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Temperature Profile in Fuel and Tie-Tubes for Nuclear Thermal Propulsion Systems

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Abstract. A finite element method to calculate temperature profiles in heterogeneous geometries of tie-tube moderated LEU nuclear thermal propulsion systems and HEU designs with tie-tubes is developed and implemented in MATLAB. This new method is compared to previous methods to demonstrate shortcomings in those methods. Typical methods to analyze peak fuel centerline temperature in hexagonal geometries rely on spatial homogenization to derive an analytical expression. These methods are not applicable to cores with tie-tube elements because conduction to tie-tubes cannot be accurately modeled with the homogenized models. The fuel centerline temperature directly impacts safety and performance so it must be predicted carefully. The temperature profile in tie-tubes is also important when high temperatures are expected in the fuel because conduction to the tie-tubes may cause melting in tie-tubes, which may set maximum allowable performance. Estimations of maximum tie-tube temperature can be found from equivalent tube methods, however this method tends to be approximate and overly conservative. A finite element model of heat conduction on a unit cell can model spatial dependence and non-linear conductivity for fuel and tie-tube systems allowing for higher design fidelity of Nuclear Thermal Propulsion.

Keywords: Nuclear Thermal Propulsion & Tie-Tubes & Heat Transfer & LEU

INTRODUCTION

Interest in Nuclear Thermal Propulsion (NTP) has been renewed with NASA [1] suggesting NTP as a good choice for a Mars mission. There is also an effort to make NTP compatible with NNSA's Global Threat Reduction Initiative by using low enriched uranium (LEU) rather than highly enriched uranium (HEU). It has been shown [2] that with design modification, LEU NTP designs are feasible. This has created a need to redesign the NTP since heritage designs to branch from are not available. These designs are completely new reactors, similar to reactors proposed in the Generation IV International Forum [3]. Even HEU designs will have similar "new design" characteristics because all NTP designs will need to be licensed by the US Nuclear Regulatory Commission. Predictive computer codes that agree with experimental results are needed to design and license reactors

Experiments requiring nuclear materials tend to be very expensive and difficult to create due to many regulatory and safety concerns. This has led to the creation of predictive computer codes that are validated by experiments whenever possible. Many of the tools used to create historical NTP designs are either outdated or unavailable. Modern, sophisticated CAD tools require highly skilled software users and a large amount of computer time to produce very detailed results. These tools are very useful when a point design is available to study, however they should not be used for quick parametric design scoping studies.

An initial design of any nuclear reactor begins with a hot channel analysis where the hottest section of the core is analyzed. This analysis is well studied in a single-pass core typical in terrestrial Light Water Reactors (LWRs), however a "hot channel" in an NTP core consists of a fuel element and a tie-tube (or moderator) element. There is a downward supply H₂ channel and an upward return H₂ channel within a tie-tube, and there are several coolant channels within the fuel element. This makes for a difficult geometry to solve flow and heat equations over. This

paper presents a method to determine the temperature profile in an NTP that contains fuel and tie-tube elements. This tool can be applied to any fuel choice such as composite or cermet with any fuel enrichment as long as material properties are available.

BACKGROUND

Thermal analysis of NTP has been the subject of many studies in the past. One of the most important aspects of NTP performance and safety is to maintain temperature under prescribed values. It's very easy to design a small neutronically critical NTP core, and very easy to design an NTP core that can be easily cooled. However obtaining both a small and coolable core is difficult. To have the best performance in an NTP, high thrust to weight with high specific impulse is required. This forces NTP designers to optimize performance and safety to multiple constraints. In order to accurately analyze cores the temperature profile in the fuel element and tie-tube (if applicable) must be known, and there are many methods to estimate these values.

A typical method as done in [2] used to capture maximum fuel temperature in a hexagonal geometry is to transform the geometry into an equivalent tube that conserves volume of fuel and the inner surface area of the coolant channel. A 1D heat equation with an appropriate thermal temperature dependent conductivity can analytically be solved on this geometry for fast determination of maximum fuel temperatures. The circularization method can under calculate the fuel centerline in some cases where surface area to fuel volume ratio is high.

Another method [4] is to use an analytical expression that takes into account geometry variations but neglects non-linear thermal conductivities. The analytical expression neglects temperature dependent conductivity, which is important when there is a large difference between the fuel centerline and wall temperatures.

A shortcoming of both methods is that the fuel region is only cooled through the coolant surface and thus heat conduction into tie-tubes is not present and so higher fuel centerline temperatures can be found which limits performance. Both methods also do not capture geometry where fuel is adjacent to fuel so the potential increased fission rate that would cause peak temperatures at the interface between fuel is not captured.

A third method [5] was to assume a portion of heat is transferred to the tie-tubes from fuel and use that known source in a 1D cylindrical heat equation model of the tie-tube. This assumes radial symmetry of the tie-tube, which is always not present, and works only when the heat into the tie-tube is known well, which is not the case unless experimental data is available for the geometry or more complex computer methods are used.

The Small Nuclear Rocket Engine (SNRE) final report [6] overviews an axially integrated finite element analysis used to predict temperature distributions in the fuel of SNRE core. The implementation details are not very clear and references cited in the report are not easily available. However, from what is known, a quarter-symmetry fuel element was modeled with thermal insulation at the fuel edges. The insulation had a presumed flux and sink temperature boundary condition. The analysis shows peaking near the insulation; however the real impact of tie-tubes with hydrogen flow and change of fuel/TT geometry cannot be found with the report's methods.

Computational fluid dynamics (CFD) has been performed in a few studies that focus on NTPs. A full core analysis [7] and hot channel analysis [8,5] both present results for a few point designs that use HEU W-Cermet fuel. Neither of these studies model tie-tubes so although they are much more complex than previous studies, the results are not useful for NTP systems with tie-tubes.

METHODOLOGY

A 1D compressible flow model using real hydrogen (H_2) gas properties [9] was implemented in MATLAB [10]. A 2D heat equation was implemented in MATLAB's PDE Toolbox [10]. These two implementations were coupled together to determine the maximum fuel temperature and H_2 outlet temperature of a hot channel in an NTP. This section details the models used and the solution implementation.

Flow Model

A 1D compressible flow modeled using real H₂ gas properties were implemented using a friction factor correlation to take into account pressure drop due to fluid-wall interactions. The governing equations and closer relations are

$$\rho v = G, \quad (1)$$

$$\frac{dP}{dx} - \left(\frac{G}{\rho}\right)^2 \frac{d\rho}{dx} = -\frac{G^2}{2\rho_{avg} D_H} f, \quad (2)$$

$$\frac{dh}{dx} - \frac{G^2}{\rho^3} \frac{d\rho}{dx} = \frac{q}{\dot{m}}, \quad (3)$$

$$f = f_{Haaland} = \left(-1.8 * \log_{10} \left(\frac{6.9}{Re} + \left(\frac{\epsilon_{rel}}{3.7} \right)^{1.11} \right) \right)^{-2}, \quad (4)$$

$$P(0) = \text{specified}, \quad (5)$$

$$h(T(0), P(0)) = \text{specified}, \quad (6)$$

$$\rho = F(P, h), \quad (7)$$

where ρ is the fluid density, v is fluid velocity, G is the mass flux, P is the pressure, x , is the dimension, f is the friction factor, D_H is the hydraulic diameter, h is the enthalpy, q is the total heat added to the fluid, \dot{m} is the mass flow rate, Re is the fluid Reynolds number, ϵ_{rel} is the relative pipe roughness, and $F(P, h)$ is a table lookup function to find the fluid density. Boundary conditions are supplied at the pipe inlet.

The flow equations are calculated on N nodes that create $N-1$ cells where heat transfer occurs for the fuel temperature solutions. These nodes and cells can be seen in Fig. 1.

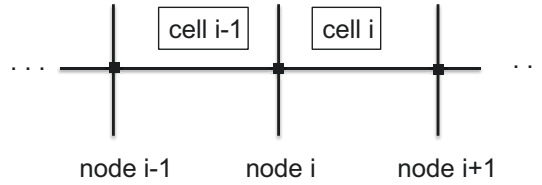


FIGURE 1. Node and Cell Stencil for Computations.

Average quantities are evaluated at the center point between nodes (i.e., the cell centers). The derivatives are discretized using first order forward differences as

$$\Delta x \frac{dp}{dx} = P_n - P_{n-1} = -\frac{G}{2\rho_{avg} D_H} \frac{f \Delta x}{\rho} + \left(\frac{G}{\rho}\right)^2 (\rho_n - \rho_{n-1}) = b_n^p, \quad n \in [1, N], \quad (8)$$

$$\Delta x \frac{dh}{dx} = h_n - h_{n-1} = \frac{q \Delta x}{\dot{m}} + \frac{G^2}{\rho^3} (\rho_n - \rho_{n-1}) = b_n^h, \quad n \in [1, N], \quad (9)$$

where Δx is the width of a cell, n is the node number, N is the total number of nodes with the first nodes containing boundary conditions, and b_n^p & b_n^h as labels to make notation simple. The heat flux used is the one from the previous cell that the n th node defines. These equations are assembled into a non-linear matrix equation,

$$Ax = b(x), \quad (10)$$

$$\begin{bmatrix} 1 & & & & & \\ -1 & 1 & & & & \\ & -1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & -1 & 1 & \\ & & & & 1 & \\ & & & & -1 & 1 \\ & & & & & -1 & 1 \\ & & & & & & \ddots & \ddots \\ & & & & & & & -1 & 1 \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ \vdots \\ P_N \\ h_1 \\ h_2 \\ h_3 \\ \vdots \\ h_N \end{bmatrix} = \begin{bmatrix} b_1^p \\ b_2^p \\ b_3^p \\ \vdots \\ b_N^p \\ b_1^h \\ b_2^h \\ b_3^h \\ \vdots \\ b_N^h \end{bmatrix}, \quad (11)$$

where blank spaces in the A matrix are zeroes. A fixed-point iteration scheme is used to solve the non-linear system with the matrix inversion handled by the ``backslash`` MATLAB operator so that an efficient inversion algorithm is used by default. The iteration scheme is

$$g(x_{i+1}) = A^{-1}b(x_i), \quad (12)$$

where the function $g(x_{i+1})$ is evaluated repeatedly until a convergence criteria of the L_2 norm of the error is met. The error is defined as

$$\|err\|_2 = \frac{\|x_{i+1} - x_i\|_2}{\|x_i\|_2}, \quad (13)$$

using $\|\cdot\|_2$ as the typical L2 norm operator.

Heat Conduction Model

A 2D heat equation was implemented into MATLAB using the PDE Toolbox. Typically with the PDE Toolbox, the frontend GUI interface is used to solve PDEs whereas in this implementation the backend was used directly by calling various toolbox functions. This allows for changing the mesh quickly for many different NTP cases.

Heat Equation

The heat equation is solved on a 2D mesh that is discretized using finite elements. The heat equation,

$$-\nabla \cdot (k \nabla T) = q''', \quad x \in \Omega \quad (14)$$

$$q''(x) = h(T(x) - T_{bulk}), \quad x \in \partial\Omega, \quad (15)$$

where k is the conductivity, T is the temperature, q''' is the volumetric heat generation rate, q'' is the areal heat generation rate, h is the heat transfer coefficient, x is the position on the domain Ω , and T_{bulk} is the bulk fluid temperature that is adjacent to the domain. The heat equation is cast into weak form and the solution is expanded using linear Lagrange elements, numerical integrals are solved using mid-point rule, and further solution implementation details are found in the toolbox manual [10]. The volumetric heat rate is taken to have no spatial dependence and is only present in the fuel meat.

Mesh

The PDE Toolbox can model 2D geometry using an unstructured mesh with triangular mesh elements. The geometry is meshed automatically at the beginning of a calculation automatically from various properties inputted into the code. The fuel channel radii, webbing thickness, and number of holes (up to 169) can be varied for 4 different combinations of fuel and tie-tube pairings ranging from 3 to 1, 2 to 1, 1 to 2, and 1 to 3 fuel to moderator ratio respectively. The smallest symmetry that arises from each of the fuel and tie-tube pairs is also implemented. Figure 2 shows a typical fuel element and moderating tie-tube. The fuel can be modeled as any fuel as long as material properties are available and the tie-tube dimensions and materials can be changed. Figure 3 shows the full lattice and the implemented symmetry. Cladding is not considered currently but will likely be added to the tool later. This study focuses on the 2 to 1 symmetries, as proof of concept. The other configurations have been considered and will be utilized to study different fuel and tie-tube element patterns.

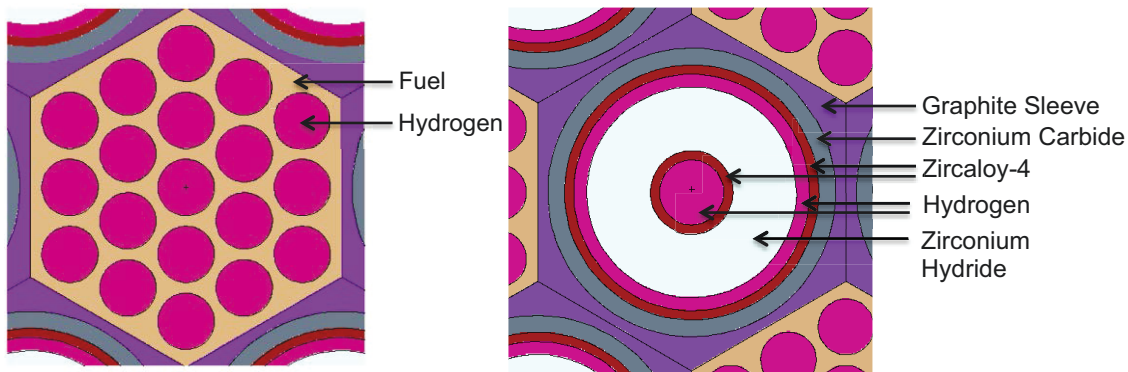


FIGURE 2. Fuel and Moderating Tie-Tube Geometry.

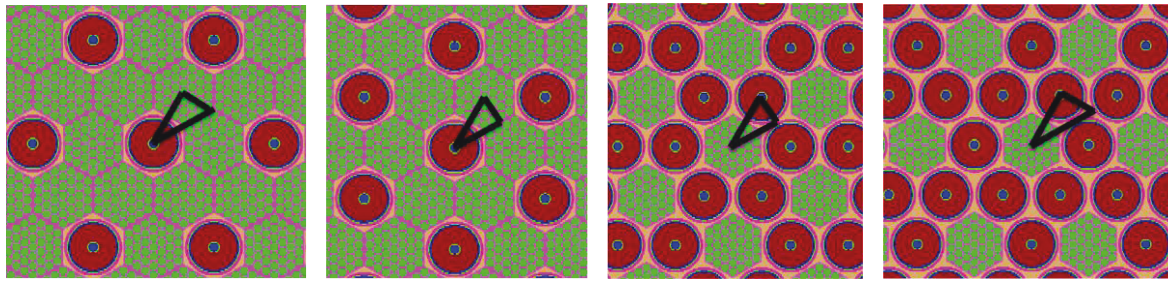


FIGURE 3. (a) 3 to 1 (b) 2 to 1 (c) 1 to 2 (d) 1 to 3 Fuel to Moderator Ratios with their Respective Symmetries in black.

The heat equation needs material properties for each material in the mesh. The heat equation can be solved as a linear or non-linear equation. The non-linear equation takes much more time to solve so the linear equation is solved with a few checks against the non-linear solution for the same case to determine how much error is introduced into the calculations. Both forms of the heat equation are initially solved using an adaptive mesh algorithm built into the PDE toolbox such that a good mesh can be created that is based on the solution.

Solution Implementation

The flow and temperature distribution implementations are coupled by heat transfer coefficient, fluid temperature, and heat profile into the fluid. The flow solution needs a heat profile input, and the fuel and tie-tube temperature distribution needs a heat transfer coefficient and a bulk fluid temperature input. The solution method is a staggered operator splitting with convergence criteria based on the information being passed between the two operators (flow and temperature) to not change by a given tolerance after some iteration. This section overviews the algorithm.

Algorithm Overview

All required parameters are initialized and then an initial guess of the heat into the fluid for the supply H , return H , and each coolant channel is made. The fluid temperature is then calculated using the assumed heat input with the 1D flow solver. This fluid temperature along with the assumed heat flux into the fluid is used to solve for the heat transfer coefficient and wall temperature. The heat transfer coefficient and the bulk fluid temperature found are used as the boundary conditions on all boundaries for the heat equation solver. A known (input) heat source is used as the heat source in the fuel region. A mesh is generated for the given geometry automatically and each cell is looped over until all cells have been calculated. The first cell on the first iteration of a calculation uses an adaptive mesh algorithm [10] to refine the mesh. This mesh is used in all further calculations because the adaptive mesh routine is time consuming and the same approximate mesh would be generated at each cell. Once the temperature distribution in each cell is found, the heat flux out of the edges is approximated using the mesh solution. Due to the mesh not being able to capture the true curvature of the circular coolant regions, the heat flux calculated is not equal to the known heat flux. Therefore, the total heat flux found is normalized to the known heat flux out. This heat flux out is used as the input to the 1D flow solver and the algorithm is looped. Before the loop a tolerance condition is evaluated such that the L_2 norm of the heat transfer coefficient for the central fuel coolant channel and heat flux profile does not change by a specified tolerance between iterations.

Boundary conditions are imposed onto the tie-tube coolant entrance and the fuel coolant entrance. A pressure drop from the tie-tube exit to the fuel inlet should be used; however the pressure is assumed so that the systems causing this pressure drop do not have to be modeled.

Pressure Drop Approximation

The flow solution is solved for each coolant channel. The proper boundary conditions should be the same inlet temperature and pressure with and outlet pressure for each coolant channel. The mass flow rate in the channel should be adjusted until the exit boundary condition can be met. Currently the outlet boundary condition is not enforced. By evaluating the difference between the maximum and minimum pressure drops out of the coolant channels, there is about a 15% difference in the pressure found so it is likely the mass flow rates would differ by a

non-negligible amount once the proper boundary conditions are met. However, in a real NTP, each coolant channel has a special orifice that introduces a pressure drop so the desired coolant mass flow rate can be achieved. Without these special orifices, it is likely proper cooling could not be established.

The physical impact of this approximation will likely be little as orificing can be introduced to match flow rates in channels. A real NTP design would likely need to cool hotter areas of fuel more than cooler areas so the orificing would take that into account too.

A numerical impact of this approximation is that pressure drops for different meshes are not all the same. This is due to heat flux into the fluid found from a coarse mesh will be slightly different than a fine mesh so a higher or lower heat input will result in a higher or lower pressure drop in the channel. This also means that convergence plots of the error introduced by the mesh do not follow the mathematical convergence rates predicted by theory. It is still valuable to create convergence plots, as they should still show similar trends.

Implementation Checks

Several checks were created to determine if the code written was correctly implemented. First, the flow solution was decoupled from the heat equation by inputting a known heat flux and increasing the mesh size. Since the derivatives in the flow equations are discretized by first order finite-difference, first order accuracy should be demonstrable. Figure 4 shows first order accuracy in the solution implementation. The "known" solution is a very fine mesh solution and the error is defined by an L2 norm between the found solution and the "known" solution.

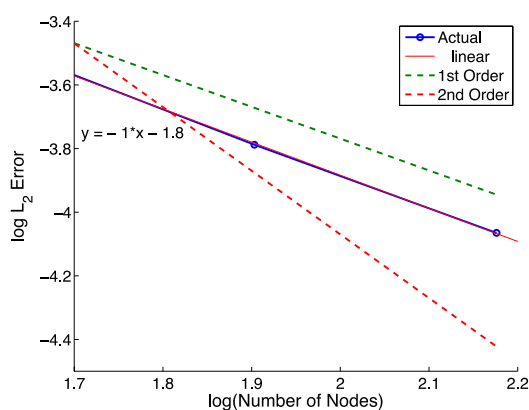


FIGURE 4. Convergence Plot for Flow Solution.

Next the PDE solution coupled with the flow solution was checked for dependence on the mesh. A 3 to 1 fuel to moderator ratio NTP was used with power densities and flow rates that seemed reasonable. The results should not be used as a performance merit. This was compared to a non-linear heat equation solver to demonstrate the inaccuracy of using a linear heat equation. Figure 5a shows that about 2.5E4 mesh elements are needed until the mesh does not have much effect on the maximum fuel temperature. Due to the approximation of not setting the pressure drop for each fuel channel and adjusting mass flow rate; there is some dependence on mesh for this implementation. A finer mesh is able to capture the heat flux into the fluid better than a coarser mesh. Small changes in the heat flux into the fluid cause changes in the pressure drop of the fluid and thus lead to changes in the temperature found in the fluid for different mesh sizes. This is believed to be the reason why the maximum temperature decreases with finer mesh up to a point then increases between 2.5E4 and 6E4 mesh elements. Similar behavior is seen in the non-linear solve. The difference between the linear and the non-linear equations is about 20 degrees at maximum and in general agree fairly well.

The total number of nodes used in the nodalization also has an effect on the solution. A 2 to 1 fuel to moderator ratio NTP was used with power densities and flow rates that seemed reasonable. The results should not be used as a performance merit. Not using enough nodes can lead to non-convergence and poor accuracy. Too many nodes can

lead to very long solution times or difficulties in the solver when root finding algorithms are needed and there is too small of a change between solutions to accurately find roots. Figure 5b shows the maximum fuel temperature does not vary more than about 2 degrees after 50 axial nodes are used. Sixty nodes are used in the studies show in this paper unless otherwise noted. Similar reasoning as the mesh dependence can be applied to the node dependence to explain why a solution is not converged upon refining the nodes.

One of the important figures of merit from each of the calculations is the maximum fuel temperature found. To verify that the convergence tolerance for the full calculation was set to a proper value, the change of maximum fuel temperature with the solution tolerance is shown in Fig. 5c—a tolerance of 10^{-4} is used for all results in this paper.

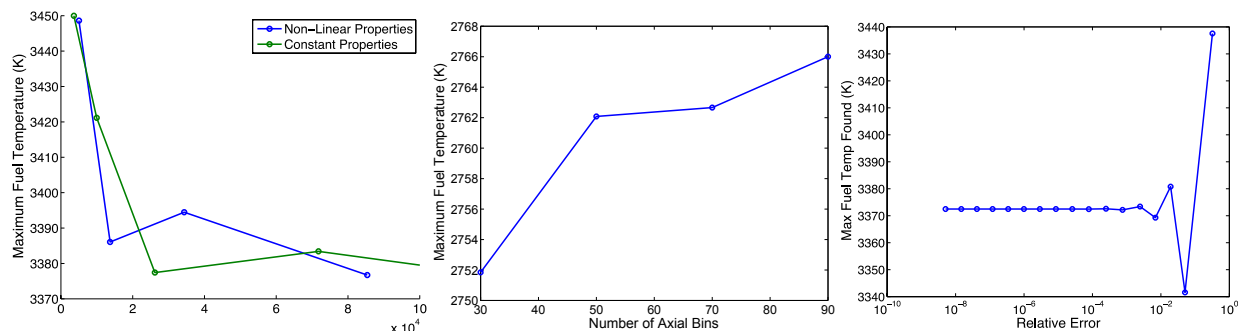


FIGURE 5. (a) Maximum fuel temperature dependence on mesh. (b) Maximum fuel temperature dependence on axial nodalization. (c) Effects of Solution Tolerance on Fuel Temperature.

Simple Performance Estimation Method

Simple methods to determine flow profiles and fuel temperatures involve neglecting the presence of tie-tubes. This was implemented by using the flow solutions described here and a maximum fuel temperature was found by using methods in [4]. This method is essentially a table lookup with a geometry correlation to take into accounts of 2D fuel geometry but does not take into account non-linear conductivities or tie-tubes.

INITIAL RESULTS

The tool developed takes about 30 minutes to run for a single case using about 120,000 mesh elements and solving the linear heat equation on a relatively old processor (2.66 GHz Intel Core i7) on one core. The MATLAB PDE Toolbox is not designed for multicore acceleration but multiple tasks may be spawned using the MATLAB Parallel Computing Toolbox.

The flow rate and power density to get approximately 2850 K maximum fuel temperature for a 2 to 1 fuel to moderator ratio core was found. This flow rate and power density was used in the simple performance estimation method to determine flow profiles and fuel temperatures. The power density shape was approximately cosine in shape with a slight bias for the peak of the cosine to be closer to the top of the core. The simple, linear-PDE and non-linear-PDE results are shown in Fig. 6.

Figure 6a compares the mean coolant temperature found from the PDE solution to the simple solution. The maximum and minimum coolant channels are also shown to show the relatively large difference between coolant channel temperatures. The mean coolant temperature is well predicted by the simple solution, however the simple solution cannot show the difference between maximum and minimum flow channels.

Figure 6b compares the maximum fuel temperature found from the PDE solution to the simple solution. There is a very large difference between temperatures predicted. All cases have the same inlet temperature and pressure. This shows that the simple method is not a good method to determine maximum fuel temperature in the fuel.

To further investigate the temperature profile in the fuel, the temperature solution along the cell where the maximum fuel temperature occurs is plotted in Fig. 7a. It can be seen that the maximum temperature occurs along the bottom fuel edge where the fuel meets another fuel element. This makes sense since more fuel would be present at the peripheries. In Fig. 7b a line segment of the fuel is plotted to better visualize the temperature distribution. It can be seen that about a third of the fuel element is hotter than the remaining two thirds.

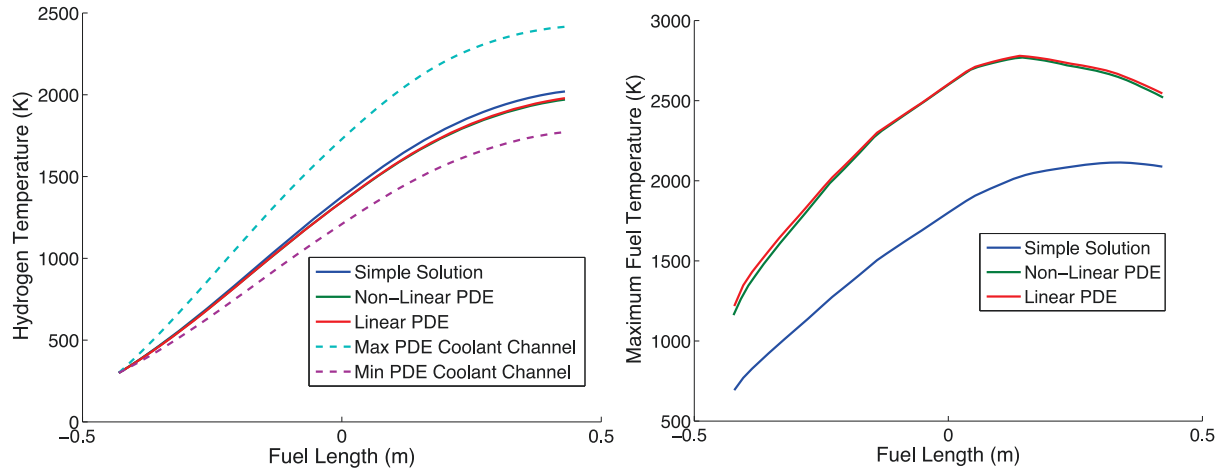


FIGURE 6. Comparing Simple Solution and PDE Solutions: (a) Coolant Temperature (b) Fuel Temperature

The simple method agrees much better to the minimum temperature found in Fig. 7b. This is reasonable since in the simple method, the fuel temperature is predicted by assuming there are no tie-tubes, which is approximately the case near the second two thirds of the fuel element plotted. Even if the maximum temperature in the two-thirds part of the fuel element was compared to the simple method, the simple method would be over predicting the temperature.

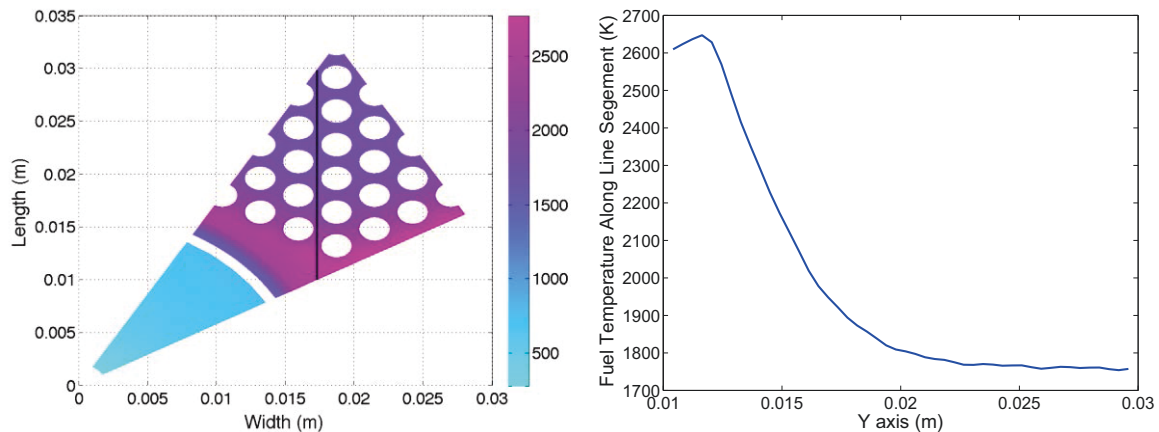


FIGURE 7. (a) Temperature Distribution in a Fuel Cell, (b) Temperature Profile Along Line Segment Shown in (a).

Future Works

The code may now be used for many different purposes. First methods to mitigate the large temperature peak in the fuel element should be evaluated. One simple method to do this would be to increase the mass flow rate in the channels near the peaked temperature in order to cool those areas more. This can also be easily physically accomplished by orificing each coolant channel to control flow rates. Another method would be to reduce the distance between the outer fuel wall and the outer fuel channels. This would reduce the amount of fuel meat between coolant channels when two fuel elements meet. This adjustment would be dependent on fuel manufacturing abilities. Another method could be to increase the distance between coolant channels in the central portion of the fuel in order to increase the heat generation in the central portion to increase the temperature there.

In order to decreasing the overall neutronic power peaking factor, several arrangements of fuel to moderator ratio may be used. This generally breaks symmetry in the core which makes it much more difficult to analyze temperature and flow profiles. It is likely CFD must be used in these cases though this tool might be useful for initial approximations of performance by estimating boundary conditions that would allow to partially model the non-symmetry of these cases.

Currently a constant power generation rate is used in the fuel. This approximation should be relaxed by using detailed power distributions based on neutron heating profiles. Portions of the fuel touching moderator tie-tubes will see a larger fission rate than portions of fuel touching other fuel. This might be enough to mitigate the large temperature peaks currently seen in the fuel. Furthermore neutron and gamma heating should be added as heat sources in the tie-tube in order to get the best estimate of the true temperature profile.

CONCLUSION

A tool to determine the temperature profile in an NTP that include fuel and tie-tubes has been developed and its implementation was detailed and demonstrated. Temperature profiles in the fuel and tie-tubes were coupled to a 1D flow channel solution in a staggered operator split in order to account for cooling by hydrogen coolant and to find NTP performance parameters. A 2 to 1 fuel to moderator ratio representative problem was examined to compare a simple solution scheme and the newly developed solution scheme. Flow profiles were found to be similar on the average between the two schemes but fuel temperatures were very poorly predicted by the simple scheme. The temperature profile in the fuel element was shown in detail and ideas to mitigate the large temperature peaks found were suggested. Improvements to the code were also discussed.

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