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The Role of COMSOL Toward a Low-Enriched Uranium Fuel Design for the High Flux Isotope Reactor

Abstract Design and safety analyses are underway to convert the High Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory (ORNL) from a high-enriched uranium (HEU) fuel to a low-enriched uranium (LEU) fuel. The primary constraint for the project is that the overall fuel plate dimensions and the current neutron flux performance must remain unchanged. This allows minimal impact on the facility and cost for the conversion, and provides transparency to the HFIR customer base and research projects that depend on the facility for isotopes and neutron flux. As a consequence, the LEU design demands more accuracy and increased definition and focus on safety margin in the analysis efforts than the original design.

Several technical disciplines are required to complete this conversion including nuclear reactor physics, heat transfer, fluid dynamics, structural mechanics, fuel fabrication, and engineering design. The role of COMSOL is to provide the fully-coupled 3D multi-physics analysis for heat transfer, turbulent flow, and structural mechanics of the fuel plates and flow channels. A goal is for COMSOL to simulate the entire fuel element array of fuel plates (171 inner, 369 outer). This paper describes the progress that has been made toward development of benchmark validation models of the existing HEU inner-element fuel plates.

Keywords nuclear fuel, heat transfer, fluid flow, structural mechanics, COMSOL

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1 Research Goals

A primary constraint on HFIR operations is the thermal limit obtained from design and safety analyses. The present limitations at a power level of 85Mw using HEU fuel is based on steady-state analysis using the SSHTC [1] code and transient analysis using the RELAP5 [2] code. RELAP5 remains under active maintenance by the NRC and DOE (depending on which version used) and the HFIR facility will update their RELAP5 models when the LEU design is committed. The current set of calculations that provide the RELAP5 portion of the safety basis will likely require repeating. Much of the input into the RELAP5 models depends directly on the results from the design-based SSHTC.

The SSHTC code was developed at the time HFIR was originally designed and constructed in the mid-1960s and has changed very little since. The basis for the thermal limits include a strong validation history of testing and experiments. The HFIR has operated safely since approximately 1966 and is now on HEU fuel cycle #423 (about 6-10 cycles per year) and counting. The code documentation and design/structure are not convenient for changing the code to accommodate an LEU design change; i.e., classic ’60s vintage FORTRAN along with difficult documentation and few embedded code comments. Further, in order to meet the design goal of achieving an equivalent neutron flux performance within the same overall external dimensions, the analysis must be carried out well beyond the capabilities of the present SSHTC code. Therefore, in order to perform an equivalent design and safety analysis for LEU fuel using the legacy codes, a major code development effort would be required if the SSHTC were to be retained as the basis code.

The major item of analysis improvement required to achieve a new HFIR LEU design is a significant reduction in the “hot spot factor” (HSF). The HSF is a direct accounting for the uncertainty in manufacturing tolerances and defects such that a reduction in heat transfer capability (increase in thermal resistance) occurs. The resulting increase in temperature causes a reduction in the safety margin and therefore restricts the operating range of HFIR. Based on present 1-D SSHTC analysis, the hot spot is verified to be acceptable by X-ray scanning during the manufacturing process if the defect area is less than approximately 0.25-inch square.

This same HSF is also used in the 1-D transient analysis carried out by RELAP5. The HSF is implemented in RELAP5 by modeling a separate host spot area, and imposing a power distribution increased by the HSF. Several hot spots are modeled in this manner with the worst case being at the core exit. A “hot streak” is also modeled in RELAP5 in a similar manner.

The application of the HSF is made in a single direction normal to the fuel plate; also the same direction as the main convection between the plate and the coolant. The dominant mode of heat transfer by conduction in the fuel plate is not credited in the other two dimensions. In utilizing a modern analysis code, such as COMSOL, on this problem, heat transfer by conduction and convection is accounted for in all three directions of space. Furthermore, additional physics are also fully coupled to the problem in full detail including structural mechanics. It is expected that the enhanced analysis will significantly reduce the HSF and a companion increase in the margin of safety. It may also be possible to improve the performance level of the HFIR.

The essential research goals are:

- Validate COMSOL results for the existing HEU fuel plate in pseudo-1D/2D against the SSHTC and companion test/experiment data taken during the era of the HFIR core design,
- Develop a detailed, realistic 3D COMSOL model of a single HEU fuel plate and coolant channel for flow, heat transfer, and structural mechanics coupled multiphysics, and demonstrate the improvement in HSF and safety margin, and
- Develop a companion LEU fuel-plate model (significantly different internals) at the proposed 100 Mw power level and compare performance. It is anticipated that a test program will be conducted to validate the LEU model results.

It is also proposed that an “enhanced HEU” HFIR core will be tested to demonstrate the improved safety margin realized prior to testing of an LEU-fueled HFIR core.

2 Tasks Currently Underway or Identified

An entry-level study[3] was conducted by a separate research group to evaluate the fundamental capabilities of COMSOL on this problem. The results were only marginally acceptable; primarily due to the inexperience of the researchers in using COMSOL causing many fundamental flaws in the analysis.

A new research team has been formed composed of individuals with extensive COMSOL experience. The first task of this team has been to check and review the initial findings. This work is approaching the completion stage and will result in a revised or new report. The tasks nearing completion are:

- verify the models and results from the prior report,
- document and verify SSHTC inputs required for input into COMSOL,
- verify finite-element accuracy by energy-norm methods as compared to graphical solution results,
- develop a COMSOL material library for HFIR-specific materials including water that is temperature and pressure dependent,
- develop a 2D non-isothermal turbulent model of the HFIR HEU fuel plate,
- verify proper boundary conditions to be used in the modeling with particular attention to the entrance and exit regions,
- develop a COMSOL-fitted nuclear fuel power distribution curve and verify proper integrated power levels, and
- overlay COMSOL results against SSHTC results.

After completion of these tasks, several additional tasks are to be completed while still focused in the 2D solution mode. These tasks include

- developing proper boundary layer meshing and determine valid ranges for y^+ and T^+ mesh dependence,
- investigate options for turbulent Prandtl number provided by COMSOL,
- develop a consistent local hot-spot model revision,
- develop a consistent entrance and exit model revision,
- accommodate a fitted-curve power distribution function provided by separate nuclear physics calculation, and
- compare and document the final, best-estimate 2D representation generated by COMSOL against equivalent SSHTC and/or RELAP5 results.

The lessons learned from these 2D studies are directly applicable to the 3D models. An efficient transition to the much more complex and computationally-intensive 3D extension can be achieved with minimal waste with this type of geometric representation of a HFIR fuel plate. For example, the near-wall mesh requirements will have been established, all the material-property libraries developed, and power distribution methodology verified. Four additional areas of development have been identified and started in the 3D framework:

- development of 3D geometry and meshing extruded from a 2D working plane,
- in parallel, develop the 3D geometry with *Solidworks* and generate the mesh with COMSOL using the “live

connection" capabilities of the two codes (early results with this approach show the additional benefit of a reduced number of surfaces to specify for boundary conditions),
- application of consistent boundary conditions upon the increased number of surfaces now present in the 3D model; including the application of extrusion coupling to provide for symmetry to the coolant channel, and
- development of the 3D iterative solution methods required to obtain a converged steady-state solution within the computing environment.

These 3D tasks are well underway and some preliminary results are presented here and in the conference presentation material.

3 Areas of Intense Focus

The HFIR fuel plate is designed with a very thin (0.050-inch) thickness across which is the predominant direction of heat transfer by convection from the nuclear-heated fuel to the coolant. In the span-wise direction, the scale is a few inches (3.6" for the inner element, and 3.2" for the outer). The length-wise direction, which is the predominant direction of the coolant flow, is 24-inches. Therefore, the aspect ratio is $\sim 74-72$ in the span-wise direction and ~ 480 in the length-wise direction. To compound the situation, because the Reynolds number, based on the channel width, is approaching 10^5, a fine mesh is required near the wall in the coolant region in order to capture the turbulent boundary layer profile and produce a reasonable y^+ range. Therefore, the aspect ratio demands on the finite elements are extremely large in the length-wise direction in order to be able to obtain a solution. Fortunately, experience has shown that because the flow is dominant in the length-wise direction, large aspect ratios are acceptable for consistent solutions. Therefore, even though the COMSOL mesh generation tools will show a poor quality element resulting from these large aspect ratios, a careful study of the axial (or length-wise) mesh spacing caused by the mesh extrusion process should reveal solutions consistent with the available test data. Hence, a primary research focus is the maximum acceptable mesh spacing in the axial direction.

The HFIR was designed to provide the highest neutron flux in the world for the production of neutrons and isotopes. As a consequence, the demands for heat flux management are high, hence, the high Reynolds number flow mentioned earlier. Therefore, it is possible that the range of applicability of the COMSOL turbulence models provided by the heat transfer and/or chemical-engineering application modes; i.e., $k-\varepsilon$ and $k-\omega$, may be deficient in accuracy for this range of heat and momentum flux. If this turns out to be the case, COMSOL provides the tools to be able to modify these models by either a better model obtained from literature and/or industry or by derivation of a new model. Hence, another primary area of research focus is on the accuracy and proper application of the given turbulent models and changing these models should it become necessary.

Early results from the 3D model solutions have found that a single fuel plate and adjacent coolant channel can be solved with a reasonable level of accuracy with about 100 axial mesh spacings yielding approximately 5×10^6 degrees of freedom (to be solved). The resulting multigrid-based iterative solution method requires about 40 GB of memory and takes about a cpu-week to solve on a single 8-core, shared memory, dual-processor, 64-bit AMD cluster node. We are interested in solving the entire HFIR core which consists of 171 inner fuel plates and 369 outer fuel plates. Needless to say, we are most interested in the potential gains to be obtained from the upcoming release of the COMSOL distributed parallel processing. We expect this to be a difficult goal to achieve and will occupy much of our research focus.

4 Current Status and Results

2D Results

The 2-D, vertical cross-section, non-isothermal HEU fuel plate model exhibits a strong dependence on the chosen meshing scheme. The mesh must be sufficiently dense at the solid-fluid boundary in order to produce the required range of y^+ for the turbulent boundary layer simulation. Our first approach was to utilize the free mesh (FM) capabilities of COMSOL for all domains in the geometry. A quality analysis of the model revealed large relative errors in the energy balance of the fluid domain, while the energy balance in the solid retained very good agreement, on the order of 1×10^{-3}%. The large errors in the fluid domain were obtained regardless of the number of mesh refinements conducted. Utilizing the COMSOL adaptive mesh feature brought no improvement in this error.

Mapped meshes (MM) are recommended by COMSOL for thin structures such as the HFIR fuel plate. The mesh was changed to a MM approach for those regions that did not involve a curvature in the geometry. This change allowed a suitable mesh to be generated in the fluid domain adjacent to the fuel plate. Also, the number of elements decreased significantly with the MM relative to the FM. While the mesh was visually acceptable in terms of sufficient density at the solid-fluid boundary, the large relative error in the energy balance of the fluid remained.

A boundary layer meshing (BLM) approach was then investigated. One advantage of the BLM is suitability along the curved leading edge of the fuel plate. With minimal refinements, the large relative error in the energy balance of the fluid was reduced below 4%. The trade off for this acceptable model quality is the increase in CPU time and RAM consumption. While the number of elements ($\sim 2\times10^5$) in the BLM was less than the FM, the total degrees of freedom was still significant at $\sim 2\times10^6$

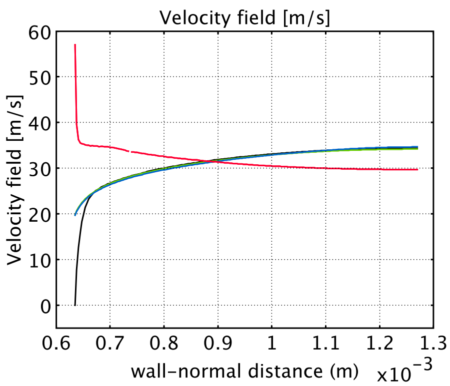

Fig. 1 Preliminary 2D Results: Velocity Profiles at flow channel entrance (red), start of heated section (blue), end of heated section (green), and exit of the flow channel (black).

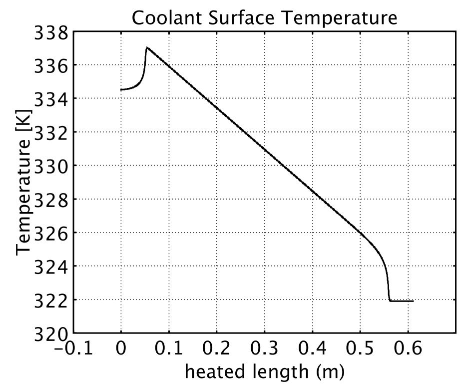

Fig. 3 Preliminary 2D Results: Coolant surface temperature along the turbulent flow wall interface. Note: left to right indicates exit to entrance of the flow channel.

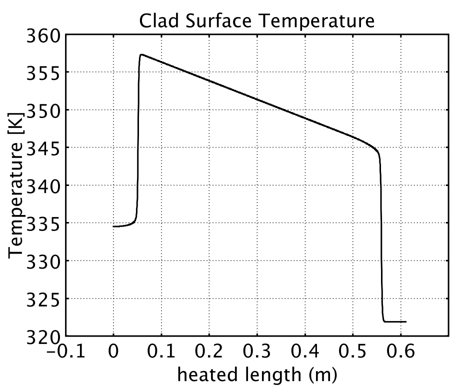

Fig. 2 Preliminary 2D Results: Clad surface temperature along the turbulent flow wall interface. Note: left to right indicates exit to entrance of the flow channel.

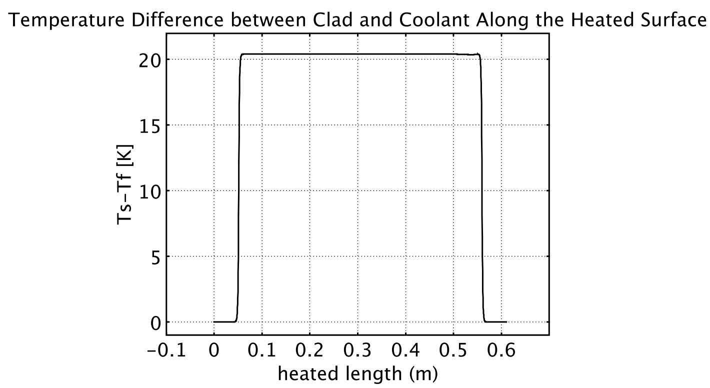

Fig. 4 Preliminary 2D Results: Clad-Coolant Temperature difference along the turbulent flow wall interface. Note: left to right indicates exit to entrance of the flow channel.

Some preliminary 2D results in Figure 1 demonstrate the classic development of the turbulent boundary layer profile in the coolant channel. The high Reynolds number and narrow channel width is apparent.

Close examination of the temperature profile at the solid and fluid interface is shown by Figures 2 through 4 inclusive. The coolant entrance is at ~ 0.6096 meters (24 inches) above the core exit and temperature increasing toward the exit (left). A near constant temperature difference of ~ 20K is shown in Figure 4.

A typical 2D result obtained in an earlier study of the total temperature of the fuel and coolant system overlayed with velocity contours is shown by Figure 5 demonstrating the importance of the entrance and exit effects on the velocity. Note that the velocity contours are of non-zero slope at the exit which implies that not all the convection heat transfer is complete in the system as it is currently modeled. The dominant mode of heat transfer is by convection in the wall-normal direction perpendicular to the coolant flow direction. However, since the goal is to credit all heat transfer mechanisms in this system, we anticipate an extension in the exit flow recovery length just as the actual HFIR core is designed.

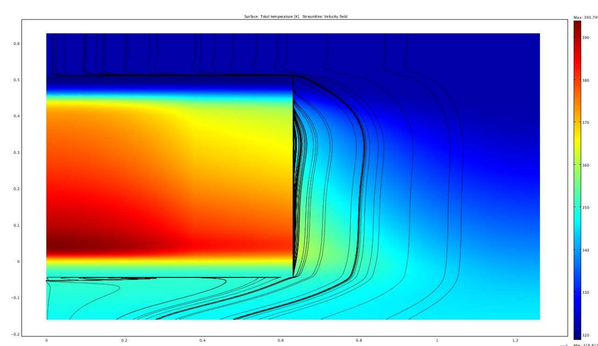

Fig. 5 Preliminary 2D Results: Total temperature overlayed by constant-velocity contour lines.

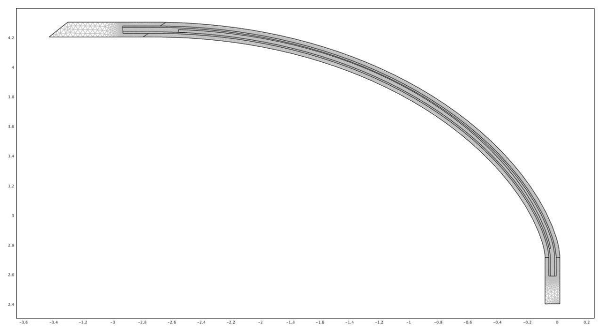

Fig. 6 COMSOL Cross Section Meshing of the HFIR Inner Fuel Element.

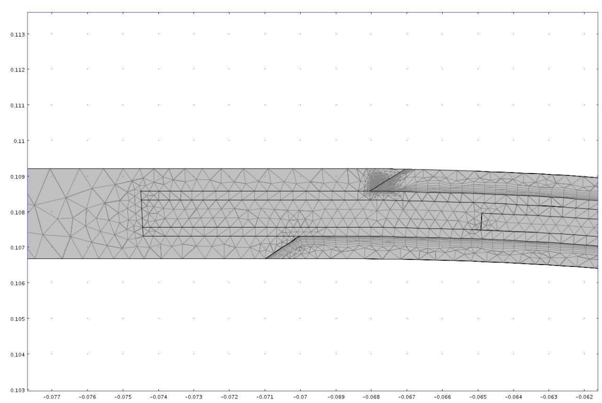

Fig. 7 Mesh Details of the HFIR Inner Fuel Plate COMSOL Model.

3D Results

The geometry of the HFIR fuel plates is an involute shape. This basic shape and fuel internals are modeled with COMSOL tools to yield the following mesh as shown in Figure 6.

A closeup of the meshing details showing the side plates, coolant, clad, filler, and fuel regions is in Figure 7. Troublesome areas near the coolant corners required extra mesh density to resolve.

This cross-section mesh was then extruded in the axial (z) direction to provide a full 3D simulation of the fuel plate and adjacent cooling channel. The computational requirements are extensive due to the large aspect ratio of the actual geometry (24” high , 0.050” fuel plate thickness) and the boundary layer mesh requirements of the variable-density Navier-Stokes equations.

Figure 8 shows the boundary segments used to produce the outer limits of the fuel plate and flow channel.

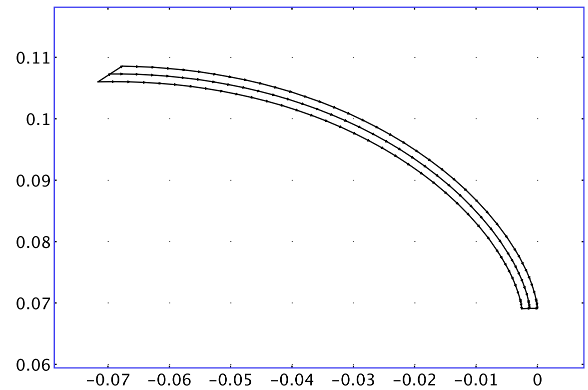

Fig. 8 COMSOL Boundary Elements of the HFIR Inner Fuel Element.

The number of boundary elements is determined by the construction method, i.e. constant arc length or constant angle between construction points. This type of geometry construction results in at least 126 boundaries. Even more boundaries or construction points would be needed to refine the curvature of the involute. In contrast, a similar Solidworks model would result in only 11 boundaries because each face is imported as a boundary.

Constructing the 3D model in Solidworks provides a straight-forward implementation of boundary conditions. However, more effort is required upfront to construct and repair the CAD model so that it will mesh successfully. In the draw mode, the imported geometry may look disjointed, but applying a mesh will refine the curvature in COMSOL so that it better resembles the initial solid model. Once meshing is completed, the assignment of boundary conditions and extrusion coupling variables is greatly simplified.

A typical result of the simulation is shown in Figure 9 for the metal surfaces. This model solves the non-isothermal form of the Navier-Stokes equations, along with the $k-\varepsilon$ turbulence model. This set of equations results in 8 independent variables $(u, v, w, p, logk, logd, Ts, Tf)$ to be simultaneously solved in 3D steady-state. The present model utilizes a geometry without the entrance and exit regions (the importance of which was demonstrated in Figure 5), and creates the 3D mesh by simple extrusion of the working-plane mesh shown in Figures 6 and 7. The most-detailed axial spacing solved thus far using this simple extrusion method was 96 elements ($\frac{1}{4}$-inch spacing) using linear-basis elements for all the variables and resulted in approximately 5×10^6 degrees of freedom to be solved. Even at this resolution, it is not clear that a sufficient level of mesh refinement (particularly in the axial, or length-wise, direction) is sufficient for this model (to be determined).

Even on our 64-bit AMD64 computer with 64GB of memory, this model is prohibitively large to be solved using the COMSOL direct solvers. Therefore, the recommended approach, based on the GMRES iterative solver, is utilized. The problem is first split into three groups by using the segregated stationary solver (u, v, w, p) , $(logk, logd)$, (Ts, Tf). Each group uses the GMRES iterative solver with the multigrid preconditioner. The multigrid meshing is set up manually by creating, and saving the mesh to file, mesh spacings of 12, 24, 48, and 96 axial elements and naming the sets mesh case 4, 3, 2, and 1 respectively. Mesh case 0 is identical to mesh case 1 with the element basis increased to quadratic everywhere (but has not been solved yet).

Within each preconditioner iteration, all mesh cases are both used and assembled. 4 outer preconditioner iterations are performed using the V-cycle multigrid cycle. For all the segregated set, a blocked SOR presmoother is performed at 4 iterations and a relaxation factor of 0.8. The postsmoother is set up identically as the presmoother. The coarse solver is solved directly using the PARDISO solver (mesh case 4).

Within each segregated step, a constant damping factor is set at 0.5 and 2-3 iterations are performed with minimal Jacobian update. The iterations are stopped at either step numbers 2-3 or tolerance of 1.0×10^{-2}. The overall convergence criteria for each segregated step was set at 1.0×10^{-4}.

With these settings, the model took about a week of clock time to converge using 8 cpu shared-memory processors on a 64-bit AMD64 Debian/Gnu-Linux machine using version 3.5 of COMSOL. The memory required was about 40 GB of the 64 GB available during this time. On average, about 6 load factor was constantly used indicating only 75% utilization of the processors available. The model could be stopped and restarted, and the new plot while solving feature was nice. We have not tried version 3.5a, having the new SOR enhancements, on this problem yet, but hope to do this soon. Our main goal was to demonstrate that we could solve the problem in a reasonable time frame and obtain a meaningful solution. We anxiously anticipate further improvements in solution time with the distributed parallel processing capabilities of COMSOL to be released soon.

5 Conclusions

It is early in the COMSOL model development for this project, but these preliminary simulations look very promising. The challenge will be to determine the number of axial mesh levels and boundary layer resolution such that a good match with early test data on the fuel design is sufficiently matched. With confidence gained from validation of the HEU fuel simulations, extended simulations of the LEU fuel redesign will be forthcoming.

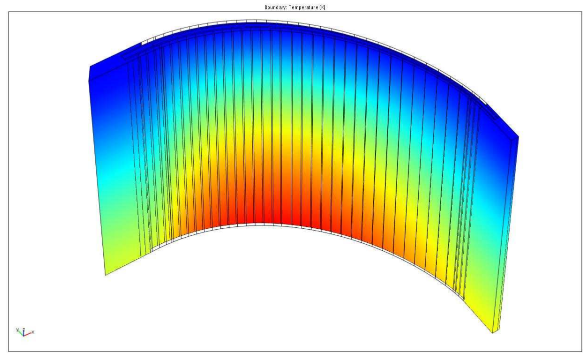

Fig. 9 Metal Surface (non-coolant) Temperature for a Typical COMSOL Simulation of a HFIR Inner Fuel Plate.

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