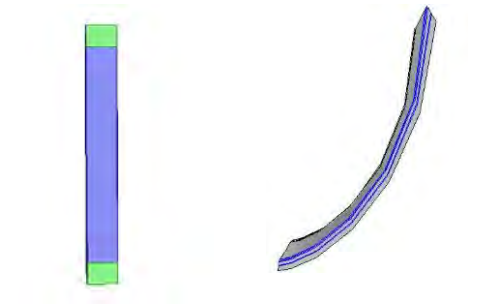
Because of the azimuthal symmetry of the HFIR fuel elements, only one fuel plate and one coolant channel of each HFIR fuel element (IFE and OFE) needs to be modeled in three dimensions (called 1P1C—one plate, one channel models) (Fig. 1), and the coupling to adjacent plates and channels can be modeled through periodic boundary conditions.



a. Inner fuel element b. Outer fuel element

Figure 1. Cross-sectional views of HFIR's one-plate, one-channel models.

In each HFIR fuel plate, there is an unfueled region present in the top and bottom 2 in. (Fig. 2a). LEU fuel meat and filler (and poison in IFE) are sandwiched by 10 mil (1 mil = 0.001 in.) thick layers of Al cladding, forming a 50 mil thick fuel plate (Fig. 2b).

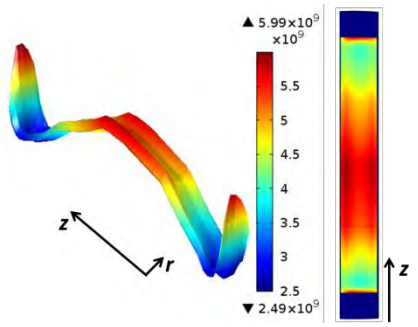


a. Side view with top and bottom unfueled regions shown in green b. Top view with 10 mil thick cladding layers shown in blue

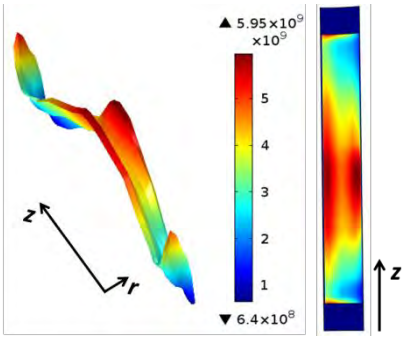
Figure 2. One plate, one channel model for the HFIR inner fuel element.

In the developed models, LEU fuel meat is assumed to be homogenized across the sandwiched region; hence, its radial contouring is not explicitly captured in the modeled geometry. However, the effects of contouring are being accounted for through approximate variations in volumetric heat sources.

The volumetric heat source for the homogenized fuel region is obtained from separate Monte Carlo N-Particle (MCNP) calculations for the axially non-contoured LEU fuel design at the beginning of the reactor cycle (Fig. 3). Note that, in contrast to the OFE, the heat source profile for the IFE in the radial direction is symmetric across its longitudinal center plane. Non-uniform heat generation in the *r*-direction of the OFE can be attributed to the continuously decreasing neutron flux in the peripheral region of the core. One should expect to see similar variations in steady state surface temperatures for IFE and OFE as in Fig. 3. Furthermore, a hot streak can develop in the OFE due to relatively high heat generation along its inner side edge (see Fig. 3b).



a. Inner fuel element



b. Outer fuel element

Figure 3. Volumetric heat source in the low enriched uranium fuel at the beginning of the reactor cycle for 100 MW reactor operation (unit: W/m^3) (Notice the unfueled region in the top and bottom of the plate and along the side edges in the longitudinal direction).

The models presented here are also being used to assess and quantify the impacts of fuel fabrication tolerances and uncertainties in the LEU fuel performance on overall thermal margin for

HFIR. Currently the effects of (a) geometric tolerances, (b) uncertainty in heat generation sources, (c) neutron flux peaking, and (d) oxide layer growth on the effectiveness of core heat removal are being examined. These models will then be benchmarked against more detailed three-dimensional COMSOL models currently under development.

3. Model Details

The geometry for the 1P1C model was developed to be fully parameterized, allowing various thicknesses of HFIR inner and outer fuel elements to be independently selected (e.g., cladding thickness, thickness of fuel meat, coolant channel thickness, and oxide layer thickness). These thicknesses can be varied independently to study the effects of geometrical tolerances on HFIR thermal safety. Conjugate heat transfer and the standard k-ε turbulence model in COMSOL v4.3 have been used to simulate turbulent flows and heat transfer. The modeled fuel meat region has been assigned properties of the U-10Mo alloy [5], whereas the properties of aluminum-6061 and water in the COMSOL material library were used for the cladding and coolant region, respectively.

3.1 Boundary Conditions

The various boundary conditions chosen for the model are shown in Fig. 4. The steady state inlet velocity (15.6 m/s), coolant inlet temperature (120 ^{o}F or 48.89 ^{o}C) and outlet pressure (366 psig or 2.52 MPa) boundary conditions for IFE and OFE models were based on data from HFIR's design and operational experience. It was presumed that each IFE and OFE channel has the same inlet velocity. Periodic heat conduction was applied on the convex and concave sides of the 1P1C model to couple to adjacent plates and coolant channels. A no-slip interface condition was used at the coolant-cladding interface.

3.2 Meshing

A mapped mesh was generated based on the two-dimensional involute geometry of the fuel plate and coolant channel and swept through the entire length of the fuel element. A boundary layer mesh for the coolant channel adjacent to the wall was also used in order to capture the steep velocity and temperature gradients. A 10-element-thick boundary layer was used in the simulations with the first layer thickness equal to 0.005 mm (wall lift off in viscous units y^{+}~11.06). In addition to the boundary layers, 10 elements were used to further subdivide the coolant channel thickness and 60 elements in the direction of the involute span (Fig. 5). Based on mesh refinement studies, this appropriately-designed mesh provided a mesh-independent solution. During the mesh refinement studies, various parameters were gradually varied such as the number of boundary layers, first layer thickness, and number of elements along the plate's involute span, thickness and height. A comparison of the COMSOL-predicted pressure drop with actual measurements was used to identify the optimum mesh density.

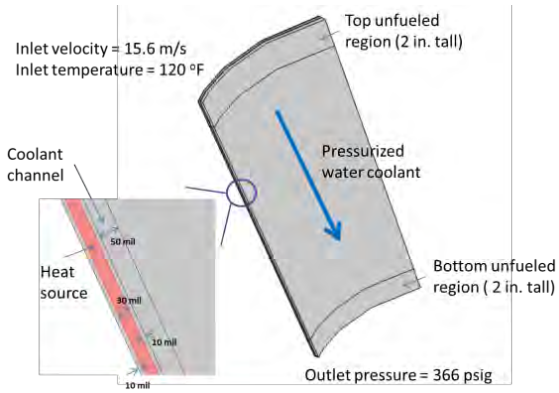


Figure 4. Boundary conditions for the one plate, one channel COMSOL model.

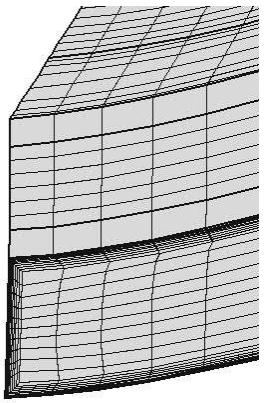


Figure 5. Mesh across the fuel plate and coolant channel thicknesses. Boundary layer mesh is used alongside the channel walls.

3.3 Solver Settings

The COMSOL non-isothermal k-ε turbulence model was used from the CFD module to simulate the turbulent flow of the coolant. COMSOL's direct PARDISO solver [6] was used to solve partial differential equations associated with this

simulation study. A relative-error convergence criterion of 10^{-3} was chosen for all the simulation variables [velocity components (u, v, w), pressure (p), temperature (T, T_{wall}), and turbulence parameters (k and ε)].

3.4 Simulation Cases

Design basis thermal-hydraulic analyses of the 1P1C model for the inner and the outer fuel element were carried out at 100% full power (FP) for the beginning of the reactor cycle. Note that the limiting control setting for the HFIR safety system is 1.3 times the normal operating power level [7–8]. Hence, analyses at 130% FP operation are also needed to estimate available thermal margins. This case was also simulated in COMSOL, and the results obtained are reported in Section 4. Because the geometrical tolerances for the LEU fuel plate are not yet established, HEU tolerances were used in these preliminary analyses of the LEU fuel plate. Using a maximum allowable HEU fuel plate thickness of 51 mil [7], two such neighboring fuel plates could result in a coolant channel 48 mil thick. Therefore, a case with a 48 mil thick coolant channel and operation at 130% FP was also simulated.

An oxide layer buildup occurs on the fuel plate surface during HFIR operation. The oxide layer is composed of boehmite (a monohydrate of aluminum oxide), which has a significantly lower thermal conductivity (~2.25 W/m-K) than the aluminum cladding [8]. In turn, this causes additional thermal resistance in the heat removal path and leads to a significant increase in the fuel centerline temperature. It is conservatively assumed[‡] that the oxide layer can grow up to a thickness of 3 mil, beyond which it would spall off from the surface [8]. Therefore, a case with a 3 mil thick oxide layer on both sides of the fuel plate has been simulated at 130% FP operation of HFIR. This 3 mil oxide layer on either side of the fuel plate results in a 6 mil reduction of the coolant channel thickness. The COMSOL results obtained for these cases are presented in the following section.

[‡] Griess correlation [8] with water-oxide interface temperature (T_s) of 133°C and 26 days gives the oxide thickness (χ) of 1.003 mil. At normal power (T_s=115°C) and 26 days, χ is 0.59 mil.

4 Results and Discussions

4.1 CFD Model Calibration

The Nuclear Regulatory Commission's Computational Fluid Dynamics Best Practice Guidelines in Nuclear Reactor Safety Applications [9] defines CFD calibration to be the ability to test a given CFD code to accurately predict global quantities of interest, for example, pressure drop and overall temperature difference. These quantities can easily be measured using simple experimental techniques and therefore can be used for model calibration.

In 1P1C models of HFIR, mesh density was systematically increased to identify an optimum mesh providing reasonable agreement with the measured pressure drop data. In Table I, computed pressure drops for IFE and OFE are compared with the measurements. Note that the COMSOL pressure drop values are about 10% less than the measured data across the core. These COMSOL model predictions are expected to be lower than the experimental values since the entrance and exit regions are not included in the model; hence inlet and exit form losses are not present in the model. Further increasing the mesh density of the model will yield better agreement with the measured pressure drop data; however, at a cost of significantly increasing the computational burden. Heat balance calculations, carried out using COMSOL predicted average coolant exit temperature, were also in good agreement with HFIR operational data. These assessments justify the use of a pressure drop calibrated mesh for design and safety basis thermal hydraulics analyses of the HFIR core.

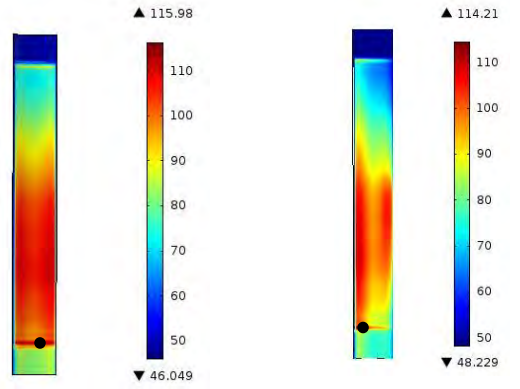
Table I: Comparison of COMSOL pressure drop predictions with measured data

Cases	Overall Pressure Drop (ΔP, in psi)		
	Measurement across the core	COMSOL predictions	
		IFE	OFE
100% full power	100	92.2	89.3

4.2 Results at 100%FP and 130%FP

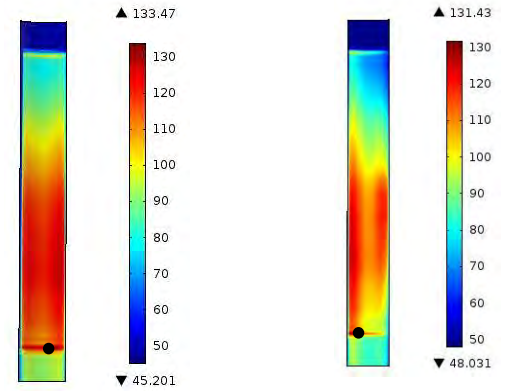
Steady state cladding surface temperatures for IFE and OFE at 100% and 130% FP operation are presented in Figs. 6 and 7. The maximum cladding surface temperature at specific axial locations on the plate, local pressure at that location, corresponding saturation temperature T_{sat}, margin to onset of nucleate boiling (ONB), overall

pressure drop, and average coolant exit temperature are tabulated in Tables II through IV. The maximum cladding surface temperature for IFE was found to be higher than that for OFE. (Table II).



a. Inner fuel element b. Outer fuel element

Figure 6. Surface temperature plots (in °C) at 100% FP (black dot shows the location of peak cladding temperature).



a. Inner fuel element b. Outer fuel element

Figure 7. Surface temperature plots (in °C) at 130% FP (black dot shows the location of peak cladding temperature).

Table II: Peak cladding surface temperature and its location

Cases (% full power)	Max. Cladding Surface Temp. (in °C) $T_{clad,m}$		Axial Location of Max. Cladding Surface Temp. (in inches from inlet)	
	IFE	OFE	IFE	OFE
100	115.9	114.2	21.78	22
130	133.4	131.4	21.8	21.8

The margin to ONB was calculated by using the local pressure at the point of maximum cladding surface temperature to find the corresponding saturation temperature (T_{sat}). A superheat of about 5°C–10°C above the saturation temperature of water is required for ONB to occur [7] and therefore, a conservative value of T_{sup} = 5°C was taken into account when evaluating the margins (Table III).

Table III: Saturation temperature at local pressure and margin to onset of nucleate boiling (ONB)

Cases (% full power)	P_{local} at Respective Axial Locations (in psia*)		T_{sat} at Local Pressure (in °C) T_{sat}		Margin to ONB (in °C) $(T_{sat} + T_{sup})$- $T_{clad,m}$	
	IFE	OFE	IFE	OFE	IFE	OFE
100	387.7	387.3	227.5	227.5	116.4	118.2
130	387.6	387.8	227.5	227.5	99	100.9

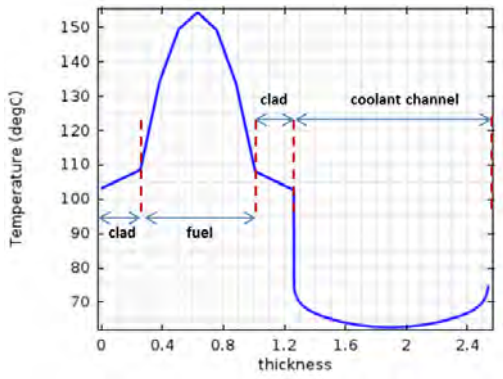
* psia = psig + 14.7 psi

The average coolant exit temperature was found to be higher in IFE than in OFE for both the cases (Table III). This is expected because IFE produces more heat per plate than OFE. The net pressure drops predicted for IFE and OFE were found to be in good agreement.

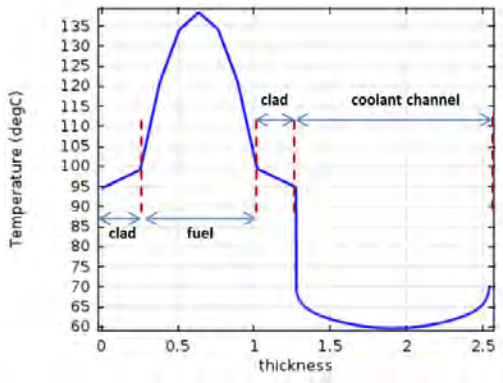
Table IV: Average coolant exit temperature and net pressure drop

Cases (% full power)	Avg. Coolant Exit Temp. (in °C)		Overall Pressure Drop (ΔP, in psi)	
	IFE	OFE	IFE	OFE
100	80.4	76.4	92.2	89.3
130	89.6	84.5	90.9	88.2

Figure 8 shows line plots for the steady state temperature variation across the thickness of the fuel plate for IFE and OFE. Temperatures were evaluated at the mid-height and mid-span of the fuel plate. As expected, a parabolic temperature profile is observed in the fuel region with the peak at the centerline. Note that there is sufficient mesh resolution available inside the fuel region to allow the first order linear elements to capture the temperature variation. The steep wall gradient at the cladding-coolant interface is also captured in the model results. Temperature variation in the coolant channel is of the typical flat profile associated with the turbulent forced convection. The trends observed are the same for IFE and OFE. Higher centerline temperatures and higher cladding surface temperatures are observed for IFE compared to the OFE.



a. IFE



b. OFE

Figure 8. Temperature line plot at 100% full power (at mid-height and mid-span of 1P1C model).

4.3 Results for 130% FP with 48 mil Thick Coolant Channel

A comparison of Table VI with Table II shows that the peak cladding surface temperatures for IFE and OFE were slightly increased because of the reduction in coolant channel thickness from 50 mil to 48 mil. The same trend was observed for the average coolant exit temperature and the overall pressure drop (Tables V and VI).

Table V: Average coolant exit temperature and net pressure drop

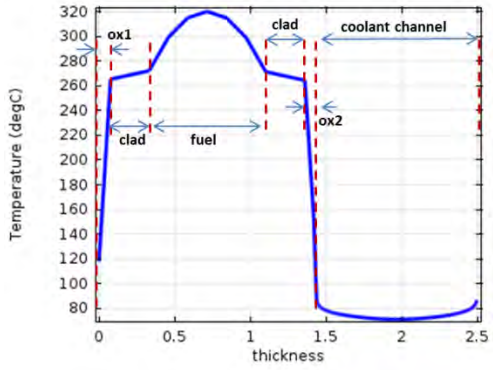
Cases (% full power)	Avg. Coolant Exit Temp. (in °C)		Overall Pressure Drop (ΔP, in psi)	
	IFE	OFE	IFE	OFE
130 with 48 mil coolant channel	91.5	85.8	92.3	90.7
130 with two 3 mil oxide layers	99	89.6	105.9	101.5

Table VI: Maximum cladding surface temperature and margin to onset of nucleate boiling (ONB)

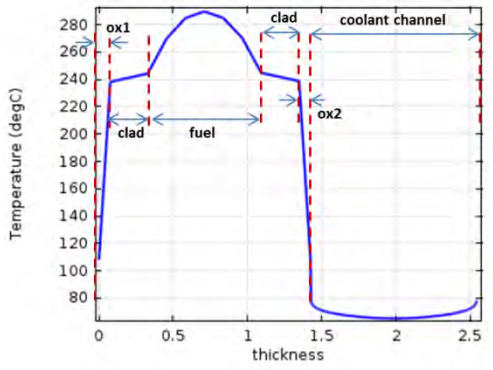
Cases (% full power)	Max. Cladding Surface Temp. (in °C)		Margin to ONB (in °C)	
	IFE	OFE	IFE	OFE
130 with 48 mil coolant channel	134.7	133.3	99.8	99.2
130 with two 3 mil oxide layers	117	110.6	117.2	123.4

4.4 Results for 130% FP with 3 mil Thick Oxide Layer on Both Sides

Figure 9 shows the temperature line plots at the mid-height of the fuel plate for the case where 3 mil thick oxide layers were considered on both sides. Note that the fuel center line temperatures are increased as a result of the thermally resistive oxide layer; however, are still significantly less than the melting temperatures of U-10Mo (~1200°C) and aluminum (~650°C).



a. IFE



b. OFE

Figure 9. Temperature line plot for 130% full power operation with 3 mil thick oxide layers on both sides (ox1 and ox2 denote oxide layers 1 and 2).

Because there is a rapid drop in temperature across the oxide layer due to its poor thermal conductivity, peak cladding surface temperatures

were found to be less than in the case of 130% FP operation with no oxide layer.

5. Summary and Conclusions

Parametric simulation models for the HFIR inner and outer fuel elements have been developed in COMSOL Multiphysics. In these models, only one fuel plate and one coolant channel of IFE and OFE were modeled in three dimensions; the coupling of adjacent plates and channels in each element were modeled through periodic boundary conditions. Heat source input in these models was obtained from separate MCNP calculations for the axially non-contoured LEU fuel at the beginning of the reactor cycle. Initial and boundary conditions were derived from operational experience at HFIR.

Thermal hydraulic analyses of the HFIR core are being carried out using these parameterized models. Cases for (a) 100% FP operation, (b) 130% FP operation, (c) 130% FP operation with a 48 mil thick coolant channel, and (d) 130% FP operation with 3 mil thick oxide layers on both sides were simulated in COMSOL. Mesh refinement studies were also carried out, and pressure drop predictions for different mesh densities were used as a means to calibrate and choose the optimum mesh density.

Results obtained using the appropriately-chosen mesh were analyzed for (a) peak cladding surface temperature and its location, (b) margin to ONB, (c) overall pressure drop, and (d) temperature rise across the core. It was found that peak cladding surface temperatures are higher in the IFE compared to the OFE. Temperature line plots show the parabolic temperature profile across the fuel meat thickness. It was also found that as a result of a thermally resistive oxide layer on the cladding, fuel center line temperatures were significantly increased. As expected, a steep wall temperature gradient was observed at the cladding-coolant interface.

This is an ongoing project, and different designs of the LEU fuel are currently being analyzed; therefore, these results may change depending upon the chosen fuel design and associated heat source variation. The models presented here can be used to identify bounding limits on the uncertainties associated with various factors and to quantify their effects on thermal margins.

6. References

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