

# Simulating HFIR Core Thermal Hydraulics Using 3D-2D Model Coupling

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**Abstract:** A model utilizing interdimensional variable coupling is presented for simulating the thermal hydraulic interactions of the High Flux Isotope Reactor (HFIR) core at Oak Ridge National Laboratory (ORNL). The model's domain consists of a single, explicitly represented three-dimensional fuel plate and a simplified two-dimensional coolant channel slice. In simplifying the coolant channel, and thus the number of mesh points in which the Navier-Stokes equations must be solved, the computational cost and solution time are both greatly reduced. In order for the reduced-dimension coolant channel to interact with the explicitly represented fuel plate, however, interdimensional variable coupling must be enacted along all shared boundaries. The primary focus of this paper is in detailing the collection, storage, passage, and application of variables across this interdimensional interface. Comparisons are made showing the general speed-up associated with this simplified coupled model.

**Keywords:** Interdimensional, Model Coupling, Thermal Hydraulic, HFIR, Involute

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## 1. Introduction

As the process of converting HFIR from high-enriched uranium (HEU) to low-enriched uranium (LEU) fuel is being researched, the computer models used to predict the reactor's LEU performance continue to evolve. In order to obtain ever more accurate and detailed

estimates of the core's operating conditions, it is desirable to create more efficient models that allow for a larger portion of the core to be modeled at once.

The reduced-cost model detailed in this paper, referred to as the coupled model from this point forward, seeks to fill this gap by providing the capability to obtain quick and reasonably accurate approximate solutions that capture key characteristics of the thermal hydraulic conditions in the reactor core.

Three primary variables of interest are the maximum temperatures in the fuel meat, the fuel plate, and the coolant channel. The first two must remain below the melting points of their respective materials while the third must remain below its incipient boiling point. Although the third criterion is most likely to be reached first, it can also be extrapolated roughly as a function of the first two. Therefore, the maximum temperatures in the solid domains—and, to a lesser extent, the temperature profiles in each solid domain—are the primary focuses of the coupled model. As a consequence, the coolant domain is simplified to a 2D slice while the solid domain is left largely intact.

The pairing of these two domains is achieved through interdimensional model coupling. Since the solid domain is the primary focus of the coupled model, the coolant domain essentially serves the role of an adaptive boundary condition.

Blanco, *et al.* [1] make a case for the use of interdimensional model coupling in this capacity, versus the implementation of a static Dirichlet or Neumann boundary condition, which imposes a certain degree of rigidity on the evolving solution's ability to adapt to changing conditions. They coin this adaptive feedback across the interdimensional coupling the "systemic response" of the entire coupled domain.

Interdimensional model coupling has appeared in many applications across many fields ranging from thermal circuitry analysis to structural mechanics and computational fluid dynamics. In the vein of producing a systemic response, the method has been applied in

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particular to systems modeling in which a complex, or at least multi-component, system is modeled with varying degrees of detail throughout. For any given component in a system, it at once influences the rest of the system even as the system imparts an influence back upon it. This breeds a looped dependency across coupling interfaces in which boundary conditions must be formatted and shared [2].

There has been a particular interest in coupling fluid domains in an effort to reduce the computational costs associated with solving the Navier-Stokes equations in three-dimensions in large solution domains [3]. Systems in which the flow impedance of a single component—ranging from a valve [4] to a burst dam [5]—requires detailed modeling have been attached to pipe flow models as a means of enforcing reactive boundary conditions. This has been applied in the automotive industry using the full 3D N-S equations to model the cavitation flow around fuel injection nozzles while utilizing 1D upstream systems to provide accurate inlet conditions [6].

Interdimensional model coupling has also found prevalence in the study of large flow environments such as rivers, lakes, and ocean currents where 2D surface flow mingles with 3D sub-surface flow effects [7-10]. Similar work has been done with a focus on locally selected regions of detailed resolution amidst a broader solution domain, especially with regards to flows with impeding structures and blockages [11,12] and flows over uneven surfaces [13-15].

Interdimensional model coupling has even been used in nuclear reactor core modeling efforts in the past. In the heavily regulated environment of nuclear reactors, any computer code or simulation software used in a safety basis calculation must be vetted for accuracy and dependability. As such, there are a number of codes, both commercial and open-source, which have found widespread use in the nuclear industry. RELAP5, for instance, is a widely used code for simulating the entire reactor loop from a systems level approach. Cobra and CFX are two common CFD codes used to model reactor core coolant flows. Multiple coupling links have been engineered that combine the systems level feedback of RELAP5 with the CFD capabilities of Cobra [16,17] and CFX [18]. Many of these codes are still used at HFIR, even

as COMSOL is being used to explore new modeling approaches.

Miglio, *et al.* [19] lump model coupling efforts into two categories: dimensionally homogeneous-physically heterogeneous couplings and dimensionally heterogeneous-physically homogeneous couplings. The former is concerned with the coupling of dissimilar physics models, such as fluid flow and solid heat conduction, in dimensionally consistent domains. The latter category constitutes interdimensional model couplings in which the same physics model is considered across dimensionally inconsistent domains. The bulk of examples cited above fall into this latter category.

The groupings are incomplete, however, due to their mutually exclusive nature. They assume that if one form of coupling is present then the other must not be. In order to rank the coupled model according to this rubric a third category must be introduced—that of the dimensionally heterogeneous-physically heterogeneous coupling. This constitutes a coupling occurring across dissimilar physics models and dimensionally inconsistent domains.

Not only does this provide a convenient interface across which to couple, but it also breaks the model down into two discrete domains with only minimal interaction between them. This results in a much smaller model which is the focus of this work. Note that this model requires neither the computational resources nor the solution time of a fully three-dimensional model while still returning comparable results. This makes it an efficient and reasonably accurate alternative to the full-3D approach.

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## 2. Geometry

The HFIR fuel plates are shaped as involute curves, governed by the base parametric equation given as

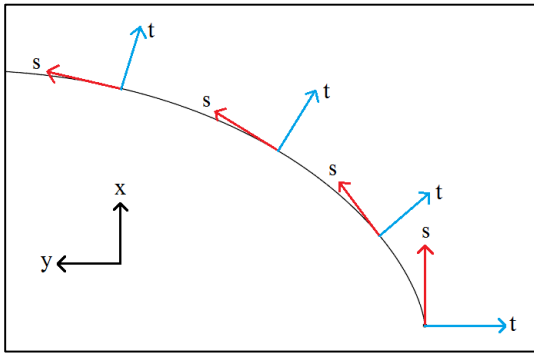
$$x = r_b [\cos(\theta) + \alpha \sin(\theta)], \quad \alpha \geq 0 \quad (1)$$

$$y = r_b [\sin(\theta) - \alpha \cos(\theta)], \quad \alpha \geq 0 \quad (2)$$

$$\alpha = \mathfrak{I}(\theta) \quad (3)$$

where  $r_b$  denotes the radius of the base circle,  $\theta$  and  $\alpha$  represent the angular displacement along the length of the base circle and the involute curve in radians, respectively, and the operator  $\mathfrak{S}$  denotes a linear function.

Rather than dealing with the two abstract coordinates  $\theta$  and  $\alpha$ , these angular dimensions can be recast as two length dimensions,  $s$  and  $t$ , as shown in Fig. 1. Here,  $s$  represents the arc length and takes the place of  $\alpha$ , the angular displacement along the curve. The coordinate  $t$  is everywhere perpendicular to the base involute curve in the  $r$ - $\theta$  plane.



**Fig. 1. Involute Coordinate System.** The coordinate  $s$  is measured positive out from the origin of the curve and  $t$  is measured positive out from the convex side of the curve.

The perpendicular coordinate  $t$  can be introduced directly into the involute parametric equation by setting  $\alpha$  such that

$$\alpha = \theta + \frac{t(\theta)}{r_b}, \quad \theta \geq 0 \quad (4)$$

The arc length,  $s$ , is defined by

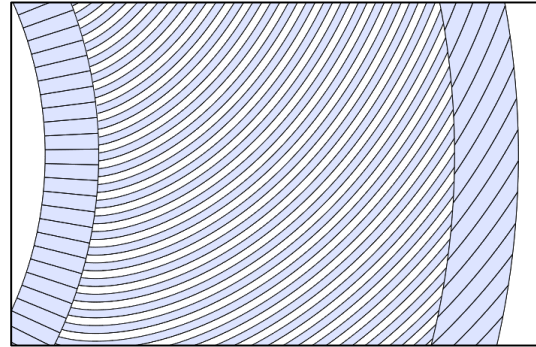
$$s_{a \rightarrow b} = \int_a^b \sqrt{\left(\frac{dx}{d\theta}\right)^2 + \left(\frac{dy}{d\theta}\right)^2} d\theta \quad (5)$$

where  $dx/d\theta$  and  $dy/d\theta$  are given by the derivatives of Eqns. (1), (2) and (4). This yields

$$s = \frac{r_b \theta}{2} + t\theta \quad (6)$$

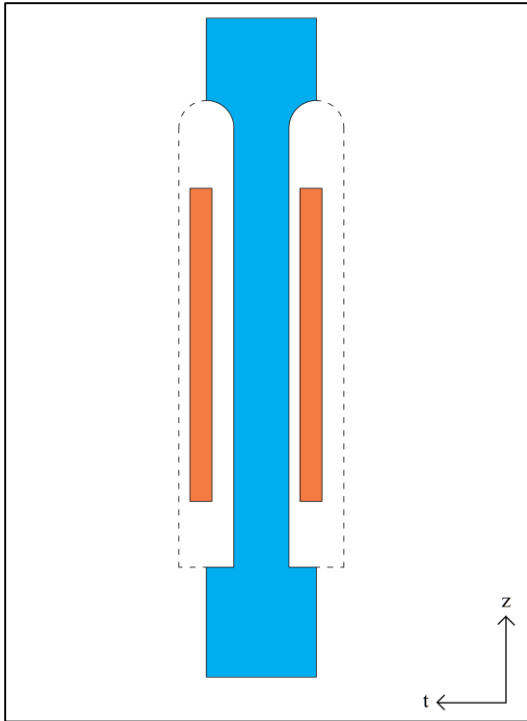
assuming all values are evaluated at point  $b$  and  $a$  is taken to be the origin as a datum.

These three equations also form the basis for creating the required involute fuel plate geometry. The involute geometry is noteworthy for its constant separation between successive spirals and its constantly varying radius of curvature. This second feature complicates the geometry creation process. As a result, the 3D fuel meat and fuel plate geometries were created in SolidWorks and imported into COMSOL. The first feature, however, is integral to HFIR's performance as it allows for every fuel plate in the radial core array to maintain a constant thickness while also being separated by constant-width coolant channels, creating near-constant operating conditions throughout, as shown in Fig. 2.



**Fig. 2. HFIR Core Inner Element Fuel Plate Configuration.** The fuel plates maintain a constant separation except in the region very near the outer side wall (shown on the right) where the coolant channels taper to a point. The direction of coolant flow is into the page.

It is due to this constant separation between plates that the coolant channels can be approximated as 2D slices oriented perpendicular to the surface of the fuel plates, as shown in Fig. 3. This orientation removes the coordinate  $s$  from the coolant domain.



**Fig. 3. 2D Coolant Domain Diagram.** The coolant domain, highlighted in blue, is not drawn to scale. The imprints that the two adjacent fuel plates make on the coolant channel are outlined with dotted lines. The asymmetric position of the fuel meat inside each plate is highlighted in orange. Fuel meat and plate position are only shown for reference. Flow is in the  $-z$  direction.

The simplified 2D coolant channel is oriented such that it is everywhere perpendicular to the fuel plate placing it in a  $t$ - $z$  plane.

### 3. Coupling Mechanisms

#### 3.1 Physics of the Coupled Domains

The 3D fuel plate is composed of a solid fuel meat consisting of LEU fuel and the surrounding clad made of aluminum. The fuel meat is solved as a steady-state heat equation with internal generation and varying properties in three dimensions resulting in a quadratic temperature profile modeled by

$$\nabla \cdot (k \nabla T) = -Q \quad (7)$$

In this model, the surrounding clad is analyzed without internal heat generation,

resulting in a linear temperature profile. The entire geometry has an extremely high aspect ratio with a width in the  $t$  direction of 0.05 inches, an arc length in the  $s$  direction of approximately 3 inches, and a height in the  $z$  direction of 24 inches. The external coolant flow couples to the concave and convex axial faces of the fuel plate, passing in the  $-z$  direction.

The coolant channel solves the  $k$ - $\omega$  Reynolds-averaged Navier-Stokes (RANS) equations. The flow conditions in the coolant, composed of light water, are set by specifying inlet pressure, velocity, and temperature along with outlet pressure. The domain itself is a single coolant channel with entrance and exit regions inserted above and below the fuel plate, respectively. The domain's side boundaries are lines of periodicity corresponding to the centerline of two adjacent fuel plates. As a result, there is an impression on either side of the coolant channel representing the cut-out of half of a fuel plate impinging the flow, as seen in Fig. 3.

Both domains are solved simultaneously using a segregated PARDISO solver. A single iterate consists of two segregated steps. Traditionally, one step is allotted to the solution of the solid domain and another step to the solution of the coolant domain. In order for the coupling to function properly, however, all of the variables directly involved in the computation of the two coupling variables must be solved in the same step. Temperature in both domains is thus solved in the first step along with coolant pressure and velocity. The turbulence variables  $k$  and  $\omega$  are solved separately in the second step.

#### 3.2 Implementing the $s$ - $t$ Coordinate System

The coupling occurs between the surface of the fuel plate and the body of the coolant channel. The coolant channel, in its simplified form, is already conveniently arrayed in a  $t$ - $z$  coordinate plane. The fuel plate, however, is defined in 3D Cartesian space. In order to be able to reference the convective surfaces in an  $s$ - $z$  coordinate plane, the  $s$  coordinate must first be introduced into the model.

Due to  $s$  being a nonlinear function of  $\theta$ , and  $\theta$  having no definitive solution in  $x$  and  $y$ , it is best to define  $s$  using the curvilinear coordinate system function. This approach also defines the normal  $t$ -coordinate.

### 3.3 3D to 2D Coupling

Nuclear heat generation is produced by a source in the LEU fuel meat. The heat then flows through the surrounding clad and to the coupled boundaries on the concave and convex surfaces. The coupling functions pass these surface temperature values from the 3D fuel plate to the boundaries of the 2D coolant channel. In order for that coupling to occur, however, the collected variables must be reduced by a dimension. Inherently, the surface temperature profile on an axial face of the fuel plate is represented by

$$T_s = T(s, z_p) \quad (8)$$

where the subscript  $p$  denotes a coordinate variable in the fuel plate domain. The boundaries of the 2D coolant channel corresponding to these axial faces, by contrast, are functions of only  $z$ . Thus the map of surface temperatures must be integrated in the  $s$  direction to produce a new variable

$$\lambda_T(z_p) = \int_s T_s(s, z_p) ds \quad (9)$$

This new variable  $\lambda_T$  now has the correct spatial dependency but not the correct units. In order to correct this incompatibility, it is divided by the length it was integrated over, transforming it into a spanwise-averaged surface temperature as a function of axial position

$$\bar{T}_s(z_c) = \frac{\lambda_T(z_p)}{\Delta s} \quad (10)$$

where the subscript  $c$  denotes a coordinate variable in the coolant channel domain. A datum is placed at the bottom of the fuel plate, setting its axial position  $z$  at a specific value. If this same datum is enforced in the 2D coolant channel (i.e. the fuel plate's bottom surface in the channel is set to this same value) then the coordinate mapping is a direct translation, resulting in

$$z_c = z_p \quad (11)$$

The spanwise-averaged surface temperature values resulting from Eqns. (10) and (11) are then directly enforced in the coolant domain via a combined Dirichlet-Neumann boundary condition in conjunction with the imposition that

$$\frac{d}{dt} \bar{T}_s(z_c) = \frac{\lambda_{dT/dt}(z_p)}{\Delta s} \quad (12)$$

where the derivative  $d/dt$  is with respect to the space dimension normal to the clad surface, not time. This gradient condition is automatically implemented when the coupled temperature boundary condition is imposed. Together, these two boundary conditions enforce a continuity of temperature and its gradient across the coupling, transmitting surface temperature values from the fuel plate to the coolant channel.

This coupling only applies to axial faces. There are two additional faces, the curved leading surface and the flat trailing surface, which are exposed to the coolant flow. These two surfaces are separated from the fuel meat by two inches of unfueled plate in the axial direction, however, and heat transfer through the fuel plate occurs predominantly in the  $t$  direction. Heat transfer in the  $s$  and  $z$  directions is insignificant enough that any heat flux through the trailing and leading surfaces is negligible. The couplings on these faces are, therefore, ignored and the faces are assumed to be insulated instead. If implemented, the coupling would function the same, only with a different coordinate transformation in the  $t$  direction linking the trailing surface coupling.

### 3.4 2D to 3D Coupling

The reverse effect of the coupling mechanism is that bulk temperatures are gathered from the coolant and passed to the fuel plate surfaces as part of a boundary condition. This coupling was chosen, in lieu of simply applying coolant boundary surface temperatures right back to the clad surfaces, due to its weak effect on the temperature profile in the fuel plate. Coupling coolant surface temperatures back to the clad would set the entire clad surface to a single temperature, thus invalidating the entire model. The clad surface temperature profile is set directly by the profile of the nuclear heat generation in the fuel meat. The bulk

temperature coupling serves only to specify the magnitude of the profile, allowing each point on the clad surface to vary, up or down, according to its local heat flux.

Bulk temperature for any given boundary point is calculated by integrating flow and fluid properties on a vector normal to the wall. For the axial boundaries in the coolant channel, this vector is confined to the  $t$ -direction. Bulk temperature is thus calculated according to

$$T_B(z_c) = \frac{\int_t \rho u c_p T dt}{\int_t \rho u c_p dt} \quad (13)$$

where  $u$  denotes the axial velocity component and integrals with respect to  $t$  are in the space dimension, not time. The process of formatting the bulk temperature values into a form compatible with the fuel plate domain is much simpler than the process of formatting surface temperature values for application to the coolant channel. In fact, the process is non-existent. Given the division of two integrals, the units and spatial dimensions of the resultant values come out perfectly formatted for application to the fuel plate domain. Therefore, the relation

$$T_s(z_p) = T_B(z_c) - \frac{k}{h} \frac{d}{dt} T_s(z_p) \quad (14)$$

in concert with the coordinate transformation in Eqn. (11) forms the basis for the coupling from the coolant to the fuel plate.

### 3.5 Exclusion from the Jacobian

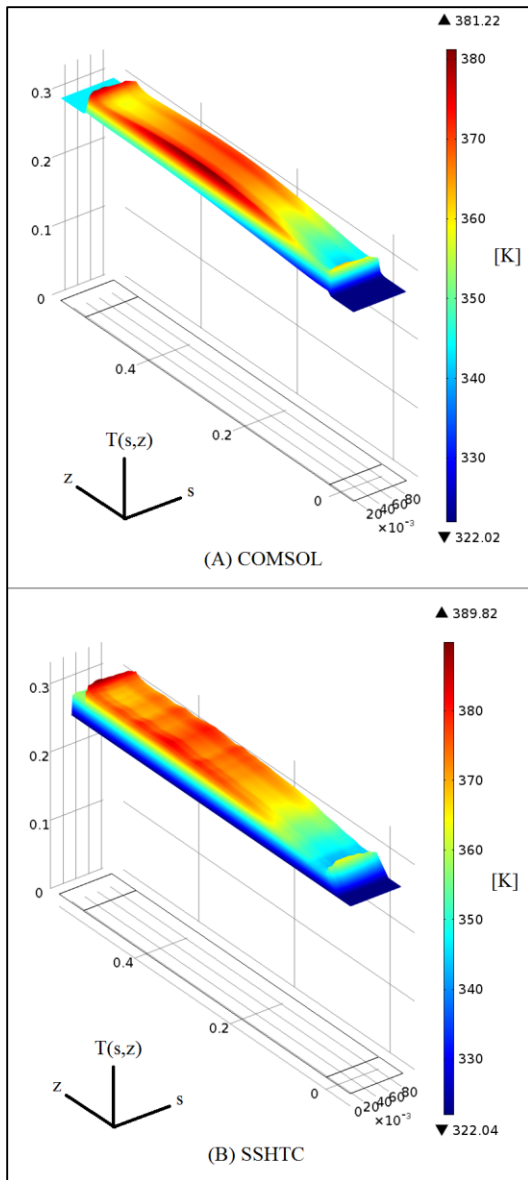
The coupled model's speed-up comes entirely from the simplification of the coolant channel. This advantage is largely negated, however, if the coupled variables are included in the Jacobian matrix formed automatically by COMSOL during the solution assembly process. Not including the coupling terms in the Jacobian matrix could reduce the stability of the model. Yet, given the weak interaction across the coupling, this turns out not to be an issue for this particular model. Both of the coupling variables, that is, the surface temperatures and the bulk temperatures, can be wrapped in a *nojac* operator

to remove them from the Jacobian. This significantly reduces the memory requirements for the solver.

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## 4. Results

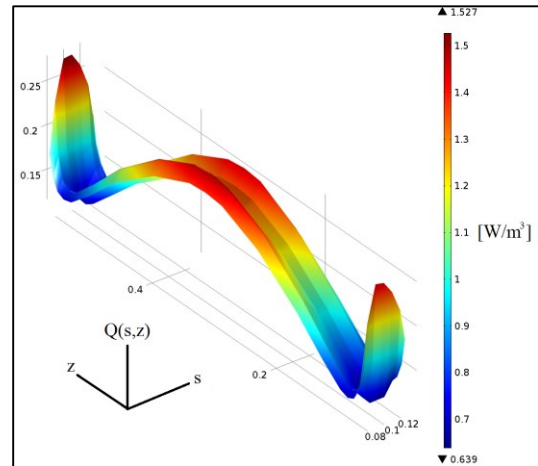
The coupled model is still in an evolving stage. Preliminary results, however, show a respectable agreement with validated safety analysis simulation tools already in use at ORNL. The Steady-State Heat Transfer Code (SSHTC) [20,21] is one such in-house code developed at ORNL for studying the surface temperature profile in reactor core fuel plates. The code is effectively 1D, breaking the fuel plate surface up into discrete nodes along an  $s$ - $z$  coordinate plane grid. Conduction is restricted to the  $t$ -direction in this model, neglecting any heat transfer that is not normal to the axial surfaces of the fuel plate. Given this simplification, there is no communication between nodes. A convective boundary is specified to simulate the coolant's effect. Local bulk temperatures and heat transfer coefficients are calculated at each iterate. Due to its 1D nature, the SSHTC model is considered a conservative estimate, producing higher temperatures than those that are realistically expected. The model also does not compute internal fuel plate temperatures and is only useful for comparing surface temperatures. A comparison of the surface temperatures calculated for the concave side of the fuel plate are shown in Fig 4.



**Fig. 4. Clad Surface Temperature Comparison.** The fuel meat is positioned asymmetrically inside the fuel plate with its center of mass located closer to the concave side than the convex side. As a result, the maximum surface temperature is always found on the concave side and provides a convenient means of comparing solutions. The direction of flow is in the positive  $z$ -direction.

In analyzing the two concave surface temperature profiles it becomes immediately clear that both models capture the general profile of the heat flux driven by the nuclear heat generation in the fuel meat. This volumetric heat generation profile is shown in Fig. 5 for

reference. As evidenced in all three profiles, there are sharp peaks near the beginning and end of the fuel meat along with a gradual rise in the center. The heat generation profile is also higher along its edges than down its center. This topographical trait was captured nicely by the COMSOL surface temperature profile.



**Fig. 5. Volumetric Heat Generation Profile.**

As expected, the two surface temperature profiles are in fairly close agreement even though the SSHTC profile does have higher peaks than the COMSOL model. The difference is due to SSHTC's exclusion of heat conduction in the  $s$ - and  $z$ -directions as well as the coupled model's coolant channel simplification. By using a single bulk temperature value for every spanwise point at a given axial position, the coupled model is, in effect, smoothing out the peaks and valleys of the clad surface temperature profile. At points of above-average surface temperature the bulk temperature is too low, lowering the maximum recorded temperature. Conversely, at points of less-than-average surface temperature the bulk temperature is too high, increasing the minimum recorded temperature.

As can be seen, the SSHTC temperature profile is rougher than the COMSOL profiles. This is again due to what is in effect a 1D solution technique. Given the lack of communication between nodes in SSHTC, each surface temperature is dependent purely upon the local volumetric heat generation and the bulk temperature.

The coupled approach proposed herein is developed as a simplification of a fully three-

dimensional COMSOL model representing an explicitly modeled fuel plate and coolant channel. A general comparison of run-times and model complexity is given in Table 1.

Model	Degrees of Freedom (Million)	Solution Time
3D COMSOL	Total: ~3.5 Clad: ~1.0 Coolant: ~2.5	~72 hrs
Coupled COMSOL	Total: ~2.2 Clad: ~1.2 Coolant: ~1.0	~6 hrs

The coupled model is obviously more efficient in terms of computation time. While it might sacrifice a level of the full 3D model's detail, its close agreement with SSHTC shows that it is still producing an accurate representation of the temperature profile in the fuel plate and meat. This is partially due to the distribution of its degrees of freedom. By simplifying the coolant domain, additional fidelity is able to be gained in the clad domain through the use of quadratic elements.

## 5. Conclusion

The coupled model has proven its usefulness as a relatively inexpensive and time-efficient model. As the LEU conversion research project moves forward with new potential fuel designs, the coupled model provides an alternative and sufficiently accurate means of obtaining temperature profiles in the fuel meat and plate. An advantage of the coupled model, in comparison to the full 3D model, is its scalability. As the periodicity of both models is increased to encompass multiple fuel plates, the computational requirements for the full 3D model increase much more rapidly than the requirements for the coupled model. The ability to extend the length of the simulated core domain permits the study of localized disturbances such as fuel defects or channel blockages, with an eventual goal of modeling the entire core consisting of 540 fuel plates. With its increased efficiency, the demonstrated coupled model takes an important step in the direction of

actualizing this capability without a substantial sacrifice to solution accuracy.

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