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Multiphysics Simulations of the Complex 3D Geometry of the High Flux Isotope Reactor Fuel Elements Using COMSOL

Abstract A research and development project is ongoing to convert the currently operating High Flux Isotope Reactor (HFIR) of Oak Ridge National Laboratory (ORNL) from highly-enriched Uranium (HEU U_3O_8) fuel to low-enriched Uranium (LEU U-10Mo) fuel. Because LEU HFIR-specific testing and experiments will be limited, COMSOL is chosen to provide the needed multiphysics simulation capability to validate against the HEU design data and calculations, and predict the performance of the LEU fuel for design and safety analyses. The focus of this paper is on the unique issues associated with COMSOL modeling of the 3D geometry, meshing, and solution of the HFIR fuel plate and assembled fuel elements. Two parallel paths of 3D model development are underway. The first path follows the traditional route through examination of all flow and heat transfer details using the Low-Reynolds number k-ε turbulence model provided by COMSOL v4.2. The second path simplifies the fluid channel modeling by taking advantage of the wealth of knowledge provided by decades of design and safety analyses, data from experiments and tests, and HFIR operation. By simplifying the fluid channel, the level of complexity and computer resource requirements are significantly reduced, while also expanding the level and type of analysis that can be performed with COMSOL. Comparison and confirmation of validity of the first (detailed) and second (simplified) 3D modeling paths with each other, and with available data, will enable an expanded level of analysis. The detailed model will be used to analyze hot-spots and other micro fuel behavior events. The simplified model will be used to analyze events such as routine heat-up and expansion of the entire fuel element, and flow blockage. Preliminary, coarse-mesh model results of the detailed individual fuel plate are presented. Examples of the solution for an entire fuel element consisting of multiple individual fuel plates produced by the simplified model are also presented.

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

1 Introduction

The fundamental design of the HFIR is a beryllium-reflected, light water cooled, HEU-fueled research reactor operating at 85 MW power. The original HEU design for HFIR was at a power level of 100 MW. 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. Several physical phenomena — including turbulent flow, conjugate heat transfer, thermal-structure interaction, and fluid-structure interaction — are of significant interest for the thermal safety analyses of the new HFIR LEU fuel core.

The HFIR core assembly resides in an 8-ft diameter pressure vessel (operable up to 1000 psi) which is located in an 18-ft diameter cylindrical pool of water. HFIR has a total of 2 fuel elements called 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 that make up the HFIR core. These involute-shaped fuel plates are uniformly spaced so as to provide equal coolant flow area for each plate within each element. To remove the heat generated in the fuel plates, light water coolant is forced through the gaps between the plates at an average inlet velocity of 15.8 m/s. A total of 13,000 gallons of water passes through the HFIR core every minute. Because of the (i) manufacturing tolerances in fuel plate dimensions, (ii) thermal expansion of plates due to radially and axially varying time-dependent heat generation rates, (iii) possible local segregation of fuel and non-bonds with cladding, (iv) pressure and turbulence induced structural deflections, (v) build-up of oxide layers on the plate surfaces, and (vi) other uncertainties, there is a possibility to develop unwanted hot regions within the HFIR fuel elements. A reasonably accurate prediction of

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these hot regions becomes necessary to ensure the safety of the reactor while converting it to a LEU core.

As mentioned earlier, several physics are considered in order to properly simulate the HFIR. A proper accounting of all of these physics will provide the desired predictive capability for the conversion of HFIR to LEU fuel. It is anticipated that the COMSOL multiphysics environment will fulfill the need for a robust simulation of all these physics and more. Efforts have started at ORNL to build the multiphysics modeling capability for the HFIR IFE and OFE. There are three other papers in the proceedings from this conference that describe some of the additional ongoing research and development related to COMSOL modeling of the HFIR[1–3]. This paper will focus on details of 3D modeling that is unique compared to other aspects of the overall project.

2 Creation of the HFIR Involute Geometry

The fundamental shape of the HFIR fuel plate is the involute. This geometry has been described in previous reports [4–6]. With earlier versions of COMSOL, it has been difficult to precisely describe the involute geometry. The most successful way was to connect a series of points to create an approximation to the involute curve in COMSOL. At each input point in the approximate curve, an artificial “corner” was created in 3D which lead to inconsistent viscous recirculation zones that were obviously not desired in the solution. In addition, handling of both the geometry and mesh requirements became time consuming and complicated due to the large number of surfaces present in the model. These surfaces were created from the extrusion of lines joining the initial points used to approximate the involute curve. The above approach, which was prone to both numerical as well as human errors, turned out to be very undesirable. Alternatively, a popular CAD package was utilized to create the involute geometry. That effort was partially successful, but ultimately caused difficulty in meshing the resulting geometry.

Upon the release of v4.1 of COMSOL, the new feature to input a parametric curve brought about a dramatically improved capability to create the HFIR fuel plate involute curve. Indeed, not only is the involute curve created precisely, but the resulting surfaces created by extrusion or extension from the basic shapes are simpler, which allows for more-consistent specification of boundary conditions, and other geometry-dependent items in fewer mouse “clicks.”

The mathematics of an involute has been described previously in detail, with particular attention to construction of the involute geometry in COMSOL[4]. The following equations of the involute curve are directly included as one of the first inputs in the geometry development process using s as the free parameter:

$$x(s) = R_{b_i}\left[sin(s) - s \cdot cos(s)\right],$$

$$y(s) = R_{b_i}\left[cos(s) + s \cdot sin(s)\right], \quad \text{where}$$

$$\theta_{\min} \leq s \leq \theta_{\max},$$

R_{b_i} = base radius of the involute, and

$\theta_{\min}$ = angle for the starting point of the involute, and

$\theta_{\max}$ = angle for the end point of the involute.

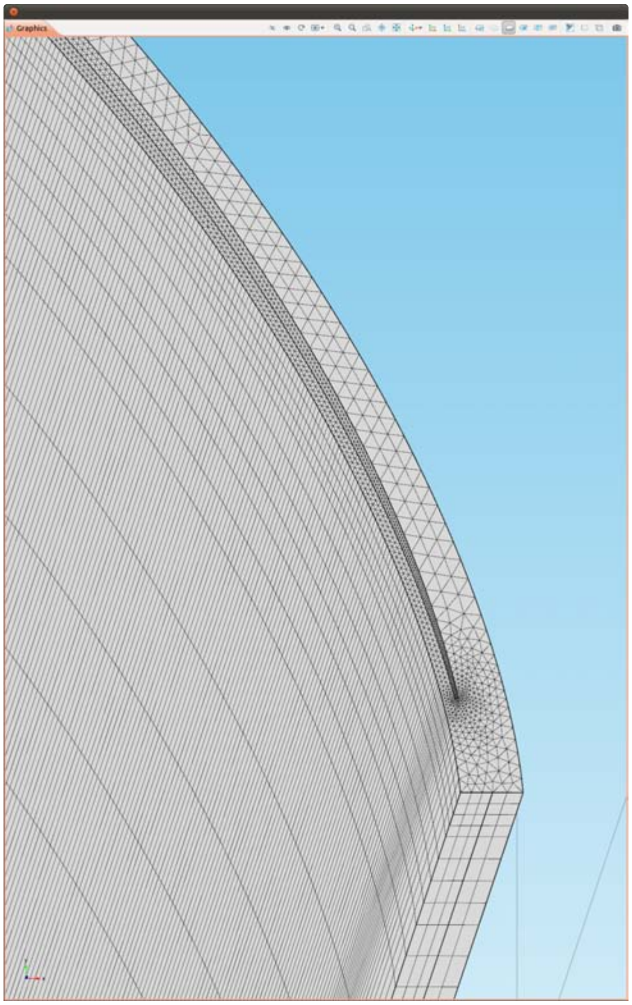

Fig. 1 Meshing details of a 3D slice as viewed from the top of the fueled section of the HFIR involute-shaped inner fuel plate.

Remaining steps for the geometry generation are rather straightforward, and therefore, not discussed herein. Fig. 1 shows the meshing details which preserve the involute geometry shape. Notice the additional involute-like shape internal to the fuel plate which represents the fuel meat. The details of this piece of the geometry are described in another paper [3] of this conference.

With continuous improvements in COMSOL meshing capabilities and CAD interface, it is expected that additional investigation into some newly-improved CAD packages could meet the needs of our HFIR COMSOL models. COMSOL technical support has also recommended the CAD import route since our geometry is testing the limits of what the internal COMSOL geometry creation can do.

3 Meshing Sequence Towards a Detailed Solution of a Single HFIR Fuel Plate

In earlier studies[5], it was determined that the resolution in the axial meshing must be at least the same as the resolution of the power profile defined as input from the nuclear physics obtained by a separate calculation. Therefore, if the power profile contains 20 points in the axial direction (same as the flow direction), then it is necessary and sufficient to have at least that many axial-direction points in the COMSOL model for the simulation to be accurate. As a starting point, the mesh is generated along exactly the same axial points as the power profile within the fueled section of the model. The adjacent domain meshing is meshed axially with similar resolution and acceptable finite-element mesh growth rate.

An initial coarse-mesh uses the k-ε turbulent model (law-of-the-wall) and overrides the wall offset computation by setting $y^+ = 100$. This coarse-mesh has only 4-5 elements spanning the half-width coolant channel. Since the model takes advantage of periodic boundary conditions, only a half-width coolant channel is modeled on each side of the fuel plate. Of course, this level of meshing is very coarse for the problem being solved, and it may become necessary to eventually arrive — through successive restarts — at an adequately refined mesh to resolve all the details.

Yet even with this very-coarse mesh, the solution space yields approximately 1 Mdof. We expect the final mesh resolution to be approximately 20 Mdof for this single-plate model. The current plan is to restart 2-3 times using the k-ε turbulence model with successive higher mesh density in the coolant. The metal mesh density is already adequate even at the initial mesh (very-coarse). Then additional boundary-layer mesh will be added to arrive at the final wall-offset (y^+) of approximately 10-30 for a law-of-the-wall simulation. Then, the Low-Reynolds number k-ε model will be restarted from the highest-resolution k-ε wall function model with an even-finer near-wall mesh such that the criteria $l_c^* \leq 1$ will be satisfied. And finally, the axial mesh spacing will be refined by doubling the mesh density until a mesh-independent solution is obtained. We expect the final mesh density to yield on the order of 20 Mdof.

4 A Coarse-Mesh Solution Comparing Two Different Fuel Designs

The project is interested in a "quick-look" solution comparison of the difference between two different designs of the LEU fuel meat. In one design[7], the meat is additionally contoured at the lower section of the fuel to reduce the neutron reflection effects due to the water at the base of the fuel element. This first design is in contrast to a second design whereby the LEU fuel meat is not contoured axially at the end, and hence, the local power peaks at the coolant channel exit. This second design, without axial contouring, is expected to have a higher fuel-clad surface temperature. The question is then, how much higher is the surface temperature, and is it sufficiently different to justify the additional cost of producing an axially-contoured LEU fuel element for HFIR in the future ? It turns out that the exit clad surface temperature of the HFIR is the critical point of interest for the nuclear safety analysis of the facility.

The "quick-look" solution on our Linux cluster for the coarse-mesh model of ≈ 1 Mdof with COMSOL is produced in about a day. Solutions with the 5-6 Mdof have been produced by restarting from this coarse-mesh solution in approximately 1 week of computation time; but this has only been done this with the axially-contoured fuel design. Therefore, only the coarse-mesh solution comparisons are shown here between the two LEU fuel designs. Fig. 2 shows the steady-state surface temperature between the clad and coolant for the coarse-mesh model where the LEU fuel is contoured at the exit. Fig. 3 is a similar solution for the case where the LEU fuel is not contoured at the exit.

The maximum temperature for the axially non-contoured (more easily manufactured) LEU fuel element is found to be about 395.6 K and is located at the exit plane of the fueled-section of the plate. [1] The bulk coolant temperature is heating continuously from inlet (top) to outlet (bottom) and is a maximum at the outlet. Therefore, the combination of a large peak in fuel heat generation rate and a maximum in bulk coolant temperature is the reason that the peak clad temperature is located at the exit for the axially non-contoured LEU fuel design.

On the other hand, the solution for the axially-contoured fuel reveals that the peak temperature has shifted away from the exit plane and is, instead, near the midplane of the fuel plate. Furthermore, the maximum temperature is also slightly increased to about 401.1 K. Since the only change made to the model is in the power density profile, this is the primary reason for the change in position and magnitude of the peak clad surface temperature. Note that both design analysis options produce the same total power in the single fuel plate. Therefore, the axial-contouring appears to be desirable, but this single analysis alone is not sufficient to answer all the questions about the final design choice.

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[1] It will be necessary for the reader to zoom in on the .pdf form of this paper to be able to see the details showing the maximum temperature value and location on the plots.

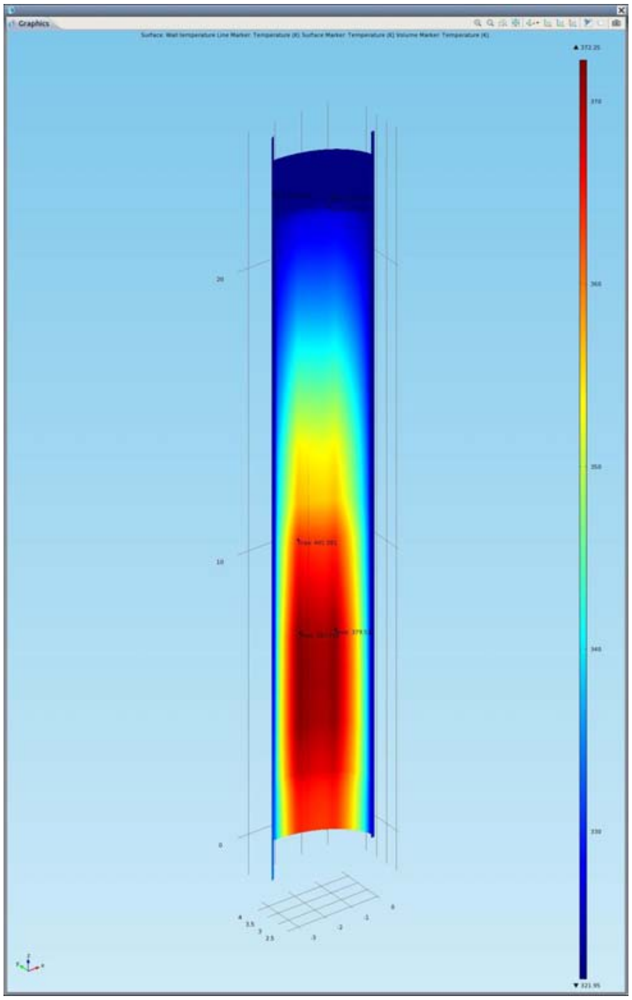

Fig. 2 Steady-state surface temperature (K) between the clad and coolant for the coarse-mesh model where the LEU fuel is contoured at the exit.

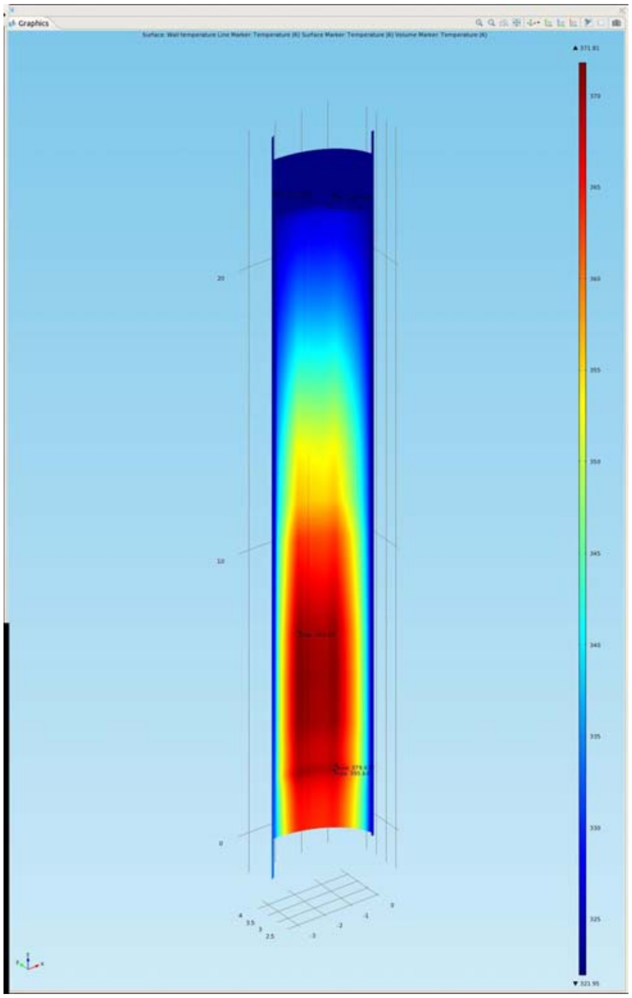

Fig. 3 Steady-state surface temperature (K) between the clad and coolant for the coarse-mesh model where the LEU fuel is not contoured at the exit.

5 Thermal Expansion Simulations of the HFIR Outer Fuel Plate in 3D

During the HFIR design development in early 1960s, several experimental investigations, often referred to as the *Kelley-Cheverton Tests* [8], were performed to ensure that the core will always remain under its thermal limits. One of the prime concerns at that time was the possibility of longitudinal buckling of the thin (0.05 inch) and long (24 inch) HFIR fuel plates under non-uniform thermal loading of the fuel elements and the side plates. To address this concern, several experiments were performed to quantify the amount of structural deformations of HFIR fuel plates under their anticipated thermal operating conditions. In these experiments, a single involute fuel plate from the OFE was constrained to its sides and heated in an oven up to 400°F, and the ensuing structural deflections due to thermal expansion were measured using the apparatus shown in Fig. 4. Note that the outer involute fuel plate was chosen in the experiments because it is relatively flatter than the inner fuel plate of HFIR, and is therefore more susceptible to buckling at a lower critical load. In the experiments, no longitudinal buckling was observed.

At ORNL, COMSOL is now being used to simulate the *Kelley-Cheverton Tests* in an effort to validate the developed models, and to provide a predictive platform to evaluate structural response of LEU fuel plates to subjected thermal loads. Preliminary 3D simulation results, as shown in Fig. 5 and Fig. 6, suggest that COMSOL is able to properly capture the thermal expansion physics and will be able to provide the desired predictive capability. Note that the relative deformation of the plate is significantly scaled up (20x) in the Fig. 5 and Fig. 6 panels for visual clarity.

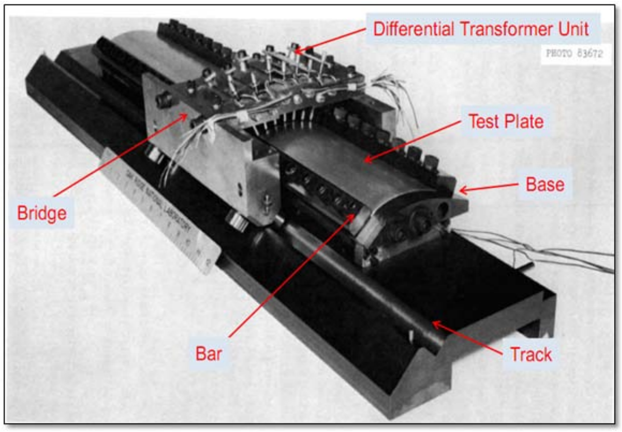

Fig. 4 Experimental setup to investigate temperature induced HFIR fuel plate deflections.

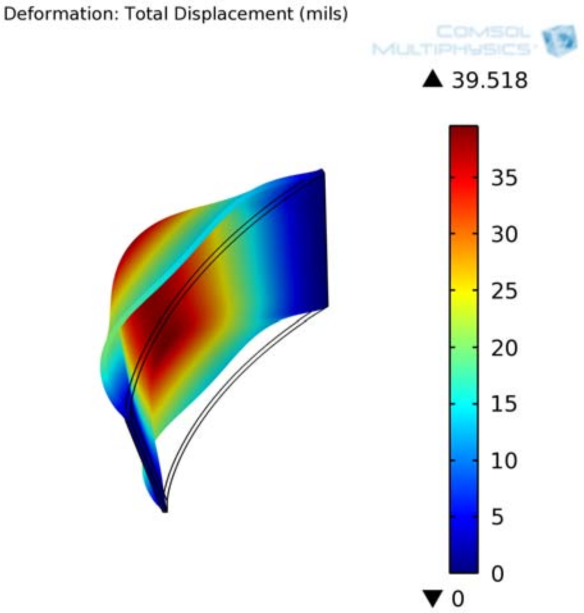

Fig. 5 Deformation in the HFIR outer plate due to thermal expansion caused by its convective heating from 80°F to 400°F. The plate is fully constrained on both of its longitudinal sides.

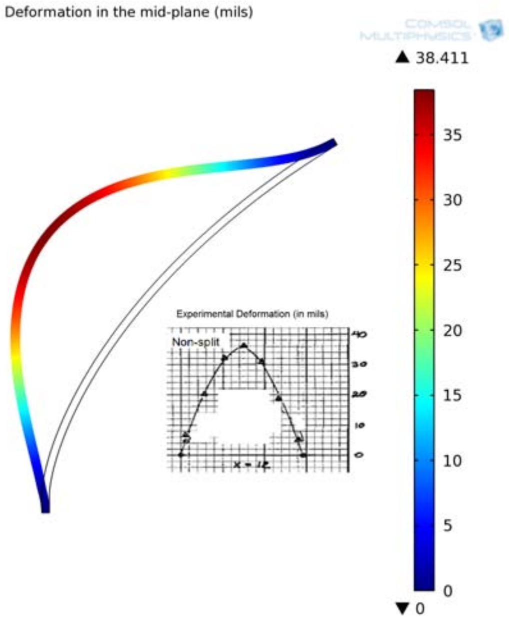

Fig. 6 COMSOL simulated deformation profile and maximum deformation (=38.4 mils) agree well with the experimental data (=37 mils).

6 Multi-channel Simulations of the HFIR Inner Fuel Element in 3D

A multi-channel COMSOL model for simulating 5 inner fuel plates and their adjacent coolant channels is currently being developed, and some preliminary results are shown in Figs. 7-9. In the multiphysics model represented by these figures, laminar flow with conjugate heat transfer is coupled with the thermal expansion physics. Several simplifications are introduced in this model to keep the associated mesh requirements and the wall-clock execution time reasonably low. Some of the simplifications include using the homogenized material for the fuel plate (i.e., not explicitly accounting for the fuel, clad, filler, and poison in the plate) and use of the laminar flow model to simulate flow. More realistic models are to be developed at a later time.

Efforts have also started for the "full-core" COMSOL model developments for the HFIR core. Fig. 10 and Fig. 11 show a 1-inch high cross-section of the HFIR IFE. To verify the proper assembly of the geometrical components in this model, a hypothetical heat conduction problem was solved along with the coupled thermal expansion physics. Both the inner and the outer side plates were kept at a constant temperature equal to 50°C and 500°C respectively. The inner side plate was fully constrained while the outer side plate was allowed to freely deform. Fig. 10 and Fig. 11 show the steady state temperature and associated deformations for this model verification problem.

7 Conclusions

The extension to 3D modeling increases the demands on COMSOL modeling in many respects. Because our geometry is quite complex, and no existing CAD-based design files yet exist at the detailed level required to describe the fuel-plate internals, creating the geometry initially was troublesome. The generalized parametric 3D curve capability introduced in COMSOL v4.1 has enabled the HFIR involute-plate geometry to be created precisely. The meshing requirements for this geometry with high-aspect ratio has been met by COMSOL. The solution procedure required for a high-resolution simulation of the fuel-plate surfaces with high-heat-flux has been identified, demonstrated to be adequate, and takes full advantage of our

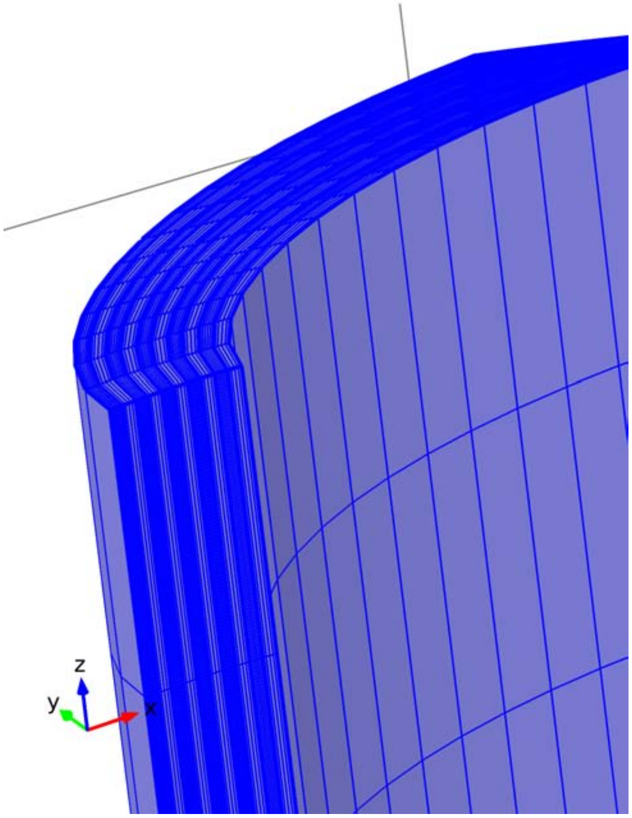

Fig. 7 Multi-channel simulation mapped mesh with 15 elements in radial, 24 elements in axial and 4 (or 8) elements in the thickness direction for each plate (or channel).

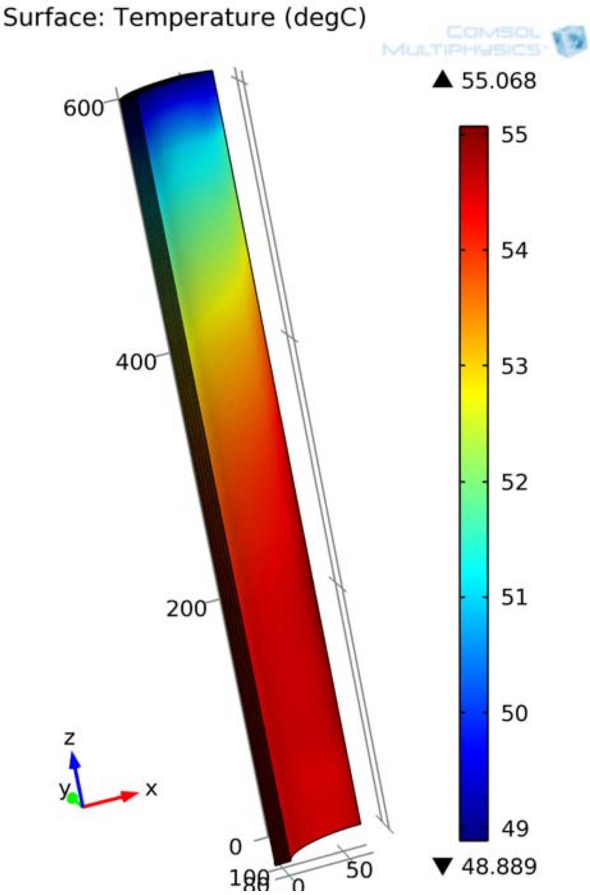

Fig. 8 Multi-channel simulation steady state temperature distribution (in °C).

distributed parallel processing Linux cluster. COMSOL-based multiphysics simulations of thermal-structure interactions have been shown accurate for both a single HFIR involute plate and multiple fuel plates and flow channels. Step-by-step development and analyses of COMSOL models for the single and multiple channels are expected to lead to the desired full-core multiphysics simulation capability for HFIR.

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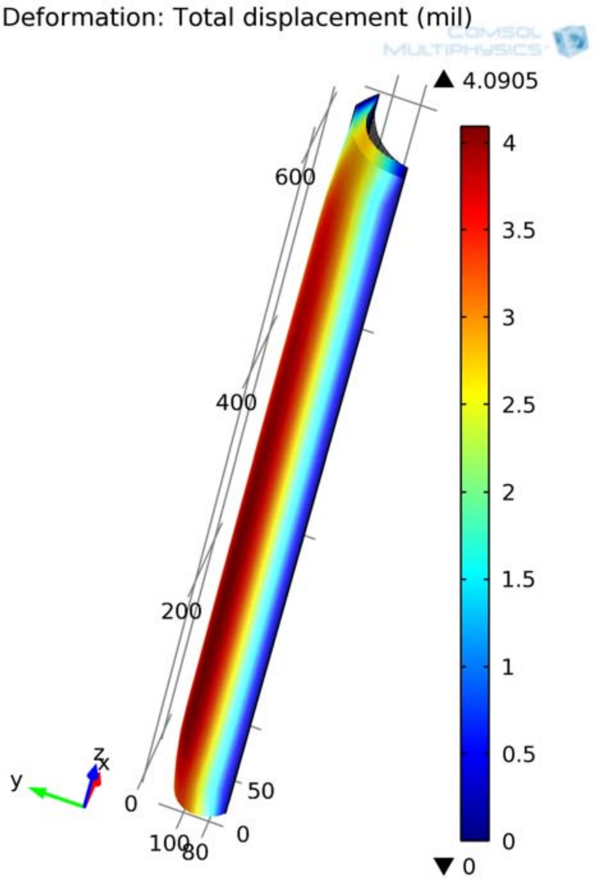

Fig. 9 Multi-channel simulation steady state deformations (in mils).

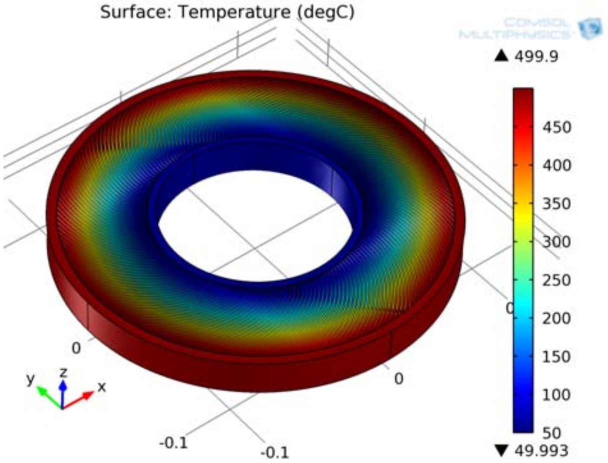

Fig. 10 Full-core simulation steady state temperature distribution for the heat conduction model problem used for model verification (in °C).

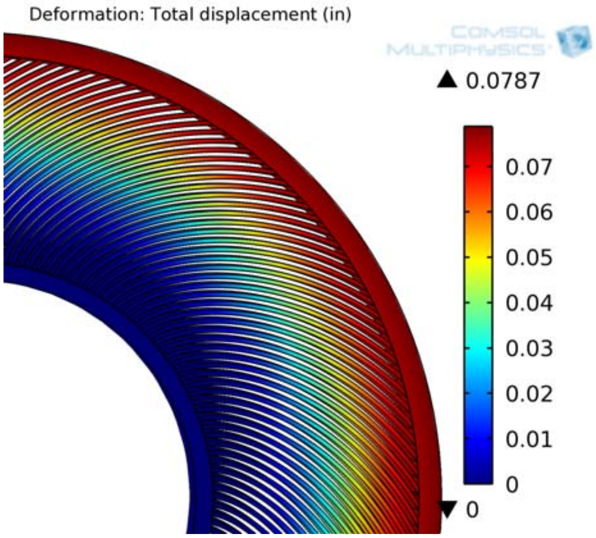

Fig. 11 Full-core simulation steady state deformation due to thermal expansion of the plates (in inches).