Upgrading the HFIR Thermal-Hydraulic Legacy Code Using COMSOL

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Abstract: Modernization of the High Flux Isotope Reactor (HFIR) thermal-hydraulic (TH) design and safety analysis capability is an important step in preparation for the conversion of the HFIR core from a high enriched uranium (HEU) fuel to a low enriched uranium (LEU) fuel. Currently, an important part of the HFIR TH analysis is based on the legacy Steady State Heat Transfer Code (SSHTC), which adds much conservatism to the safety analysis. The multi-dimensional multi-physics capabilities of the COMSOL environment allow the analyst to relax the number and magnitude of conservatisms, imposed by the SSHTC, to present a more physical model of the TH aspect of the HFIR.
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1. Introduction

The TH analysis of the HFIR core is currently based upon the legacy SSHTC. The SSHTC is a one-dimensional, steady state heat transfer code. The dimensionality of the code refers to the way in which thermal energy is distributed in the system by diffusion in a direction normal to the clad surface only. A representation of the computational domain for the SSHTC is presented in Figure 1.

The SSHTC uses a distributed power density profile as an input within the fuel which is determined and provided by separate neutron physics calculations. The assumption of thermal energy diffusion in a direction normal to the clad surface only, assures that the clad surface heat flux maintains the input power density profile. This constraint simplifies the calculation of the clad surface heat flux.

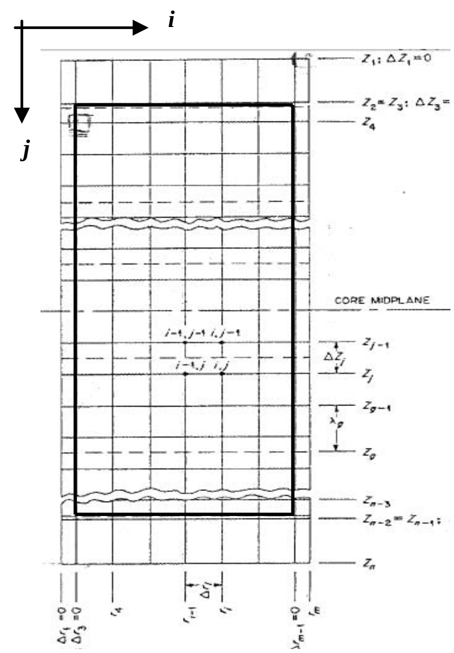

Figure 1. The Fuel Plate Computational Domain of the SSHTC [1]. The index ***i*** represents the span-wise nodal locations of the fuel plate and ***j*** represents the axial nodal locations of the fuel plate. The leading edge of the fuel plate has nodal position ***j*** = 1. The heavily outlined area of the fuel plate represents the active fuel region. Fluid flow is from top to bottom.

The SSHTC does not account for thermal energy diffusion in the ***i, j*** direction. All thermal energy generated in the fuel is diffused in a direction normal to the plane of the paper relative to the orientation of the fuel plate in Figure 1. This presents a constrained estimate of the local quantity of heat leaving the clad surface by confining regions of local thermal energy generation into cells represented by the active fuel portion of the lattice structure in Figure 1. As a result regions of high local power density produce regions of high local clad surface heat flux and high local clad surface temperatures.

A further restriction imposed by the SSHTC on the TH analysis of the HFIR core, is the use of a Nusselt number correlation to determine the film coefficient. Often, many assumptions are made in the determination of an appropriate Nusselt number correlation for a given convection process. As a result, these assumptions have the potential to greatly affect the numerical representation of the physical system. This Nusselt number correlation, in effect, predetermines the quantity of thermal energy leaving the fuel plate and being deposited in the coolant. Because both the film coefficient and the bulk water temperature are not dependent on the simulation of coolant flow, the SSHTC is essentially a thermal energy conduction model.

Geometric assumptions are also present in the SSHTC. The HFIR core is cylindrical in geometry with an inner and outer section. The inner section consists of 171 fuel plates while the outer section houses 369 fuel plates [1]. Each fuel plate is geometrically involute in the radial or span-wise direction from the center of the core. The SSHTC considers a single plate and assumes the fuel plate has a planar surface from which heat is being convected.

A simulation should incorporate as few physical and geometrical assumptions as possible to accurately represent the physical process to be simulated. This is especially true in the nuclear industry where strict standards must be followed to ensure public safety. COMSOL provides such a computational environment. The multi-dimensional multi-physics aspect of the COMSOL environment is well suited to provide a more physically accurate simulation of the thermal-hydraulic phenomena that is key to the HFIR core safety analysis.

As a first step toward the goal of a full 3-D model of the HFIR core, it was necessary to demonstrate that COMSOL was a viable replacement for the legacy safety analysis code, the SSHTC, i.e. using the same inputs, the COMSOL environment would yield similar results to that of the SSHTC.

2. Geometric and Mathematical Representation of the HFIR Fuel Plate in the COMSOL Environment

The above discussion describes the way in which the SSHTC calculates clad surface heat flux and clad surface temperatures. The assumptions listed above (i.e., quantity of heat distributed on the clad surface, film coefficient, and bulk water temperature) should be determined by the physics in the simulation.

Without initially adding the inherent complications of a 3-D analysis, a 2-D geometry was created that represented an axial strip of the fuel plate depicted in Figure 1 at position $\boldsymbol{j} = 6$. This position was chosen based upon the physical geometry of the fuel, i.e., influences of other material was minimized at this position.

The HFIR fuel plate is 0.050 inches (1.27×10^{-3} m) thick and 24 inches (0.6096 m) long [1]. The flow channels have the same dimensions. Figure 2 shows the 2-D geometry used to establish the viability of COMSOL with respect to the SSHTC. The geometry of the COMSOL model is half the width of a fuel plate, 0.025 inches (6.35×10^{-4} m), which is justified by symmetry while the length is preserved [2].

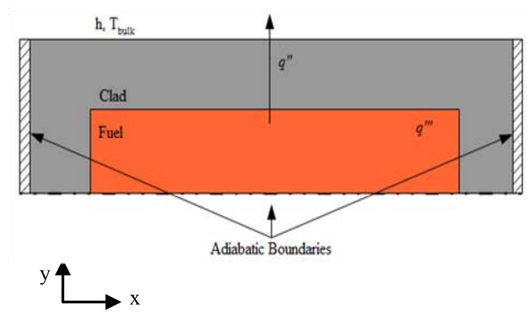

Figure 2. 2-D COMSOL geometry used to reproduce the SSHTC results [2]. The hatched regions signify adiabatic boundaries not due to symmetry. The scale is greatly exaggerated for visual purposes. The aspect ratio of the HFIR fuel plate is 480, length to width. Fluid flow is from left to right.

Since the film coefficient and the bulk temperature are specified inputs in the SSHTC, the model is strictly a conduction problem. The film coefficient used in the SSHTC is shown in Figure 3.

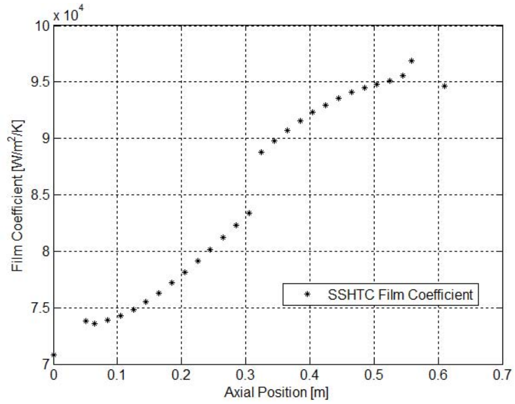

Figure 3. Heat transfer coefficient as a function of axial position used in the SSHTC [2]. The flow is from left to right.

The bulk water temperature used as an input in the SSHTC is shown in Figure 4.

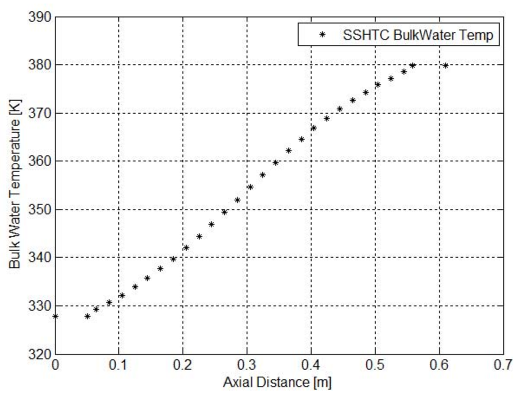

Figure 4. Bulk water temperature as a function of axial position used in the SSHTC [2].

The power density in the fueled region of the plate was back calculated from the clad surface heat flux found in the SSHTC. This calculation was greatly simplified due to the constraint of the diffusion of thermal energy normal to the clad surface. The power density in the fuel is depicted in Figure 5.

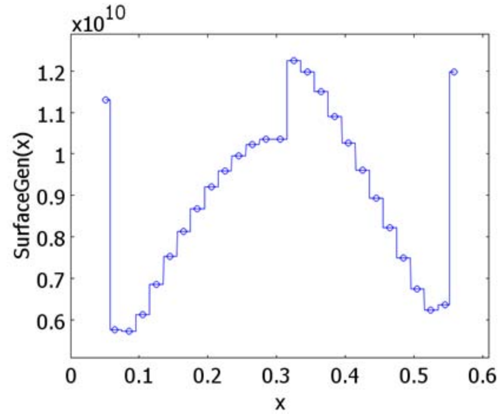

Figure 5. Power density profile used in the SSHTC at position $\boldsymbol{j} = 6$ [2]. Flow is from left to right.

The power density was implemented as tabular data in the COMSOL environment then interpolated with the nearest neighbor scheme.

Because this is a 2-D representation, an inherent assumption is that aspects of the model extend normal to the plane of the paper through a unit distance. While this does present a flaw in modeling the actual physics of the HFIR, it provides a simulation with which to compare results between COMSOL and the SSHTC.

2.1 Governing Equations and Boundary Conditions for Conduction Analysis

As discussed earlier, the specification of a film coefficient and the bulk water temperature reduce the analysis to a conduction problem. Thus the governing equation for the conduction problem is the heat equation which has the general invariant form

$$-\vec{\nabla} \cdot \vec{q}'' + q''' = \rho C_p \frac{\partial T}{\partial t} \qquad (2.1).$$

In equation 2.1, q'' represents the Fourier law for heat conduction, formally given as

$$\vec{q}'' = -\boldsymbol{k}\,\vec{\nabla} T \qquad (2.2)$$

where $\boldsymbol{k}$ is the thermal conductivity tensor of the material and $\vec{\nabla} T$ is the gradient of the temperature field. The other constituents of Equation 2.1 are the thermal energy generation or power density in the material, q''', the material density, ρ, the material specific heat, C_p, and the temporal derivative of the temperature, $\frac{\partial T}{\partial t}$. The boundary conditions associated with equation 2.1 are shown in Figure 2, namely three adiabatic conditions, formally written as

$$\vec{\nabla} T = 0 \tag{2.3}$$

and the convection boundary at the fluid-clad interface given as

$$q'' = h(T - T_{\infty}) \tag{2.4}$$

In order to provide similar inputs in the COMSOL model as those used in the SSHTC, the thermal conductivity tensor, $\boldsymbol{k}$**,** was made to have the following form

$$\boldsymbol{k} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & k_{yy} & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{2.5}$$

This formulation of the thermal conductivity tensor ensures that the heat will only diffuse in the y direction, i.e. normal to the clad surface. The adiabatic conditions on the boundaries normal to the x direction in Figure 2 are consistent with the SSHTC constraint of zero energy diffusion in the axial direction. The adiabatic fuel centerline boundary condition is a physical condition produced by the symmetry of the uniform thermal energy generation. The fuel-clad interface is represented by the continuity condition, which is an idealized condition, i.e., it represents perfect thermal contact. The eventual safety analysis extends this approach by accounting for non-bonding of this interface; causing a degradation in heat transfer. Indeed, it is the non-bonding and hot-spot effects that are of primary emphasis for this advanced analysis capability in COMSOL.

2.2 Constraint Relaxation Model Geometry

The heat transfer coefficient and bulk water temperature are required quantities in convection processes. Eliminating a priori knowledge of these quantities places the burden of their determination on the dynamics of the flow field. As a result the simulation geometry must be changed to include the flow field. This geometry is shown in Figure 6.

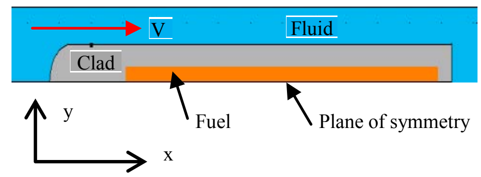

Figure 6. 2-D HFIR Fuel Plate Geometry Including Fluid Flow.

2.3 Turbulent Fluid-Thermal Interaction

In order to relax the constraints imposed on the TH of the HFIR core by the SSHTC, the fluid flow physics needs to be modeled. The volumetric flow rate of the coolant through the HFIR core is approximately 13,000 gallons per minute (GPM) [3]. That translates into a relatively high fluid velocity, u, of 15.88 m/s [1]. The hydraulic diameter of the flow channel, D_h, is 0.0025 m [3] and the dynamic viscosity of the fluid, η, is 0.5693×10^{-3} Pa·s [4]. The Reynolds number based on the hydraulic diameter of the flow channel and fluid density, ρ = 980.28 kg/m^3 [5], is given by

$$Re = \frac{\rho u D_h}{\eta} \tag{2.6}$$

which yields a value of 68,360 which is well within the turbulent flow regime, Re > 2300. The COMSOL non-isothermal turbulent flow coupling equations, found in the heat transfer module, were employed to create a more physical simulation of the HFIR core.

COMSOL version 3.5a has two available turbulent closure models, the k-ε and the k-ω formulations. Energy and mass conservation analyses were performed for both closure models using identical mesh structures and varying the mesh density through adaptive refinements. The k-ω model outperformed the k-ε formulation in mass and energy conservation for this particular problem over the entire range of mesh densities. Thus k-ω was the turbulence model used in the 2-D HFIR TH simulation.

The turbulent equations of fluid flow are

$$i)\ \rho(\vec{u}\cdot\nabla)\vec{u} = \nabla\cdot[-p\boldsymbol{I} + (\eta+\eta_T)(\nabla\vec{u} + (\nabla\vec{u})^T - (2/3)\rho k_{turb}\boldsymbol{I})] \tag{2.7}$$

$$ii)\ \nabla\cdot(\rho\vec{u}) = 0$$

where $\vec{u}$ is the flow velocity vector, η is the dynamic viscosity of the fluid, η_T is the apparent eddy viscosity, p is the thermodynamic pressure, ρ is the fluid density, and k_{turb} is the turbulent kinetic energy of the flow which is represented by its own set of equations.

Equation 2.1 was used for the transport of thermal energy within the solid, with an isotropic thermal conductivity tensor, $\boldsymbol{k}$.

The equation of thermal energy transport in the fluid has the form

$$\vec{\nabla} \cdot \left[-(\boldsymbol{k} + \boldsymbol{k_T})\vec{\nabla}T_f\right] - \rho C_p\left(\vec{u} \cdot \vec{\nabla}T_f\right) = 0 \qquad (2.8)$$

where previously unmentioned quantities are the turbulent thermal conductivity, $\boldsymbol{k_T}$, and the fluid temperature, T_f. This equation represents a balance between thermal energy conduction and thermal energy convection.

Flow boundary conditions associated with equation 2.7 are listed in Table 1.

Table 1. Flow Boundary Conditions for 2-D HFIR Fuel Plate Simulation.

Boundary	**Condition**
Inlet	v0 = 15.88 m/s
Outlet	p = 0 Pa
Clad Surface	$dw^+ = 30$
Non Solid	Symmetry

Thermal boundary conditions associated with the fluid, i.e., equation 2.8, are listed in Table 2.

Table 2. Thermal Boundary Conditions for the Fluid in the 2-D HFIR Fuel Plate Simulation.

Boundary	**Condition**
Inlet	T = 321.9 K
Outlet	Convective Flux
Clad-Fluid	k = k0_chns $T = T_{surface}$ dw = dw_chns
Non Solid	Symmetry

Thermal boundary conditions for the solid fuel plate are listed in Table 3.

Table 3. Thermal Properties of the HFIR Fuel Plate.

Boundary	**Condition**
Fuel Center Line	Adiabatic
Fuel-Clad	Continuity
Clad-Fluid	q0 = -qwf_htgh

The wall offset, dw = y^+, has a valid range of $30 \leq y^+ \leq 100$. Values of y^+ closer than approximately 10 greatly diverge from experimental observations using the logarithmic wall function and over predict the velocity in the viscous sublayer of the flow. As a result unrealistic lower temperatures would be observed at the solid-fluid interface in the simulation.

3. COMSOL-SSHTC Comparison Results

The 2-D COMSOL simulation of the HFIR fuel plate successfully reproduced the SSHTC results for the same axial location, $\boldsymbol{j}$ = 6 and similar inputs. The comparison of the SSHTC clad surface heat flux results, at position $\boldsymbol{j}$ = 6, with that produced by COMSOL are shown in Figure 7.

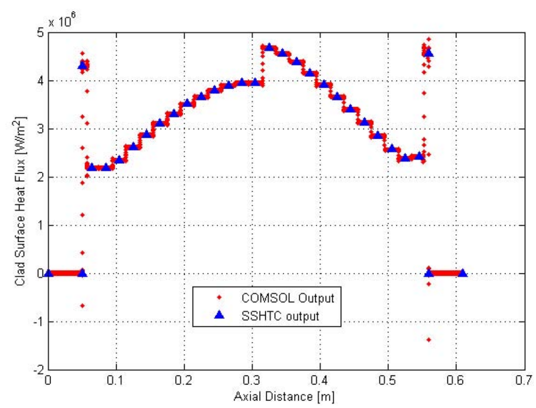

Figure 7. SSHTC and COMSOL clad surface heat flux comparison. Fluid flow is from left to right.

Very good agreement is observed between the two simulations. The comparison of the clad surface temperature determined by COMSOL and that determined by the SSHTC at position $\boldsymbol{j}$ = 6 is shown in Figure 8.

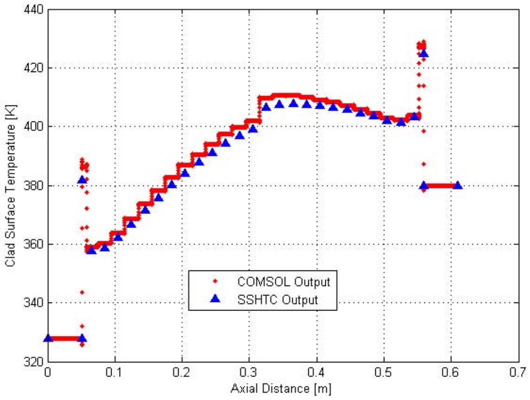

Figure 8. SSHTC and COMSOL clad surface temperature comparison. Flow is from left to right.

These results show that, given a consistent set of inputs and assumptions necessary to approximate the SSHTC simplification, COMSOL can indeed provide similar results with those produced by the SSHTC.

Having shown that COMSOL is a viable code for the TH safety analysis of the HFIR core, interest logically fell on relaxation of the aforementioned constraints imposed by the SSHTC.

3.1 Comparison of Constraint Relaxation COMSOL Model with SSHTC Results

Using the model geometry described in section 2.3, a more physical simulation of the HFIR core was created. The results of this simulation are compared with the results from the SSHTC in Figure 9.

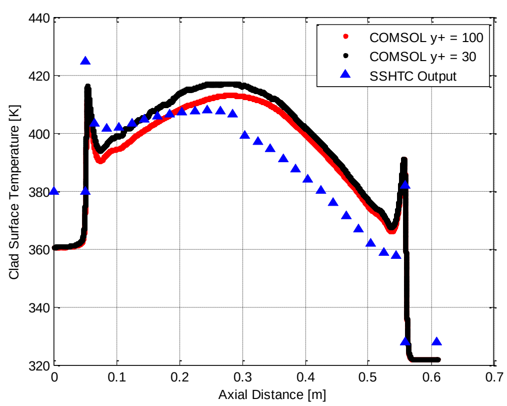

Figure 9. COMSOL Constraint Relaxation Model Compared with SSHTC. Flow is from right to left.

The influence of the wall offset is depicted in Figure 9 by the red and black curves. It is observed that larger values of the wall offset do indeed yield lower temperatures. This is a result of the higher fluid velocities encountered further from the wall.

The effect of the isotropic thermal conductivity tensor is also apparent in Figure 9. The local maxima have changed in magnitude. The SSHTC calculates the highest temperature to reside at the trailing edge of the fuel plate, i.e., axial position 0.5 m. The COMSOL simulations show that the temperature at that position has dropped approximately 10 K. The center of the plate has increased in temperature due to the axial diffusion of thermal energy and is approximately equal in temperature with the trailing edge of the fuel plate. This is important information from a safety standpoint regarding phase change in the coolant. As mentioned previously, the SSHTC determined the maximum temperature to occur at the trailing edge of the fuel plate, thus the most likely position for boiling to occur was rather localized. The present v3.5a COMSOL simulations indicate higher clad surface temperatures in the majority of the domain as compared to the SSHTC results. Preliminary v4.0a COMSOL simulations (not shown here) using Low-Reynolds number turbulence models indicate lower clad surface temperatures.

Also of interest is the thermal expansion of the fuel plate. The SSHTC results would lead one to conclude that the fuel plate will expand significantly in a local manner. This is confirmed by the COMSOL results, and further suggests that the thermal expansion is significant over most of the plate.

4. Conclusions

COMSOL is a viable code in which HFIR TH safety analysis may be performed with confidence. The use of COMSOL will increase knowledge of the TH phenomena occurring in the HFIR. As a result, nuclear safety analysts will be able to simulate nuclear safety related problems with significantly more detail and accuracy.

5. References

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6. Acknowledgements

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