COARSE-MESH-BASED REDUCED-ORDER PACKAGE FOR MULTIPHYSICS SIMULATION OF NUCLEAR THERMAL PROPULSION REACTOR CORE

A Dissertation
Presented to
The Academic Faculty

by

Jim C. Wang

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy in the
School of Nuclear and Radiological Engineering

Georgia Institute of Technology
December 2021

COPYRIGHT © 2021 BY JIM C. WANG
COARSE-MESH-BASED REDUCED-ORDER PACKAGE FOR MULTIPHYSICS SIMULATION OF NUCLEAR THERMAL PROPULSION REACTOR CORE

Approved by:

Dr. Dan Kotlyar, Advisor
School of Nuclear and Radiological Engineering
Georgia Institute of Technology

Dr. Jon McWhirter
TerraPower

Dr. Bojan Petrovic
School of Nuclear and Radiological Engineering
Georgia Institute of Technology

Dr. Massimiliano Fratoni
School of Nuclear Engineering
University of California, Berkeley

Dr. Mostafa Ghiaasiaan
School of Nuclear and Radiological Engineering
Georgia Institute of Technology

Date Approved: [Nov 19th, 2021]
To David, Wendy, and twelve-year-old Jim.
ACKNOWLEDGEMENTS

I would like to thank my advisor, Dr. Dan Kotlyar, for his guidance and support throughout my research career as a graduate student at Georgia Tech. I would also like to thank my Ph.D. committee for being part of this magnificent journey. This dissertation cannot be accomplished without the support of my family, friends, and colleagues. I am grateful for having my family as the backbone of this adventure.

Finally, I would like to tell the twelve-year-old little Jimmy who always wanted to pursue nuclear engineering that “Thank you for believing in yourself and look what we have accomplished!”
# TABLE OF CONTENTS

ACKNOWLEDGEMENTS ....................................................................................... IV

LIST OF TABLES ................................................................................................... VIII

LIST OF FIGURES .................................................................................................. X

LIST OF ABBREVIATIONS ................................................................................... XIII

SUMMARY ............................................................................................................... XIV

CHAPTER 1. INTRODUCTION .............................................................................. 1

1.1 A Selected Modern NTP Design ................................................................. 2

1.2 Modeling Considerations and Challenges .................................................. 8

1.2.1 Explicit sub-element geometry ............................................................... 9

1.2.2 Element-to-element heat transfer ........................................................... 10

1.3 Why OpenFOAM? ...................................................................................... 11

1.4 OpenFOAM as a High- and Reduced-Fidelity Computational Tool .......... 12

1.4.1 OpenFOAM for high-resolution T/H modelling ..................................... 12

1.4.2 OpenFOAM for coarse-mesh-based modelling ....................................... 13

1.5 Objectives and Goals ................................................................................... 14

CHAPTER 2. NUMERICAL THEORY FOR FULL-ORDER T/H SIMULATION 16

2.1 Navier-Stokes Equations ............................................................................. 16

2.2 Energy Balance Equation ........................................................................... 18

2.3 Turbulence Modeling .................................................................................. 19

2.3.1 RANS Model .......................................................................................... 19

2.3.2 \( k - \epsilon \) turbulence model ...................................................................... 21

2.3.3 Turbulent near-wall treatment ................................................................. 23

2.4 Conjugate Heat Transfer Algorithm ............................................................ 25

2.5 SIMPLE Algorithm ..................................................................................... 27
CHAPTER 3. NUMERICAL THEORY FOR COARSE-MESH-BASED SIMULATION ................................................................. 29

3.1 Thermal-hydraulic (T/H) Module .............................................................. 30
  3.1.1 Coarse-mesh treatment of sub-elements ........................................... 30
  3.1.2 1-D Navier-Stokes equations under coarse-mesh treatment .............. 33
  3.1.3 Finite-difference Sub-function for Sub-structure Temperature Profile .... 38
  3.1.4 Empirical Correlations for Convective Heat Transfer ....................... 42

3.2 Inter-elemental Heat Transfer Module (Inter-HT Module) .......... 46
  3.2.1 Sub-elements Interface Conditions .................................................. 47
  3.2.2 Heat Transfer Mechanism .............................................................. 50

3.3 Neutron Diffusion Module .................................................................. 52
  3.3.1 Albedo Boundary Conditions .......................................................... 55

3.4 Iterative Strategy in NTPSteadyFOAM ........................................ 56
  3.4.1 Main T/H Module ..................................................................... 57
  3.4.2 Iterative Strategy of the Inter-elemental Heat Transfer Module .......... 58
  3.4.3 Neutron Diffusion Module Iterative Strategy ................................... 60
  3.4.4 Full Coupled Package .................................................................. 61

CHAPTER 4. CHT MODELS VERIFICATION AND VALIDATION .......... 63

4.1 Mesh Structure for the CHT Model ....................................................... 64

4.2 Input and Boundary Conditions for the NRX-A6 Sample FE .......... 66

4.3 CHT Solver Mesh Sensitivity Study ................................................. 68

4.4 Validation of the CHT Solver ............................................................. 70

CHAPTER 5. RESULTS ........................................................................... 74

5.1 Description of Selected Models ......................................................... 74
  5.1.1 High-resolution CHT Model Setup .................................................. 76

5.2 Single Element Benchmark Study ..................................................... 78
  5.2.1 Mesh Sensitivity Studies ................................................................. 78
  5.2.2 Single Element V&V ................................................................... 80

5.3 Verification of Two Adjacent Elements ............................................. 87

5.4 Supercell Analysis ............................................................................. 94

5.5 Neutronic Verification ...................................................................... 99
CHAPTER 6. DEMONSTRATION OF NTPSTEADYFOAM ........................................ 103

6.1 Sample Miniature Core Description .................................................................. 103

6.2 Multiphysics Modeling ...................................................................................... 106

6.3 Summary of NTPSteadyFOAM Computational Performance .......................... 114

CHAPTER 7. CONCLUSIONS .................................................................................. 116

7.1 Summary of NTPSteadyFOAM Package .......................................................... 116

7.2 Summary of The Work Performed ...................................................................... 118

7.3 Future work ......................................................................................................... 121
  7.3.1 Geometric weighting ....................................................................................... 121
  7.3.2 Neutron Diffusion Module ............................................................................ 125
  7.3.3 Discontinuity Factors .................................................................................... 126

APPENDIX A. THERMOPHYSICAL PROPERTIES FOR T/H SIMULATION 128

APPENDIX B. CHT MESH SENSITIVITY STUDIES .............................................. 130

APPENDIX C. FEW-GROUP CROSS-SECTION DATA ........................................ 133

REFERENCES .......................................................................................................... 137

VITA .......................................................................................................................... 143
LIST OF TABLES

Table 1. Closure coefficients for the Launder and Sharma $k - \epsilon$ model. ................. 22
Table 2. Available Nusselt correlation in NTPSteadyFOAM. ........................................ 46
Table 3. Control parameters within the solution scheme................................................. 67
Table 4. FE General Parameter. ..................................................................................... 67
Table 5. CHT solver boundary conditions. ....................................................................... 68
Table 6. Mesh sensitivity study for FE in axial direction.................................................... 70
Table 7. Mesh sensitivity study at FE flow channel boundary........................................... 70
Table 8. Comparison between CHT and experimental measurements. .............................. 71
Table 9. Average fuel temperature distribution along the axial length predicted by OpenFOAM CHT and the experimental calculation....................................................... 72
Table 10. FE & ME Model Specifications........................................................................... 75
Table 11. FE & ME Operating Conditions. ......................................................................... 76
Table 12. Coarse-mesh FE model sensitivity study in axial direction................................. 79
Table 13. Coarse-mesh ME model sensitivity study in axial direction. ............................. 79
Table 14. FE model sensitivity study in radial direction (at fuel meat layer). ..................... 80
Table 15. ME model sensitivity study in radial direction (at ZrH2 layer). ................. Error!
Bookmark not defined.
Table 16. Percentage difference between codes taken at FE location of interest. ........... 84
Table 17. Percentage difference between codes taken at ME location of interest........... 87
Table 18. Summary of Supercell Analysis. ......................................................................... 98
Table 19. Neutronic model axial mesh independency study (Red-color-highlighted row indicates selected mesh parameter). ................................................................. 100
Table 20. Neutronic comparison of reactivity. ................................................................. 102
Table 21. Input and boundary conditions for the subsequent sample reactor models. ... 106
Table 22. Impact summary of inter-elemental HT in the multiphysics simulations...... 107
Table 23. Sample core model nominal vs. feedback simulations.................................. 109
Table 24. NTPSteadyFOAM solution summary for different reactor pattern designs... 113
Table 25. Computational performance results for different models executed using different numerical solvers. ................................................................. 115
Table 26. Parametric calculations for each ring............................................................ 123
Table 27. FE and ME Solid Material Definitions. ......................................................... 129
Table 28. Mesh sensitivity study for high-resolution FE model in axial direction....... 130
Table 29. Mesh sensitivity study for high-resolution ME model in axial direction. ..... 131
Table 30. Mesh sensitivity study for high-resolution FE model in radial direction taken at the coolant channel solid-fluid domain interface........................................... 131
Table 31. Mesh sensitivity study for high-resolution ME model in radial direction taken at the supply channel solid-fluid domain interface........................................... 131
Table 32. Mesh sensitivity study for high-resolution ME model in radial direction taken at the return channel (RC) solid-fluid domain interface........................................... 132
Table 33. Cross-section data for nominal NTP reactor conditions......................... 133
Table 34. Cross-section data at higher FE fuel meat temperature condition.......... 134
Table 35. Cross-section data at lower FE fuel meat temperature condition.......... 134
Table 36. Cross-section data at higher ME ZrH2 temperature condition.............. 135
Table 37. Cross-section data at lower ME ZrH2 temperature condition.............. 135
Table 38. Cross-section data at lower FE coolant density condition..................... 135
Table 39. Cross-section data at higher FE coolant density condition..................... 136
LIST OF FIGURES

Figure 1. NERVA-type core radial configuration.......................................................... 3
Figure 2. NERVA-type core axial configuration............................................................ 5
Figure 3. (a) Top and (b) side view of an FE................................................................. 6
Figure 4. (a) Top and (b) side view of an ME................................................................. 6
Figure 5. Large NERVA expander cycle........................................................................ 8
Figure 6. Iterative Strategies for: (a) SIMPLE algorithm, and (b) chtMultiRegionSimpleFoam solver................................................................. 28
Figure 7. Mesh treatments in different modeling orders of dimensionality. ..................... 31
Figure 8. Discrete full-order FE model (left) vs. Equivalent FE model (right). .................. 33
Figure 9. Schematic of the equivalent Supply (left) and Return (right) Channel models. 33
Figure 10. Nomenclature for FD representation for an annular cylinder with constant grid size [33]........................................................................................................... 39
Figure 11. Nomenclature for FD representation for an annular cylinder with variable grid size. ..................................................................................................................... 41
Figure 12. Supercell model: (left) full-order vs. (right) coarse-mesh............................... 48
Figure 13. The contact situation from the finite volume perspective. .............................. 48
Figure 14. The zoom-in contact situation from the finite volume and finite-difference overlaying perspective. ................................................................. 49
Figure 15. Reduced-geometry supercell models: (a) full-order vs. (b) coarse-mesh........ 52
Figure 16. Inter-HT Module sample mesh model.......................................................... 52
Figure 17. Main T/H module iterative strategy overview................................................. 58
Figure 18. Main T/H to Inter-HT modules iterative strategy overview............................ 59
Figure 19. Neutron diffusion module iterative strategy overview.................................. 60
Figure 20. NTPSteadyFOAM full coupling scheme..................................................... 62
Figure 21. Typical NRX-A6 fuel cluster configuration.................................................. 64
Figure 22. NRX-A6 FE High-resolution Mesh Model .................................................. 65
Figure 23. Axial power profile for the sample FE model ........................................ 67
Figure 24. Equivalent FE model generated for CHT solver mesh sensitivity study ....... 69
Figure 25. Comparison of CHT and experimental average axial fuel temperature ....... 72
Figure 26. Benchmarked FE & ME Model Configurations .................................... 75
Figure 27. Benchmark Elements Power Profile ....................................................... 76
Figure 28. Description of hybrid grid used for: (A) FE and (B) ME models ............ 78
Figure 29. Comparison between the finite-difference and analytical solutions in FE .... 81
Figure 30. Code-to-code comparison in FE axial distributions: (a) coolant (\(T_b\)) and surface (\(T_s\)) temperatures, (b) mean velocity, (c) fuel outer-edge temperature, and (d) fuel temperature ................................................................. 83
Figure 31. Code-to-code comparison of average axial: (a) coolant (\(T_b\)) temperature, (b) mean velocity magnitude, (c) flow channel surface (\(T_s\)) temperature, and (d) ME YSZ outer-edge temperature .................................................. 86
Figure 32. Comparison between the finite-difference sub-solver and analytical solution over two conjugated equivalent FE models ......................................................... 88
Figure 33. Reduced-geometry high-resolution mesh model for single FE-ME heat transfer analysis .................................................................................................................. 89
Figure 34. Comparison of ME’s axial profiles in FE-to-ME configuration: (a) coolant (\(T_b\)) temperature, (b) mean velocity magnitude, and (c) flow channel surface (\(T_s\)) temperature. ..................................................................................................... 91
Figure 35. Comparison of FE’s axial profiles in FE-to-ME configuration: (a) coolant (\(T_b\)) and surface (\(T_s\)) temperature, and (b) FE-ME interface temperature ................. 92
Figure 36. Radial temperature distribution in ZrH\(_2\) compared at different axial layers. The green dash-line represents the boundary between the ZrH\(_2\) inner edge and zircaloy-4 cladding outer-edge ............................................................. 93
Figure 37. Supercell configurations ......................................................................... 94
Figure 38. Reduced-geometry supercell mesh models generated with: (left) high-resolution full-order mesh, and (right) NTPSteadyFOAM coarse-mesh .................................. 95
Figure 39. Propellant temperature distributions for 4F2M and 2F4M supercell configurations ......................................................................................................................... 96
Figure 40. Propellant velocity distributions for 4F2M and 2F4M supercell configurations.

Figure 41. Surface temperature distributions for 4F2M and 2F4M supercell configurations.

Figure 42. Interface FE-ME surface temperature distributions for 4F2M and 2F4M supercell configurations.

Figure 43. Neutronic model overview: (left) Cross-section view of the homogenized active core region, and (right) Model’s axial distribution.

Figure 44. Two-group axial flux distribution for single physics neutronic analysis.

Figure 45. Neutronic benchmark analysis with: (a) thermal-to-fast flux ratio, and (b) axial power distribution.

Figure 46. Sample core configuration.

Figure 47. Selected solutions from a one-way multiphysics analysis: (a) Average fuel temperature distribution, (b) bulk coolant temperature distribution taken at ME return channels, and (c) volumetric power ($q''')$ distribution.

Figure 48. Axial power distribution with and without the reactivity feedback obtained for the center-most FE.

Figure 49. Radial power distributions with and without the reactivity feedback.

Figure 50. Selected reactor pattern designs.

Figure 51. Radial core fuel temperature distributions in the different loading patterns.

Figure 52. Schematic of decomposition methods for FE geometric weighting calculations.

Figure 53. Axial thermal distributions following the application of the geometric weighting technique: (a) coolant temperature, (c) fuel temperature, and (d) outer-surface temperature.

Figure 54. NTP fuel element (left) and moderating element (right) configurations with material labels.

Figure 55. Equivalent sub-element models for mesh dependency study: (a) FE, (b) ME supply channel, and (c) ME return channel.
# LIST OF ABBREVIATIONS

<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>B.C.</td>
<td>Boundary Condition</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamic</td>
</tr>
<tr>
<td>CHT</td>
<td>Conjugate Heat Transfer</td>
</tr>
<tr>
<td>FD</td>
<td>Finite-difference</td>
</tr>
<tr>
<td>FE</td>
<td>Fuel Element</td>
</tr>
<tr>
<td>FVM</td>
<td>Finite Volume Method</td>
</tr>
<tr>
<td>HALEU</td>
<td>High-Assay Low-Enriched Uranium</td>
</tr>
<tr>
<td>HEU</td>
<td>high-enriched uranium</td>
</tr>
<tr>
<td>HTC</td>
<td>Heat Transfer Coefficient</td>
</tr>
<tr>
<td>Inter-HT module</td>
<td>Inter-elemental Heat Transfer module</td>
</tr>
<tr>
<td>$I_{sp}$</td>
<td>Specific Impulse</td>
</tr>
<tr>
<td>ME</td>
<td>Moderating Element</td>
</tr>
<tr>
<td>NERVA</td>
<td>Nuclear Engine for Rocket Vehicle Application</td>
</tr>
<tr>
<td>NS Equations</td>
<td>Navier-Stokes Equations</td>
</tr>
<tr>
<td>NTP</td>
<td>Nuclear Thermal Propulsion</td>
</tr>
<tr>
<td>OpenFOAM</td>
<td>Open-source Field Operation and Manipulation</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynold-Averaged Navier Stokes</td>
</tr>
<tr>
<td>RC</td>
<td>Return Channel</td>
</tr>
<tr>
<td>SC</td>
<td>Supply Channel</td>
</tr>
<tr>
<td>SIMPLE</td>
<td>Semi-Implicit Method for Pressure Linked Equation</td>
</tr>
<tr>
<td>T/H</td>
<td>Thermal-hydraulic</td>
</tr>
<tr>
<td>YSZ</td>
<td>Yittria-Stabilized Zirconia</td>
</tr>
</tbody>
</table>
SUMMARY

Among the various proposed space propulsion technologies, the nuclear thermal propulsion (NTP) system has been identified as the technology of choice for NASA’s mission to Mars due to its high efficiency in fuel performance. Most of the legacy NTP engine designs from the NASA’s historical Rover/NERVA program relied on highly enriched (above 90% enrichment) uranium (HEU) fuel. Recent efforts focused on designing a high-efficiency engine that relies on high-assay low-enriched uranium fuel (HALEU with ~19.75% enrichment). To achieve high specific impulse and thrust to weight values, these new HALEU-based generations of NTP would require geometrical modifications associated with the elements’ thickness and pitch, as well as the core’s length and configuration. The evolution of current designs mandates setting up new experiments to alleviate some uncertainties; however, these are costly and not readily available. Therefore, there is a real need to complement these expensive experiments and capture multi-physics effects using numerical modeling and simulation tools.

This dissertation introduces a steady-state OpenFOAM multiphysics package tailored for NTP core simulation. Denoted as NTPSteadyFOAM, this package consists of three sub-modules that allow to model NTP fuel-to-coolant heat transfer, element-to-element heat transfer, and power generation through neutron diffusion. In this package, the single element fuel-to-coolant heat transfer is modeled using a 1.5-D sub-channel approach in conjunction with multiple empirical convective heat transfer models. The element-to-element heat transfer is governed by the Laplacian thermal conduction model with customized boundary interface treatments to capture heat flux across reactor sub-elements.
The neutronic simulation relies on a traditional multi-group diffusion model using the $P_1$ approximation. Moreover, the multiphysics coupling approach across modules is built upon an existing reactor solver, GeN-Foam, designed to tighten the coupling between thermal-hydraulics (T/H), neutronic, and other important feedback. The NTPSteadyFOAM package is heavily verified against higher-fidelity models (e.g., Conjugate Heat Transfer CFD solver for T/H and Monte Carlo simulation for neutronic models) that compares single sub-element T/H analysis as well as different patterns of inter-elemental heat transfer. Furthermore, full core neutronic-T/H coupling capability is demonstrated using a miniature sample NTP core.

As result, this dissertation presents the fidelity and the multiphysics capabilities of the coarse-mesh-based multiphysics package for NTP core simulations. The overarching goal of this work is to establish a multiphysics package designed to obtain full core solution with a timely-efficient computational performance.
CHAPTER 1. INTRODUCTION

For many years now, the National Aeronautics and Space Administration (NASA) has been planning human-Mars missions. However, sending humans to Mars is costly for many reasons, such as astronauts’ life support systems, space-vehicle fuel utilization, and cosmic radiation endurance. Considering that the amount of resource consumption is proportional to the travel time, the performance of the propulsion technology plays a crucial role in the feasibility and success of the mission.

Among all the proposed space propulsion technologies, the nuclear thermal propulsion (NTP) system has been identified as the technology of choice for NASA’s deep-space mission to Mars due to its high efficiency of propellant utilization. The space propulsion engine performance can be quantified using the specific impulse ($I_{sp}$), thrust, and thrust-to-weight ratio. The specific impulse is defined as time, in seconds, one pound of propellant can deliver one newton or pound of thrust (seconds per klbf or kN). A conventional chemical rocket delivers $I_{sp}$ of 300-450 seconds at a thrust of 445-2224 kN (100-500 klbf), while an electric rocket delivers 1000+ seconds at a thrust of 0.0445 N (10 mlbf), and a nuclear rocket is capable of producing 800-1000 seconds of $I_{sp}$ at a thrust of 44.5-445 kN (10-100 klbf) [1]. In addition to the specific thrust, the thrust-to-weight ratio is another performance indicator that needs to be above an optimized to enable specific maneuvers to be performed. An overall performance comparison between rocket types shows that nuclear rockets should carry an advantage over chemical rockets in specific impulse, yet a chemical rocket would provide more thrust over nuclear; this implies that a chemical engine is more suitable for rocket launch while an NTP system is
better for inter-planetary travel. Such an advantage would make NTP an ideal candidate for a long-haul mission to Mars.

The history behind the development of NTP systems can be traced back to NASA’s historical Rover/NERVA program that started in the 1960s and lasted for two decades. The early research projects on NTP system designs were heavily experiment-oriented with several significant test engines including Kiwi, Phoebus, Pewee, and the NERVA NRX series [1]. Kiwi was the very first experimental space reactor that provided $4.95 \text{ klf }$ of thrust with thermal power of 1000 MW. Designed as an upgrade of Kiwi, Phoebus program achieved $19.7 \text{ klf } \left(87.5 \text{ kN}\right)$ in thrust and 5000 MW in thermal power. The NERVA NRX reactor series further modified the Phoebus’ design and applied techniques from other programs to implement the first flight-type system to test [2]. Among the historical NTP experimental reactors, the NERVA NRX-A6 was the last uranium-fueled tested reactor with a total run time of 62 minutes at full power [2]. In 1972, the NERVA program was eventually canceled due to a shortage of governmental funds [3]. Nonetheless, these legacy NTP reactor programs have demonstrated the feasibility and the higher efficiency towards the development of space propulsion technology.

The subsequent sections will present the configuration and the specifications of a solid-fuel NERVA-type NTP core, followed by the considerations and modeling challenges of such system. This chapter will then formally introduce OpenFOAM as both high- and reduced-fidelity tool for nuclear applications and conclude with the overarching goals and objectives for the presented dissertation.

1.1 A Selected Modern NTP Design
Figure 1 presents the radial cross-section view of a typical NERVA-type reactor core. In this configuration, the core consists of two radial regions: the outer pressure vessel, and the inner pressure vessel. The outer pressure vessel contains beryllium radial reflectors with several rotatable control drums embedded within. Each control drum is partially made of neutron absorber and reflector that rotates upon operation demands. The reactor power control is achieved by rotating the control drum such that the reflective side would have a greater portion exposed to the inner core vessel when higher power is needed. Alternatively, the entire absorption side of the control drum will face the inner core vessel during reactor shutdown. The inner pressure vessel contains different sub-element patterns that are made of fuel elements (FEs) and moderating elements (MEs). In past designs, MEs were also referred to as tie-tubes. The inner vessel sub-elements are wrapped by a graphite sleeve, which acts as the core former and provides thermal-mechanical support under high temperature [4].
Figure 2 illustrates the axial configuration of the same NERVA-type core. In this figure, the active core region is located between two axial reflector plates with an internal shielding plate (and some intermediate support plates) placed on top. In a typical historical design, the fuel within the active core is about 1 to 1.3 meters in height and usually consists of a single axial layer of fuel material (i.e., uranium particles embedded in a carbon matrix). In some modern designs, the fuel material would be split into multiple axial regions (i.e., the molybdenum-based matrix on top of tungsten-based matrix) to reduce total system weight and improve the thrust-to-weight ratio [4]. As an example, the work carried out by Krecicki et al. presented an approach according to which the overall mass of the core can be minimized by adopting the axial split configuration. Although tungsten is an excellent choice in terms of thermal performance, it introduces considerable neutron absorption. The latter necessitates the use of more uranium mass loading and larger core dimensions. However, the regions closer to the propellant core inlet typically experience considerably lower operation temperatures and thus do not fully exploit tungsten’s excellent thermal properties. Therefore, tungsten can be replaced by an alternative material, i.e., molybdenum, which is still compatible thermally, but absorbs significantly less neutrons.
In a typical historical NTP core, the internal/active region is composed of hexagonal prismatic honeycomb-shaped FEs and tie-tubes. To achieve a high specific impulse, the design uses a gaseous hydrogen propellant due to its low molar mass. The FEs are inverted elements with embedded coolant channels. Modern NTP systems also use MEs that have evolved from the tie tubes previously used in the NERVA program. These tie tubes or MEs are designed to maintain structural integrity, as well as to extract additional heat from the core to drive turbopumps that are used to pressurize the cryogenic hydrogen. The additional role of the ME is to slow down neutrons by including a moderating material (e.g., graphite or zirconium-hydride) and to sustain criticality for the entire course of the mission. Figure 3 and 4 provide radial and axial cross-section views for FE and ME models. The white arrow in both figures indicates the flow direction, with the arrow’s background indicating the flow paths. The material composition and the size of each element are not specified here as these parameters vary by core design. A typical FE design consists of multiple circular channels flowing parallel in the axial core direction. These flow channels are typically arranged in a hexagonal lattice with identical pitch lengths between one another.
The ME contains multiple layers of moderating and support materials with a twice-through counter-flow design flowing along the axial direction.

![Figure 3. (a) Top and (b) side view of an FE.](image1)

![Figure 4. (a) Top and (b) side view of an ME.](image2)

The Small Nuclear Rocket Engine (SNRE) was the last engine studied by the Los Alamos National Laboratory during the NERVA program. The SNRE has designed its NTP system based on the expander cycle to improve the engine’s specific impulse, as compared to the original bleed cycle design that relied on a single path of the propellant in the core. Using the bleed cycle, the turbopump discharged hydrogen into the FE with a lower inlet
temperature [5]. In the expander cycle, however, the propellant enters and exits the ME and is pre-heated before entering the fuel elements. The latter is the second path in the reactor core followed by a discharge through the converging-diverging nozzle. The subsequent numerical analysis conducted by NASA Glenn Research Center has reinforced that the expander cycle can significantly increase system performance [4].

Figure 5 demonstrates a simplified (only for illustration purposes) block diagram of a large NERVA expander cycle system [6]. The dashed line in this figure indicates a possible connection to a secondary turbopump loop. Point 1 of the expander cycle shows hydrogen exits through the cryogenic tank as it is pressurized by the pump as it proceeds to point 2. Point 2 is where the flow splits into two paths towards $3_{a}$ and $3_{b}$. From $3_{a}$, part of the hydrogen will pass through the nozzle skirt and reflector circuit. The remaining flow at $3_{b}$ will enter through the ME supply channel and return to point 4 through the ME return channel. The flow from both paths will recombine at point 4. The total flow then proceeds through point 5, with part of the hydrogen going through turbopump and the rest going through a bypass valve. The latter procedure is needed to control the mass flow rate and pressure that is primarily needed for startup and restarts operations. Finally, the hydrogen recombines and returns to the active core region at point 6. The propellant is then heated within the FE channels and expelled through the rocket nozzle (point 7).
1.2 Modeling Considerations and Challenges

Most of the legacy NTP engine designs relied on highly enriched (above 90% enrichment) uranium (HEU) fuel, which is less favorable nowadays due to issues regarding policies and social perspectives [7]. Recent efforts focused on designing a high-efficiency engine that relies on high-assay low-enriched uranium fuel (HALEU with 19.75% enrichment) [3]. To achieve high specific impulse and thrust to weight values, these new HALEU-based generations of NTPs would require geometrical modifications associated with the elements’ thickness and pitch, as well as the core’s length and configuration. These modifications may introduce significant uncertainties into the empirical correlations (e.g.,
heat transfer for various regions such as fuel and moderator) developed during the Rover/NERVA program. In addition, the extensive legacy data generated for specific ranges of Reynolds numbers and diameter-to-height ratios might not be fully applicable to current designs [4]. The evolution of current designs mandates setting up new experiments to alleviate some uncertainties; however, these are costly and not readily available. Therefore, there is a real need to complement these expensive experiments and capture multiphysics effects using numerical modeling and simulation tools. The following subsections discuss some specific challenges associated to the modeling of sub-elements in general NTP systems.

1.2.1 *Explicit sub-element geometry*

The previous section has introduced the configuration of the reactor sub-elements in a NERVA-type core, in which both the FE and ME consist of hexagonal prismatic honeycomb-shaped cylinders with inverted flow path design (see Figure 3-4). Some specific modeling techniques (see ref. [1], [8]) for NTP sub-element analysis evolve around simplified solution routines typically applied for fuel-pin configurations. To be specific, many reduced-order solvers [9] treat a sub-element’s explicit geometry as equivalent annular cylinders. Such solvers rely on a 1.5-D approach to determine the average thermal conditions for these equivalent sub-element models. In general, the 1.5-D approach cannot directly be applied to model the thermal performance of an NTP. However, some engineering-based assumptions and iterative techniques can improve the accuracy of the 1.5-D approach while exploiting the very quick simulation times. For example, Wang and Kotlyar developed and tested a 1.5-D T/H code to estimate the average fuel temperature for a single FE. The simulation results demonstrated good agreement against measured
experimental data [10]. Nevertheless, the 1.5-D equivalent modeling approach requires heavy modification before solving a ME, specifically due to the twice-through counter flow design with multiple intermediate layers. In addition, remapping boundary conditions from a hexagon design to an equivalent cylinder may introduce inconsistencies in the thermal solution. To conclude, reduced-order engineering tools are vital for design purposes but require adopting various assumptions to maintain sufficient accuracy. Yet, before one can use such reduced-order tools, they must be properly verified via a code-to-code comparison.

1.2.2 Element-to-element heat transfer

Another substantial modeling challenge comes from the element-to-element heat transfer mechanism. Modern NTP systems incorporate many moderating elements necessary for neutron moderation. These moderating elements are placed in full contact with fuel elements such that the moderation is efficient. The typical fuel-moderating element’s configurations introduce a strong and non-uniform heat transfer from the fuel to moderating elements. The heat transfer is mostly from the fuel to the moderating element, however, at the entrance of the propellant to the fuel elements, which is also the exit for the moderating elements, an opposite heat transfer can occur. A typical reduced-order methodology used for the NTP T/H analysis often focuses on individual/decoupled reactor sub-elements study, where the solver often ignores conduction heat transfer mechanism between different sub-elements. For example, in a recent work presented by Gates et al., the 1.5D reduced-order heat transfer solver relied on treating each sub-element separately [11], neglecting to properly account for the heat flux between the moderating and fuel elements. When applied to currently proposed NTP concepts, the reduced-order approach
produces highly inaccurate results. A recent study has [12] demonstrated the importance of the inter-elemental heat flux at the interface between the fuel and moderating elements.

1.3 Why OpenFOAM?

The modern NTP designs rely on HALEU fuel as opposed to the historically developed HEU fuel. This is a considerable design modification with major impacts on the characteristics (e.g., neutron spectrum) of modern systems. As a matter of fact, the design adaptations (e.g., inclusion of moderating elements) result in many challenges that must be resolved. Numerical modeling and simulation tools are a key to successively promoting the NTP technology through the demonstration phase. The current research chooses OpenFOAM as a designated platform for NTP core analysis due to its unique capabilities for computational fluid dynamics and solving partial differential equations. In addition, OpenFOAM has been utilized in many nuclear engineering applications (i.e., CANDU [13], High Temperature Gas-cooled Reactor [14], and dynamic analysis in Lead-Cooled Fast Reactors [15]). Perhaps the most notable application is the GeN-Foam reactor multiphysics solver [16]. The current dissertation uses GeN-Foam as the inspiration and foundation for building a novel tailored, NTPSteadyFOAM, solver for NTP core simulations.

It must be pointed out that at the time of conceiving this dissertation, there was limited number of options to tackle multiphysics problems capable of performing both high- and reduced-fidelity simulations. Recently, there is a strong push to use MOOSE-based tools for NTP analysis [17]. The package and methods proposed here are complementary to the on-going research activities rather than contradictory. The methods
and tools developed during this research are novel and unique, and to the best of our knowledge are not readily available elsewhere. Some key differences between the OpenFOAM-based and MOOSE-based tools are the use of finite volume and Computational Fluid Dynamic (CFD) as opposed to the use of finite elements and heat transfer correlations respectively.

1.4 OpenFOAM as a High- and Reduced-Fidelity Computational Tool

This study focuses on capturing the T/H and the neutronic phenomena within the NERVA-type NTP active core region, as these are the most important physical considerations in NTP multiphysics analysis. After a thorough review of existing modeling and simulation tools applicable for our needs, we have selected OpenFOAM-5.0 as the primary tool for the ongoing analyses.

OpenFOAM is an open-source C++ toolbox designed to solve continuum mechanical problems such as chemical reaction, turbulence, and heat transfer phenomena with complex fluid flow [18]. This finite volume method (FVM) code has been used for various nuclear applications, such as fuel performance [19], sub-channel analysis [20], and reactor multiphysics simulations [16]. OpenFOAM was also used in a coupled neutronic-thermal hydraulic manner to analyze a PWR fuel assembly. Another advantage of using OpenFOAM is its ability to construct customized solvers and boundary conditions specifically tailored for user-desired applications.

1.4.1 OpenFOAM for high-resolution T/H modelling
The previous section mentioned that most legacy programs (with HEU-based fuel) heavily relied on experimental setups to demonstrate and deploy the NTP technology. As opposed to previous experimental efforts, modern HALEU-based design efforts heavily complemented by modeling and simulation. To remedy circumstances where the applicability of legacy experimental data could remain questionable [4], we propose to use the CFD capabilities embedded in OpenFOAM as a complementary tool to the experimental effort by relying on high-resolution modeling techniques. The current research adapts the conjugate heat transfer (CHT) approach to generate T/H models as a means of generating reference solutions for the modern sub-element designs (e.g., including multiple supercell configurations).

1.4.2 OpenFOAM for coarse-mesh-based modelling

Currently, there are not many existing computational tools that can perform large-scale T/H analysis for the NTP reactor core due to the high computational requirements associated with fine-mesh high-resolution modeling. With the specific limitation on mesh-resolution, the previously mentioned CHT method must balance between computational efficiency and scale of the simulation. An alternative way to conduct large-scale T/H analysis is to adopt a coarse-mesh-based reduced-order approach. In general, the approach uses a coarser mesh size in conjunction with approximated interface conditions to reduce the complexity of the problem. An example of an OpenFOAM solver that provides insight on large-scale core simulation is the GeN-Foam multiphysics package [16].

GeN-Foam is a novel solver characterized by tight coupling between differential equations. The code was originally developed by the FAST group at the Paul Scherrer
Institute (PSI) and was mainly built to account for the multiphysics feedback in Molten Salt Reactors (MSRs) and Sodium Fast Reactors (SFRs) [16]. GeN-Foam’s multiphysics solver is comprised of four sub-modules: coolant-based porous-medium T/H solver, sub-scale finite-difference solver, nodal neutron diffusion solver, and displacement-based thermal-mechanic solver. Decomposing Gen-Foam into multiple modules and components allows the solver to model each physics individually and in a multiphysics manner when needed.

Overall, the GeN-Foam solver provides a solid and unique framework to account for coarse-mesh-based multiphysics feedback. However, it is not possible to apply GeN-Foam directly to the analysis of NTP systems, as the source code requires heavy modifications. Moreover, the nature of the NERVA-NTP core’s sub-element configuration and heat transfer mechanism (as mentioned in Section 1.2) would be a potential bottleneck to GeN-Foam’s NTP implementation.

1.5 Objectives and Goals

The primary objective of this study is to introduce NTPSteadyFOAM, as a novel coarse-mesh-based multiphysics package for steady-state NERVA-type reactor analysis. The package contains three major sub-modules and several sub-functions to account for the multiphysics effects of typical NTP systems. The calculation sequence will consider the unique T/H characteristic that is unique to NTP cores; mainly the heat transfer within and between sub-elements, identified as part of the modeling challenge.

As a secondary objective, the study will also perform full-order T/H analysis on different combinations of sub-elements to verify and validate the solution generated by the
novel NTPSteadyFOAM package. The goal is to develop a higher fidelity tool that performs high-resolution T/H simulation for modern NTP designs where experimental data do not exist. The computational effort conducted in this objective will heavily rely on the OpenFOAM CHT approach, which can be applied to study thermal margins, geometric impact, and sub-element interface thermal effects in detail. However, this study only uses the CHT approach to generate small-scale high-definition benchmark solutions for coarse-mesh models, as such an approach is usually computationally expensive.

The presented study is structured as follows. Chapter 2 introduces the mathematical theory behind the full-order T/H model used for reference solution generations. Chapter 3 demonstrates the mathematical derivations and assumptions for the coarse-mesh-based, NTPSteadyFOAM, solver. Chapter 4 then verifies the CHT solver by performing multiple sensitivity studies. The solver’s results are then validated against experimental data set obtained from the historical NERVA NRX-A6 program. Chapter 5 applies NTPSteadyFOAM to perform T/H and neutronic simulations of multiple full-scale models (e.g., single FE, single ME, and multi-element analysis). Moreover, the results obtained with NTPSteadyFOAM are benchmarked against higher-order reference solutions including the CHT approach for T/H and Monte Carlo for neutronics. To demonstrate the solver’s full capability, Chapter 6 adopts a large-scale NTP model to perform single and multiphysics analysis and compare the results for cores with different loading patterns. Finally, Chapter 7 presents the concluding remarks as well as discussion on future work needs.
CHAPTER 2. NUMERICAL THEORY FOR FULL-ORDER T/H SIMULATION

This chapter introduces the numerical theory behind OpenFOAM’s full-order multi-region conjugate heat transfer (CHT) solver. The latter can be used to generate reference solutions for different elements (e.g., FE and ME) and different supercell configurations. The nature of the CHT methodology allows the solver to model fuel-to-flow-channel heat transfer without the need to adopt empirical convective models and correlations. The OpenFOAM CHT model iterates upon different equations: single-phase Navier-Stokes (NS) equations of mass and momentum conservation, energy balance equation, thermal conduction equation, turbulence model, and the conjugate heat transfer interface condition. The chapter will present the fundamentals of each physics and corresponding mathematical relations. Finally, the SIMPLE algorithm that governs the coupling of these equations will be discussed.

2.1 Navier-Stokes Equations

The Navier-Stokes (NS) equations are commonly used in finite volume methods (FVM) for solving the fluid motion for both internal and external flow. Eq. (1) and (2) show general single-phase steady-state NS equations for mass and momentum continuity respectively [21]. The solution of these equations describes fluid motion within a finite volume.

\[
\nabla \cdot (\rho \vec{U}) = 0 \tag{1}
\]
\(\rho (\overrightarrow{U} \cdot \nabla) \overrightarrow{U} = \overrightarrow{F}_b + \nabla \cdot \overrightarrow{\tau} \tag{2}\)

where \(\rho\) and \(\overrightarrow{U}\) represent a fluid substance’s density scalar and velocity vector. The left-hand-side of Eq. (2) represents the convective term, which describes the change of fluid momentum per unit volume. The right-hand-side of the balance equation represents the net force combined between the body force \(\overrightarrow{F}_b\) (weight) and the surface force defined by the divergence of the dyadic stress tensor \(\overrightarrow{\tau}\) [22]. The net force terms in the momentum equation can be further expanded based on the direction of shear. Eq. (3) presents the momentum equation, in which the surface force term is expanded into two normal force components: the isotropic force denoted as static pressure gradient (\(\nabla p\)) and the force performed by viscous stress tensor \(\tau'\).

\[\rho (\overrightarrow{U} \cdot \nabla) \overrightarrow{U} = \rho \overrightarrow{g} - \nabla p + \nabla \cdot \tau' \tag{3}\]

In Cartesian coordinates (with unit direction \(x_i, x_j,\) and \(x_k\)), the components of the viscous stress tensor \(\tau\) for a Newtonian fluid can be represented as

\[
\tau_{ij} = \mu \left[ \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \left( \frac{\partial U_k}{\partial x_k} \right) \delta_{ij} \right] \tag{4}
\]

where \(\mu\) represents the dynamic viscosity and \(\delta_{ij}\) is the Kronecker-Delta function (\(\delta_{ij} = 1\) for \(i = j\), otherwise \(\delta_{ij} = 0\)). The subscript notation for \(\tau_{ij}\) indicates the stress component
acts in \(x_j\)-direction on a surface normal to \(x_i\)-direction. In incompressible flow, the third term on the right-hand side of Eq. (4) can be neglected, which transforms the momentum equation into the following form:

\[
\rho(\bar{U} \cdot \nabla)\bar{U} = \rho\bar{g} - \nabla p + \nu \nabla^2 \bar{U}
\]  
(5)

Codes that use FVM (e.g., OpenFOAM) often iterate between mass and momentum equations to calculate the velocity field. Depending on fluid’s compressibility or pressure dependency, the two equations can also be used to determine pressure drop across the system.

### 2.2 Energy Balance Equation

The NS equations often include the conservation of energy equation when fluid energy is in the scope of the calculation. Eq. (6) presents the steady-state energy balance equation in terms of specific total energy \(E\) [20], where the specific total energy is the summation between specific internal energy and kinetic energy.

\[
\rho \nabla \cdot (\bar{U} E) = -\nabla \cdot (p\bar{U}) + \nabla \cdot (\tau \cdot \bar{U}) - \nabla \cdot (q''') + S
\]  
(6)

In this equation, \(q'''\) is defined as the heat flux traveling into the finite volume and \(S\) represents the external heat source and work done by body force. Moreover, the left-hand term represents the spatial diffusion of energy per unit volume. The first term and the second term on the right-hand-side represent the mechanical work done by pressure and viscous stress, respectively.
In addition to the NS equations of mass, momentum, and energy, a multi-region solver that models the thermal condition for both fluid and solid domain solver will also include the heat conduction equation. Eq. (7) shows OpenFOAM CHT solver’s thermal conduction equation in terms of specific enthalpy \( h \).

\[-\nabla \cdot (\alpha \nabla h) = q_{\text{gen}}\]  \hspace{0.5cm} (7)

where \( \alpha \) is the thermal diffusivity and \( q_{\text{gen}} \) is the heat source.

### 2.3 Turbulence Modeling

In a fluid flow dominated by a high Reynolds number, the effect of the nonlinear convective term \((\vec{U} \cdot \nabla)\vec{U}\) in Eq. (2) will become substantial in the numerical modeling of NS equations. A turbulent-dominated NS equation would require a very fine mesh grid to resolve all the turbulent scales. The unsteady nature of the turbulent flow also requires the solver to maintain fine resolution in time [23]. A truly high-fidelity approach, known as the Direct Numerical Simulation (DNS), would solve the NS equations without using any turbulence model. However, using such an approach could be computationally expensive or even unrealistic, considering practical model dimensions. Fortunately, the application of the current study does not look for the finest detail of the turbulent flow but rather the time-averaged flow condition within each flow channel. In this study, the solver will utilize the Reynold-Averaged Navier Stokes (RANS) model as a turbulence modeling technique that simplifies the turbulent flow problem in NS equations.

#### 2.3.1 RANS Model
The RANS approach separates the turbulent flow fields into a mean and a fluctuating component [23]. Eq. (8) shows the definition of Reynolds decomposition, in which \( \phi \) could be any turbulent fields described by the NS equations, with \( \bar{\phi} \) being the mean (time-averaged) and \( \phi' \) being the fluctuating component. In addition, the Reynolds decomposition comes with a property that states the time-average of the fluctuation term is equal to 0 (\( \bar{\phi}' = 0 \)).

\[
\phi = \bar{\phi} + \phi'
\]  

(8)

Applying Reynolds decomposition into the convective term of a 2-D momentum equation as an example, the expression for one of the 2-D-direction becomes:

\[
\frac{\partial (\rho \bar{u}_i \bar{u}_j)}{\partial x_i} + \frac{\partial (\rho \bar{u}_i' \bar{u}_j')}{\partial x_j} = \rho \ddot{g} - \nabla p + \nabla \cdot \tau
\]  

(9)

The second term on the left-hand-side of Eq. (9) describes the gradient of turbulent stress. In a three-dimensional problem, the RANS approach would introduce six additional unknowns of turbulent stresses in different shear directions. A simple approach to tackle these unknowns would be using the Boussinesq hypothesis. The hypothesis states that the correlation between turbulent stresses and the mean velocity gradient behaves in almost the same way as the correlation between viscous stress and full velocity gradient [24]. Using the Boussinesq hypothesis, the turbulent stress in a 3-D domain can be written in the following form:
\[-\rho \bar{u}_i' \bar{u}_j' = \left[ \mu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right] - \frac{2}{3} \rho k_t \delta_{ij} \] (10)

where \( \mu_t \) is the turbulent eddy viscosity and \( k_t = \frac{1}{2} \sum_{n=i,j,k} \bar{u}_n^2 \) is the turbulent kinetic energy. The third term on the right-hand side of the equation is added to avoid unphysical prediction where the turbulent kinetic energy could become zero for an incompressible or pressure independent assumption [21].

Applying Eq. (10) into Eq. (9) with incompressible assumption, the general form for a momentum equation (in one of the 3 dimensions) that considers the turbulent condition under RANS approximation becomes:

\[
\frac{\partial \bar{u}_i}{\partial x_i} + \frac{\partial \bar{u}_j}{\partial x_j} + \frac{\partial \bar{u}_k}{\partial x_k} = \rho \bar{g}_i - \nabla p + (\mu + \mu_t) \left[ \frac{\partial^2 \bar{u}_i}{\partial x_i^2} + \frac{\partial^2 \bar{u}_j}{\partial x_j^2} + \frac{\partial^2 \bar{u}_k}{\partial x_k^2} \right] \] (11)

The turbulent eddy viscosity \( \mu_t \) in Eq. (11) can be calculated using the solution of the turbulence model. The following section will introduce the \( k - \epsilon \) turbulence model used by OpenFOAM’s CHT model.

2.3.2 \( k - \epsilon \) turbulence model

The \( k - \epsilon \) model is the most widely implemented, two-equation turbulence model, due to its well-established performance. The model describes turbulent flow using two independent variables: the turbulent kinetic energy (denoted as \( k_t \)) and dissipation rate
(denoted as \( \epsilon_t \)). The current section only provides a brief introduction regarding the \( k - \epsilon \) model. Detailed information and implementation of OpenFOAM’s turbulence model can be found in reference [25]. For an incompressible fluid, Eq. (12) and (13) show the transport equations for solving \( k_t \) and \( \epsilon_t \) [26].

\[
\rho u_j \frac{\partial k_t}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k_t}{\partial x_j} \right] + \mu_t \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} \left( \frac{\partial (\bar{u}_i)}{\partial x_i} + \frac{\partial (\bar{u}_j)}{\partial x_j} \right) - \rho \epsilon_t \tag{12}
\]

\[
\rho u_j \frac{\partial \epsilon_t}{\partial x_j} = \\
\frac{1}{\rho} \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon_t}{\partial x_j} \right] + C_{\epsilon 1} \frac{\epsilon_t}{k_t} \frac{\mu_t}{\rho} \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} \left( \frac{\partial (\bar{u}_i)}{\partial x_i} + \frac{\partial (\bar{u}_j)}{\partial x_j} \right) - C_{\epsilon 2} \frac{\epsilon_t^2}{k_t} \tag{13}
\]

Using the solution from the above equations, the turbulent eddy viscosity is calculated as

\[
\mu_t = \rho \frac{C_\mu k_t^2}{\epsilon_t} \tag{14}
\]

Table 1 presents the corresponded closure coefficients for \( k - \epsilon \) model [23].

**Table 1. Closure coefficients for the Launder and Sharma \( k - \epsilon \) model.**

<table>
<thead>
<tr>
<th>( C_\mu )</th>
<th>( C_{\epsilon 1} )</th>
<th>( C_{\epsilon 2} )</th>
<th>( \sigma_k )</th>
<th>( \sigma_\epsilon )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.44</td>
<td>1.92</td>
<td>1</td>
<td>1.3</td>
</tr>
</tbody>
</table>

The \( k - \epsilon \) model assumes that deviatoric Reynolds stresses are linearly related to local mean strain rate, and as such the model could perform poorly in cases with strong
curvature [27]. However, the flow paths encountered in the study are all straight with no curvature and thus make the $k - \epsilon$ model suitable for the simulation.

2.3.3 Turbulent near-wall treatment

So far, Eq. (2) has presented the momentum equation as the balance between fluid convection and external force in a control volume. Assuming an internal flow condition where the fluid’s body force term is insignificant compared to the rest of the force terms, the momentum equation would simply be balancing between the fluid convection and the viscous effect asserted by the surrounding structure. Therefore, it is essential to understand the boundary layer effect while the turbulent flow is modeled. The $k - \epsilon$ model treats turbulent eddy viscosity $\mu_t$ as scalar quantity by assuming local isotropy in the turbulent field; such an assumption is valid mainly in the region with high Reynolds numbers but will become invalid close to walls with significant viscous effect. Thus, some near-wall treatment is required when using the $k - \epsilon$ model in OpenFOAM.

The turbulent boundary layer parallel to a smooth surface can be categorized into three sublayers: viscous sublayer, buffer layer, and turbulent core [21]. In the viscous sublayer, viscous effects are dominant, and the flow field is predominately laminar. In the fully turbulent zone, turbulent eddies dominate all transport process, and viscous effects are typically negligible. In the buffer zone, viscous (molecular) diffusion and turbulent effects are both important. The range of each sublayer can be described by $y^+$, which is a dimensionless value that describes the distance from the wall under turbulent effect. Eq. (15) presents the definition of $y^+$. 

23
where $U_r$ is the friction velocity, $\nu$ is the fluid kinematic viscosity, and $y$ is physical distance from the wall. The friction velocity is a form of shear stress written in units of velocity.

The value of $y^+$ at the boundary cell centroid allows many CFD codes, including OpenFOAM, to pick the suitable wall function that correlates near-wall velocity fields to the surface shear stress. Eq. (16) and (17) present the most common expression for the logarithmic velocity profile $U^+$ used by many CFD wall functions.

For viscous sublayer ($y^+ < 5$)

$$ U^+ = y^+ $$

For fully turbulent zone ($y^+ > 30$)

$$ U^+ = \frac{1}{0.4} \ln y^+ + 5.5 $$

The logarithmic velocity profile is another dimensionless value that describes the ratio between the local mean velocity and the friction velocity. When using wall functions to model turbulent boundary effect, a general rule is to avoid having the first boundary cell centroid located within the buffer zone ($5 < y^+ < 30$) because many wall functions would fail to predict velocity fields at this region accurately. For the full-order T/H model of NTP sub-elements, the current study will be using a very fine boundary mesh with a first cell
\( y^+ \) less than 1. The reason is that the full-order solver would use the same mesh structure with both turbulent wall functions and CHT boundary conditions to model heat transfer near the solid-fluid interface. Under a large magnitude of heat flux, the continuity of heat transfer under the CHT interface condition would be susceptible to grid size. Therefore, part of the mesh sensitivity study would focus on the magnitude of \( y^+ \) at the interface cell for all CHT models.

### 2.4 Conjugate Heat Transfer Algorithm

This study implements a 3-D CHT numerical solver to generate reference solutions for single FE/ME models, as well as for various supercell models. The supercell models rely on various combinations of FE and ME that are used to study the inter-elemental heat transfer. The adopted OpenFOAM CHT solver, denoted as “chtMultiRegionSimpleFoam” is a steady-state solver capable to model buoyant, turbulent flow of incompressible/compressible fluids using the SIMPLE algorithm [28]. The solver also includes a multi-region capability, which allows each sub-domain or region to have its own mesh structure. In this study, the multi-region capability is utilized to model the heat transfer and/or the fluid mechanics within the hydrogen propellant and solid fuel sub-domains. The Navier-Stokes conservation equations of continuity, momentum, and energy are solved in the fluid domain [20], while heat conduction equations are solved in the solid domain. The CHT solver also makes the use of interface boundary conditions, referred as “turbulentTemperatureCoupledBaffleMixed” to thermally couple solid and fluid regions. Such interface boundary condition allows the solver to model solid-to-fluid heat transfer without using empirical convective heat transfer models. The governing equations for CHT boundary condition are presented in Eq. (18) and (19):
\[ \lambda_1 \nabla_{\perp} T_1 = \lambda_2 \nabla_{\perp} T_2 \]  \hspace{1cm} (18)

where \( \lambda \), is the thermal conductivity and \( T \) is the temperature at the interface. The subscripts 1 and 2 correspond to domain 1 and 2 located on both sides of the interface boundary. \( \nabla_{\perp} \) represents the gradient operator at the direction normal to the interface boundary. Eq. (18) assumes continuity of the heat flux at the interface between the two connected domains. Assuming no presence of radiation heat transfer, Eq. (18) is valid at the coolant-fuel interface if the size of the first cell in the fluid domain is small enough (\( e.g., y^+ < 1 \)). The latter requirement is needed to capture laminar viscous effects under fully developed turbulent flow where the heat transfer is dominated by thermal conduction [29]. By using a linear approximation for the gradient, the heat flux \( q_s'' \) at the interface \( s \) can be estimated with Eq. (19).

\[ q_s'' \approx \lambda_i(T_s) \frac{T_s - T_i}{\Delta_i} \]  \hspace{1cm} (19)

where \( \lambda_i(T_s) \), \( T_s \), \( T_i \), and \( \Delta_i \) represent the effective thermal conductivity at the boundary, interface temperature, first cell temperature, and the corresponding normal distance from domain \( i (i = 1 \text{ or } 2) \). The surface temperature, \( T_s \) is calculated based on the thermal conditions from both domains using the following relation:

\[ T_s = \frac{\frac{\lambda_1}{\Delta_1} T_1 + \frac{\lambda_2}{\Delta_2} T_2}{\frac{\lambda_1}{\Delta_1} + \frac{\lambda_2}{\Delta_2}} \]  \hspace{1cm} (20)
where the thermal conductivity values $\lambda_1$ and $\lambda_2$ are evaluated in domains 1 and 2 by employing known thermodynamic properties in conjunction with a turbulence model.

The iteration for the CHT boundary coupling starts from an initial guess of interface surface temperature at the boundary. At each new iterate, the temperature fields ($T_i$) as well as the thermal conductivity in each domain will be re-evaluated using the interface boundary temperature ($T_s$) as the boundary condition. The interface boundary temperature $T_s$ will then be updated based on the newly evaluated fields at each domain using Eq. (20). The iterative procedure will proceed until the residual error on $T_i$ is small enough.

### 2.5 SIMPLE Algorithm

The Semi-Implicit Method for Pressure Linked Equation (SIMPLE) algorithm is a widely used CFD iterative strategy for NS equations. SIMPLE is a pressure-based algorithm commonly used to solve steady-state problems where the fluid is assumed incompressible, or the fluid density is independent of pressure. The fluid velocity and pressure solution rely on the predictor-corrector strategy applied to mass, momentum, and Poisson equations for pressure fields. Figure 6 presents the SIMPLE algorithm flow chart in OpenFOAM. More details regarding the algorithm can be found in the CFD textbook by Kajishima and Taira [30]. Finally, Figure 6 also shows the iterative strategy for the OpenFOAM’s steady-state multi-region CHT solver.
Figure 6. Iterative Strategies for: (a) SIMPLE algorithm, and (b) chtMultiRegionSimpleFoam solver.
CHAPTER 3. NUMERICAL THEORY FOR COARSE-MESH-BASED SIMULATION

This chapter presents the theory behind the main dissertation topic: the NTPSteadyFOAM, a coarse-mesh-based solver package for NTP multiphysics analysis. The package is composed of three major numerical sub-modules, each governed by different physical characteristics required to properly model the NTP active core. These numerical sub-modules include:

- **Main T/H Module** – responsible for modeling individual sub-elements using a reduced-dimension 1.5-D approach.

- **Inter-elemental Heat Transfer Module (Inter-HT Module)** - models 2-D inter-elemental heat transfer using Laplacian solver with special interface boundary conditions.

- **Neutron Diffusion Module** - calculates flux and power distributions by solving 3-D multi-group diffusion equations with user-selected cross-section data set (with feedback capabilities).

The current version of NTPSteadyFOAM only enables steady-state T/H and neutron diffusion calculations as part of future multiphysics capabilities. In this package, the T/H physics are distributed into two separate sub-modules to provide users with the freedom to decouple and couple between individual solvers (e.g., with and without inter-elemental heat transfer). The following sections will introduce the methodology and implementation of the reduced-order treatments for each sub-module and discuss the
coupled iterative strategy adopted to create a complete multiphysics framework. Again, it must be pointed out that only T/H and neutronic analysis are included in the current multiphysics capabilities.

3.1 Thermal-hydraulic (T/H) Module

NTPSteadyFOAM’s main T/H module relies on solving the 1-D NS equations of mass, momentum, and energy, in which the energy equation relies on the 1-D finite-difference sub-function (also implemented for this study) to determine the sub-structural heat source/sink embedded in each cell. Together with many other sub-functions (e.g., empirical convective heat transfer models, head loss models), the main T/H module performs 1.5-D T/H calculations for every element within the core.

3.1.1 Coarse-mesh treatment of sub-elements

Before discussing the governing equations for the main T/H module, it is crucial to identify the mesh requirements for a coarse-mesh-based solver as its mesh definition will dictate the accuracy and computational requirements of the solution. In FVMs, each control volume is associated with a polygon mesh; and each mesh stores information at the cell centroid while passing information through cell surfaces.
Figure 7. Mesh treatments in different modeling orders of dimensionality.

Figure 7 presents a simple internal pipe flow problem with two different orders of mesh treatments, in which the problem resembles the flow condition inside a NTP sub-element. In this figure, Treatment A on the left represents a full-order mesh model that discretizes the geometry into various regions using fine mesh (presented in different colors). In the fluid path region, the mesh filled in green is the boundary cell, and the mesh filled with red is the center cell. The difference between the boundary and center cells is the different impact on momentum at the boundary/interface; thus, the boundary cell may require wall treatment in a CFD calculation.

Treatment B disregards the geometric composition of the problem and treats every substance inside the control volume as a bulk. Such an approach implies that all coarse-mesh cells inside the problem shall consider the phenomenon that leads to energy and momentum generations and dissipations (e.g., sub-structure heat source/sink and surface frictions). Moreover, if the mean flow is confined to a single direction, as is within the FE and ME, the coarse-mesh treatment can reduce the fluid mechanic into a 1-D problem.
Overall, Treatment A provides a detailed solution for a given problem, while Treatment B provides the bulk solution (i.e., lump model). Considering the full core simulation scale needs for NTPSteadyFOAM, the T/H module will use Treatment B’s coarse-mesh approach to discretize the problem.

In addition to the sub-elements’ mesh treatment, the computational sequence implemented in the main T/H module relies on the equivalent modeling assumption. The equivalent model is usually an analytically well-established geometry (i.e., circular, and annular cylinders); such a geometry shall resemble the average characteristics of the original model. In NTP sub-elements, the equivalent models preserve the hydraulic parameter and fuel volume with an assumption of radial symmetry. Figure 8 presents the full-order FE model (left) in comparison to NTPSteadyFOAM’s 1.5-D equivalent FE model (right). In this figure, the equivalent outer-diameter of the 1.5-D FE model is obtained by dividing the total fuel volume of the explicit model by the number of channels (e.g., 19 channels are presented in Figure 8) and transform the divided volume into annular cylinder.

The equivalent ME model uses a similar approach to generate annular cylinders. Given a more complex twice-through counter flow design for this sub-element, the solver will decompose ME into two sub-scale models, known as the Supply Channel (SC) and the Return Channel (RC). Figure 9 presents the schematic of the two sub-scale problems. The SC and the FE equivalent models share similar geometric features; however, the SC’s outer-edge boundary condition relies on the T/H condition of the RC. The RC has an annular flow path, which is surrounded by several solid layers. The inner and outer boundary conditions play an important role in the heat transfer within the model. Both sub-
scale problems rely on the modification and the manipulation of the boundary conditions in conjunction with the FD method.

![Discrete full-order FE model vs. Equivalent FE model](image)

**Figure 8.** Discrete full-order FE model (left) vs. Equivalent FE model (right).

![Equivalent Supply and Return Channel models](image)

**Figure 9.** Schematic of the equivalent Supply (left) and Return (right) Channel models.

### 3.1.2 1-D Navier-Stokes equations under coarse-mesh treatment

This section derives the 1-D NS equations of mass, momentum, and energy based on the previously introduced mesh treatment and equivalent modelling approach. Eq.(21) and (22) present the conservation equations for a steady, compressible, subsonic turbulent flow under the coarse-mesh porous-medium assumption [16].
\[ \nabla \cdot (\gamma \rho \vec{U}) = 0 \quad (21) \]

\[ \gamma \rho (\vec{U} \cdot \nabla) \vec{U} = -\nabla \gamma p + p_i \nabla \gamma + \nabla \cdot (\mu_{eff} \nabla \vec{U}) + \gamma F_{ss} \quad (22) \]

In these equations, \( \gamma \) represents the volumetric fraction occupied by the fluid flow path with respect to the cell volume. The \( \mu_{eff} \) is the effective viscosity combining dynamic and turbulent viscosity. The \( F_{ss} \) represents the momentum sink due to sub-structure interactions. \( p \) and \( p_i \) are respectively the channel pressure and the interfacial pressure under porous-medium assumption. In this case, the balance equations have neglected the gravity-induced momentum, which is a valid assumption considering the zero-gravity operating condition in an NTP reactor.

The previously introduced coarse-mesh treatment for the NTP sub-element has allowed the solver to treat the fluid mechanic problem in a 1-D manner, where the mean flow direction would be parallel to the channel path(s) of the sub-element. For such an assumption, the diffusion term \( \nabla \cdot (\mu_{eff} \nabla \vec{U}) \) on the right-hand side of Eq. (22) can be omitted. Knowing that the cross-sectional area flow in the sub-elements does not vary axially, the gradient \( \nabla \gamma \) in respect to \( z \) is zero. The 1-D coarse-mesh-based NS equations of mass and momentum can be reduced to the following form.

\[ \frac{\partial}{\partial z} \gamma \rho \vec{U} = 0 \quad (23) \]
\[
\frac{\partial}{\partial z} \rho U^2 = - \frac{\partial p}{\partial z} + F_{ss}
\]  \hspace{1cm} (24)

where the flow path is parallel to \( z \)-axis. It is worth noting that the volumetric fraction \( \gamma \) is purposely left in Eq. (23) as in general it can vary radially and axially throughout the flow path of the sub-elements. Eq. (23) simply states that the mass flow rate is constant, and \( \gamma \) indicates that the correct volumetric flow fraction is used to calculate the velocity fields that are required as boundary conditions.

The sub-structure drag force term \( (F_{ss}) \) is usually described by a linear or quadratic correlation associated with flow path permeability, geometry, and fluid velocity in a porous-medium assumption [31]. In a complex porous flow path, the solution for the drag force term is usually obtained through experimental fit, in which the exact value for such a term is typically not available in many engineering applications [16]. Fortunately, the flow channels embedded in NTP sub-elements follow straight paths without obstacles blocking the channel. The drag force term can therefore be expressed by the following equation [16]:

\[
F_{ss} = \frac{f_D \rho U^2}{2D_h}
\]  \hspace{1cm} (25)

where \( f_D, D_h \) are the Darcy friction factor and hydraulic diameter of the flow channel.

The treatment of the energy equation requires to adopt additional simplifications and assumptions before it transforms to the final coarse-mesh representation. The
derivation begins by recalling the energy balance equation from Eq. (6) and apply fluid volumetric occupancy ($\gamma$) into each term.

$$\gamma \rho \nabla \cdot (\vec{U} h) = -\nabla \cdot (\gamma p \vec{U}) + \gamma \mu \Phi + \nabla \cdot (\gamma q'') + S_{ss} + \gamma F_{ss} \cdot \vec{U} \quad (26)$$

Here, Eq. (26) has broken down the external source term ($S_{ext}$) into energy source due to sub-structure heat generation ($S_{ss}$), and energy sink due to sub-structure friction work ($\gamma F_{ss} \cdot \vec{U}$).

In contrast to the full-order solver that solves fluid temperature using the enthalpy-based balance equation, NTPSteadyFOAM’s T/H module directly implements a temperature-based equation as the governing correlation for fluid heat transfer. To present Eq. (26) in terms of temperature, one shall use the enthalpy change correlation for a single-phase pure substance at equilibrium, given as [22]:

$$dh = \left( \frac{\partial h}{\partial T} \right)_p \, dP + \left( \frac{\partial h}{\partial P} \right)_T \, dT = C_p \, dT + \left[ v - T \left( \frac{\partial v}{\partial T} \right)_P \right] \, dP \quad (27)$$

where $C_p$ and $v$ are the specific heat capacity and fluid specific volume.

Substituting Eq. (27) into Eq. (26), recasts the energy balance equation in terms of temperature.

$$\gamma \rho C_p \nabla \cdot (\vec{U} T) = -\left( \frac{\partial \ln \rho}{\partial \ln T} \right)_p \nabla \cdot (\gamma p \vec{U}) + \gamma \mu \Phi + \nabla \cdot (\gamma q'') + S_{ss} + \gamma F_{ss} \cdot \vec{U} \quad (28)$$
where \( \left( \frac{\partial n}{\partial nT} \right)_p = 1 \) for ideal gas such as hydrogen [22].

The following additional simplifications are made to the energy balance equation. The energy equation requires to account the heat source term \( (S_{ss}) \) as potential summation of volumetric heat sources coming from different sub-structural components. For instance, the ME return flow may contain two energy sources transferred through the inner and outer heated surfaces. Moreover, the solver also treats the viscous dissipation term \( (\mu \Phi) \) as a negligible second-order effect under the 1-D coarse-mesh assumptions. Finally, the problem assumes that hydrogen density depends only on the temperature as the experiment has shown the pressure losses within the sub-elements contain negligible effect on the hydrogen thermophysical properties [32].

The final assumption is crucial to the iterative scheme between the three balance equations. By assuming the density to be pressure independent, the velocity field can be directly determined through the 1-D continuity equation (Eq. (23)). Given the solution for velocity, the momentum equation will simply become a correlation for pressure drop due to fluid accelerations and sub-structural friction interactions. Knowing the pressure-drop term has already considered all mechanical interactions within the system, the frictional work term \( (\mathbf{F}_{ss} \cdot \mathbf{U}) \) in Eq. (28) can therefore be omitted from the balance equation.

Using the Fourier law of conduction to describe the heat flux, Eq. (29) presents the final formation of the 1-D coarse-mesh-based energy balance equation adopted by NTPSteadyFOAM.
\[
\gamma pU C_p \frac{\partial T}{\partial z} = -\gamma \frac{\partial p}{\partial z} U + \sum_i S_{ss_i}
\]  

(29)

The sub-structural energy source (heat flux) term in Eq. (29) is determined through Newton’s Law of cooling written as

\[
\sum_i S_{ss_i} = \sum_i A_{vi} h_i (T_{si} - T)
\]  

(30)

In this equation, the subscript \( i \) represents the sub-structure surface index that could go from 1 to 2, depending on the element type. The \( h_i, A_{vi}, T_{si}, \) and \( T \) are respectively the convective heat transfer coefficient (HTC), the volumetric wetted area, the sub-structure surface temperature, and the bulk coolant temperature. In this solver, the HTC can be determined using user-selected empirical correlations; and the sub-structure surface temperature is calculated using a 1-D FD sub-function for conduction heat transfer.

3.1.3 Finite-difference Sub-function for Sub-structure Temperature Profile

Finding the temperature profile for the sub-structure is not only needed for the main T/H module, but also for the overall multiphysics simulation. For the main T/H module, the energy equation uses sub-structure’s surface temperature to determine heat source/sink to coolant channels. The ME model also utilizes surface temperature as part of the boundary conditions to couple between supply and return channel models. For the other modules, the Inter-HT Module uses sub-structure’s outer-edge temperature to predict heat flux across different elements. In its current version, the Neutronic Module uses the average
fuel temperature to update cross sections for reactivity feedback calculations. This section discusses the theory of the finite-difference function that is used to calculate the local radial temperature distribution as well as the surface temperature.

![Diagram of finite-difference model](image)

**Figure 10. Nomenclature for FD representation for an annular cylinder with constant grid size [33].**

The sub-elements’ local temperature ($T_{ss}$) is obtained using a 1-D, node-based, multi-region thermal conduction solver under cylindrical coordinate. The equivalent modelling assumption has allowed each FD problem to be treated as axis-symmetric annular cylinder. Eq. (31) shows the governing equation for the sub-scale thermal conduction solver.

$$\frac{d^2 T_{ss}}{dR^2} + \frac{1}{R} \frac{dT_{ss}}{dR} + \frac{1}{k} q'' = 0 \quad \text{for } a < R < b \quad (31)$$

where $k_{ss}$ and $q'''$ are the constant thermal conductivity and local volumetric heat. The relation in Eq. (31) is applied for each sub-solid domain characterized by a unique material composition with a specific conductivity value.
Figure 10 shows a general FD representation for an annular geometry with identical grid size. Using a second-order central difference scheme, Eq. (31) can be discretized into the follow form:

$$\frac{T_{i-1} - 2T_i + T_{i+1}}{\delta^2} + \frac{1}{a + i\delta} \frac{T_{i+1} - T_{i-1}}{2\delta} + \frac{1}{\kappa} q_i''' = 0$$  \hspace{1cm} (32)$$

where the nomenclature for Eq. (32) is stated in Figure 10.

The discretized thermal conduction equation is often rearranged into the linear matrix formation for the convenience of solution process. The rearranged form is presented in Eq. (34).

$$\left[ 1 - \frac{1}{2(a + i)} \right] T_{i-1} - 2T_i + \left[ 1 + \frac{1}{2(a + i)} \right] T_{i+1} + \frac{\delta^2}{\kappa} q_i''' = 0$$  \hspace{1cm} (33)$$

One important aspect that dictates the shape of the local temperature profile is the ability of the solver to treat different boundary conditions. This study has implemented multiple boundary conditions (B.Cs.) each sub-element would encounter; these conditions include fixed temperature, fixed heat flux, adiabatic condition, convective heat flux, and interface heat transfer boundary. The first four B.Cs. do not require near-boundary mesh treatments because their boundary values do not rely on the resolution of the FD mesh model. However, for a multi-layer model like ME, the solid-to-solid interface boundary value would depend on the resolution of the near-boundary mesh to account for both temperature and heat flux continuity. This section will only discuss the numerical theory.
and the mesh-refinement treatment behind the interface condition. The mathematical representation for the remaining boundary conditions can be found in reference [33].

Figure 11 demonstrates a two-layer annular model with perfect contact situation. At the interface boundary (shown by the red line), the model uses mesh refinement technique with interface B.C. to ensure continuity of heat transfer and to improve the computational cost without the need to use an ultra-fine mesh throughout the model.

\[ T_{AM} = T_{B_0} = \frac{k_A \Delta A_{M} T_{AM-1} + k_B \Delta B_0 T_{B_1}}{\Delta A_M + \Delta B_0} \] (34)

\( T_{AM} \)}

Figure 11. Nomenclature for FD representation for an annular cylinder with variable grid size.

Eq. (34) presents the correlation for the interface boundary. This interface B.C. borrows the concept from the previously mentioned CHT method, where the interface temperature is a product of heat flux continuity.
Like the previous CHT approach, Eq. (34) also depends on the mesh resolution on both sides of the interface. To avoid the additional computational cost of the fine mesh, the FD sub-function will only implement finer mesh at the interface while leaving the rest of the grid size constant. Eq. (35) presents the discretized thermal conduction equation with variable grid size ($\delta_i$). As a sanity check, Eqs. (32) and (35) should be equivalent if the mesh size $\delta_i$ equals to a constant $\delta$.

$$
\frac{(T_{i-1} - T_l)}{\delta_{j-1}} - \frac{T_l - T_{i+1}}{\delta_{j+1}} \left( \frac{1}{2} \left( \frac{1}{\delta_{j-1}} + \frac{1}{\delta_{j+1}} \right) \right) + \frac{1}{R_0 + \sum_k \delta_k} \frac{T_{i+1} - T_{i-1}}{2} \left( \frac{1}{\delta_{j-1}} + \frac{1}{\delta_{j+1}} \right) + \frac{1}{k} q'''_i = 0
$$

where $R_0$ represents the location at the layer’s innermost radius.

Finally, the linear matrix representation of Eq. (35) can be written as:

$$
\begin{bmatrix}
\frac{2}{\delta_{j-1}} - \frac{1}{a + \sum_k \delta_k} & 0 & \cdots & 0 \\
2 & \frac{1}{\delta_{j-1}} & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & \frac{1}{\delta_{j+1}} & \frac{2}{\delta_{j+1}} \\
\end{bmatrix}
\begin{bmatrix}
T_{i-1} \\
T_l \\
T_i \\
T_{i+1} \\
\end{bmatrix}
= \begin{bmatrix}
\frac{2}{\delta_{j+1}} + \frac{1}{a + \sum_k \delta_k} \\
\frac{1}{\delta_{j+1}} + \frac{1}{a + \sum_k \delta_k} \\
0 \\
0 \\
\end{bmatrix}
\begin{bmatrix}
T_{i-1} \\
T_i \\
T_{i+1} \\
\end{bmatrix}
+ \frac{R_0}{k} q'''_i = 0
$$

3.1.4 Empirical Correlations for Convective Heat Transfer

The previous discussion has mentioned the external heat source (i.e., heat flux) term from the energy equation is solved by Newton’s Law of Cooling (See Eq. (30)), in which the heat transfer correlation itself would rely on multiple sub-functions. This section
discusses the use of Nusselt’s convective heat transfer model as one of the sub-functions in the main T/H module.

NASA’s Technical Memorandum has suggested a general form of the Nusselt number correlation for turbulent pipe flow described in the following relation [1]:

\[
Nu_D = C_1 \cdot Re_b^{C_2} \cdot Pr_b^{C_3} \cdot \left( \frac{T_w}{T_b} \right)^{C_4} \cdot \left( C_5 + C_6 \cdot \left( \frac{x}{D} \right) \right)^{C_7}
\]  

(37)

where \( Re_b \), \( Pr_b \), \( T_w \), \( T_b \), \( x \), and \( D \) are the Reynolds number, Prandtl’s number, wall temperature, bulk coolant temperature, fluid location with respect to the inlet, and channel diameter respectively. The constants \( C_i \) are generated based on the flow condition, fluid type, and experimental results. In a more general form, a conventional Nusselt number correlation can be described in the following form [4]:

\[
Nu = 0.023 \cdot Re_b^{0.8} \cdot Pr_b^n \cdot \phi_v
\]  

(38)

The first part of the expression (up to \( \phi_v \)) in Eq. (38) is the standard Dittus-Boelter representation that is widely used to estimate heat transfer in a single-phase flow within circular long tube. However, the Dittus-Boelter correlation is less accurate when large temperature differences between wall surface and bulk coolant are present [34]. As the NTP sub-elements will encounter considerably different flow conditions (than typical light water reactors) characterized by high Reynolds with maximum Mach number less than 0.3, the shape function factor (\( \phi_v \)) is needed to capture the potential turbulent surface effect (i.e., viscous effect, length to diameter ratio, or surface to bulk temperature ratio).
Multiple Nusselt correlations were reported by NASA in various technical notes, e.g., [2], in which most of the correlations rely on both the ratio of the distance from the entrance to channel diameter ($\frac{x}{D}$) and the ratio of surface to bulk temperature ($\frac{T_s}{T_b}$). Among all the proposed empirical correlations, the Taylor correlation presented in Eq. (39) is the most constraint in terms of the $T_s/T_b$ and $x/D$, thus providing the most conservative heat transfer correlation adopted for our code:

$$Nu_D = 0.0023 \cdot Re_b^{0.8} \cdot Pr_b^{0.4} \cdot \left(\frac{T_w}{T_b}\right)^{(-0.57-1.59 \frac{D}{x})}$$

(39)

According to Taylor, the superscript term for the ratio between wall and bulk temperature ($\frac{T_w}{T_b}$) is generated using first order fit between various experimental data sets tested at different range of $x/D$ ratio. Taylor’s approach indicates the correlation should be valid even at the entrance region (non-fully developed region) providing that $x/D$ ratio is larger than 1.1 [35].

In addition to the empirical correlations derived from fitting experimental data, NASA’s Technical Memorandum has suggested another format of analytically derived Nusselt number model proposed by Petukhov (1970) [35]. The latter relies on extensive parametric calculation with the assumption of turbulent Prandtl’s number of $Pr_{tu} = 1$ in conjunction of using the eddy diffusivity model presented by Reichardt (1951) [36]. The model is valid within the Re ranged from $10^4$ to $5 \cdot 10^6$ and Pr from 0.5 to 2000 [37]. Petukhov’s Nusselt’s model is presented in Eq. (40)- (42).
\[ Nu_{D,m} = \frac{\left(\frac{f_m}{8}\right) Re_D Pr}{K_1(f_m) + K_2(Pr) \left(\frac{f_m}{8}\right)^{\frac{1}{2}} \left(Pr^\frac{2}{3} - 1\right)} \]  

(40)

with

\[ K_1(f_m) = 1 + 3.4f_m \]  

(41)

\[ K_2(Pr) = 11.7 + 1.8 Pr^{1/3} \]  

(42)

From the above equations set, \( Nu_{D,m} \) and \( f_m \) are the Nusselt number and the Darcy friction factor taken at mean coolant temperature. In addition to these correlations, Petukhov also suggest the following expression for smooth surface friction factor [36]:

\[ f = (1.82 \log_{10} Re_D - 1.64)^{-2} \]  

(43)

and the ratio between near surface and bulk Nusselt numbers for a heated pipe should be

\[ \frac{Nu}{Nu_{D,m}} = \left(\frac{\mu_m}{\mu_s}\right)^{0.11} \]  

(44)

where subscripts “\( m \)” and “\( s \)” represent mean and surface temperatures, respectively [36].

In summary, the Nusselt number describes the ratio of convective to conduction heat transfer in a fluid, in which the main T/H module uses the Nusselt model as a sub-function to determine HTC. The current version of the NTPSteadyFOAM (version 1.0)
allows users to choose different Nusselt model for solving heat transfer at difference sub-element surfaces. Table 2 lists out the available Nusselt correlations implemented in NTPSteadyFOAM.

<table>
<thead>
<tr>
<th>Name</th>
<th>Correlations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Taylor [35]</td>
<td>( Nu = 0.023 \times Re_b^{0.8} \times Pr_b^{0.4} \times \left( \frac{T_w}{T_b} \right)^{-0.57-1.59D/x} )</td>
</tr>
<tr>
<td>Wolf-McCarthy [37]</td>
<td>( Nu = 0.025 \times Re_b^{0.8} \times Pr_b^{0.4} \times \left( \frac{T_w}{T_b} \right)^{-0.55} \times \left( 1 + 0.3 \left( \frac{x}{D} \right)^{-0.7} \right) )</td>
</tr>
<tr>
<td>Gnielinski [36]</td>
<td>( Nu_{D,m} = \frac{(Re_D - 1000) Pr \frac{f_m}{8}}{1 + 12.7 \sqrt{\frac{f_m}{8}} \left( Pr^{2/3} - 1 \right)} ) where ( \frac{Nu}{Nu_{D,m}} = \left( \frac{\mu_m}{\mu_s} \right)^{0.11} )</td>
</tr>
</tbody>
</table>
| Dittus-Boelter (Default) [37] | \( Nu = 0.023 \cdot Re^{0.8} \cdot Pr^n \)  
\( n = 0.4 \) for heating  
\( n = 0.3 \) for cooling |

### 3.2 Inter-elemental Heat Transfer Module (Inter-HT Module)

The methodology described so far focused on the ability of the main T/H module to model the thermal conditions and distributions within each element. However, heat transfer between FEs and MEs is of uttermost importance for NTP core designs and operations. From the design perspective, the ME serves as the neutron moderator for the core and a heat sink for the high-temperature FEs. Therefore, the number and configuration of moderating and fuel elements would affect the power distribution and the thermal margins within the core. From an operation perspective, part of the hydrogen is preheated through the ME flow channel before passing into the turbopump and re-entering the active
core (See Section 1.1 for expander cycle). During the preheating process, most of the kinetic energy picked up within ME’s flow channel originates from its high-power neighbor FEs. Therefore, the correct prediction of incoming heat flux becomes essential when calculating velocity and temperature profiles inside the ME. The described inter-elemental heat transfer problem is 2-D in nature as there could be different fuel-moderating elements configurations. For example, the incoming heat flux to a central ME would depend on the conditions of the surrounding elements (both FEs and MEs). The challenge is then to exploit the quick 1.5-D\(^1\) solver relying on the axis-symmetry assumption, but also to accurately capture the 2-D heat transfer from adjacent elements. This section will discuss the implemented numerical theory behind the Inter-HT Module.

3.2.1 Sub-elements Interface Conditions

A typical schematic on how different elements is interfacing/touching is displayed in Figure 12. This figure shows both the explicit and its coarse-mesh representation in NTPSteadyFOAM. Such a cluster is typically referred to as the supercell, which will also be the denoted term here. The NTPSteadyFOAM treats each sub-element as a simple hexagon made of six triangular cells. Each is further represented by an equivalent cylindrical model solved using a 1.5-D T/H model. In principle, the coarse-mesh composition allows the solver to use triangular prism for a single sub-element analysis, however in practice hexagonal prisms must be used due to the nature of the sub-element configurations (i.e., moderating and fuel are defined as hexagons).

\(^1\) In this study, the 1.5-dimensional (1.5-D) sub-element heat transfer solver is defined as a numerical approach that generates local solutions in the radial direction with an axis-symmetry assumption. Furthermore, the heat transfer across axial layers can only be done through the sub-channel fluid flow in the axial direction, making the solution scheme 1-D at the local level but 1.5-D from a global perspective.
The following analogy explains the numerical manipulation that couples 1.5-D equivalent model to the coarse-mesh supercell. Figure 13 presents two adjacent coarse-mesh cells separated by the interface boundary shown in red. The zoom-in representation on Figure 13 shows the discretization scheme where a standard FVM nomenclature is applied. The local temperatures \((T_1\) and \(T_2)\) are stored at the center of the cell and the boundary temperature \((T_B)\) is positioned at the middle of the surface. Assuming two cells consist of different material properties (presented by sub-script 1 and 2), the continuity of heat flux and temperature at the boundary follows Eq. (45).
\[ T_B = \frac{k_1 T_1 + k_2 T_2}{\frac{k_1}{\Delta_1} + \frac{k_1}{\Delta_2}} \]  \hspace{1cm} (45)

To better represent the interface conditions between adjacent element Figure 14 overlays the 1-D finite-difference model from the main T/H module with the FVM model presented in Figure 13. In this figure, the local temperature \( T_1 \) and \( T_2 \) are shared by both finite volume and finite-difference domains, in which the finite volume domain considers \( T_1 \) and \( T_2 \) as local values stored inside the triangular cell, whereas the finite-difference domain treats \( T_1 \) and \( T_2 \) as the outer-edge temperature from the equivalent annular cylinder. Since Figure 14 is a schematic of two overlaying domains, each data point shown on the figure will correspond to its associated domain. Using this point of view, Eq. (46) recasts Eq. (45) with the consideration of the actual contact situation.

**Figure 14.** The zoom-in contact situation from the finite volume and finite-difference overlaying perspective.
\[ T_B = \frac{k_1 T_1 + k_2 T_2}{k_1 + k_2 \delta_1 + k_2 \delta_2} \]  

where \( \delta_i \) is the buffer layer thickness between the interface boundary and the outer-edge of an equivalent FD model. The magnitude of the buffer layer thickness is the distance between the equivalent geometry outer radius \( (R_{f,\text{out}}) \) and the outer fuel radius \( (R') \). The latter dictates the distance occupied by the sub-scale structure in each cell.

### 3.2.2 Heat Transfer Mechanism

Eq. (47) presents the governing equation for the heat transfer module as a steady-state thermal conduction equation balanced between thermal diffusion and heat source/sink.

\[
\nabla \cdot k \nabla T_{ss} \big|_{out} + Q_{net}''' = 0
\]

In this equation, \( k \) and \( T_{ss} \) represent the thermal conductivity and temperature evaluated near the sub-structure periphery and \( Q_{net}''' \) represents the net volumetric heat source. It is important to note that the practical evaluation of Eq. (47) includes geometric factor introduced by the previously mentioned contact situation (e.g., a geometric factor that transforms Eq. (45) to (46)). The net volumetric heat term is a summation between the heat generation and the heat dissipation acting on the same cell, which can be expressed as:

\[ Q_{net}''' = Q_{gen}''' - Q_{dis}''' \]
\[ Q_{\text{net}}''' = q''' \cdot f_v - A_v h_m(T_{ss \in} - T_b) \cdot f_v \] (48)

On the right-hand side of (48), the first term is the energy production within the buffer layer, and the second term represents the energy dissipation through sub-channel fluid convection. The heat dissipation term is equivalent to part of the external source term taken from main T/H module’s energy equation. The \( f_v \) is a geometric factor added to preserve the energy balance at the buffer layer, which is defined by the volume ratio between the buffer layer and the equivalent fuel that can be written as:

\[ f_v = \frac{R_{f,\text{out}}^2 - R'^2}{R_{f,\text{out}}^2 - R_{f,\text{in}}^2} \] (49)

The Inter-HT Module will iterate upon Eq. (47) with the assistance of mesh baffles that are used to store interface B.C. described in Eq. (46). In OpenFOAM, the mesh baffles are additional internal boundaries created to separate different mesh regions. These internal boundaries can also be equipped with special interface conditions that manipulate information passed through the baffles [18]. In addition to the interface baffles, this module also implements adiabatic baffles in both axial and radial direction for cases in which symmetry needs to be applied or to ensure zero heat flux when needed. Figure 15 presents how mesh baffles will be implemented onto a reduced-geometry supercell model, in which the red lines represent the interface baffle, and the blue lines represent the inner-element adiabatic baffles. In addition to these baffles, the module also introduces adiabatic baffles/plates at each axial layer to ensure OpenFOAM treats each axial layer as a 2-D
problem. Finally, Figure 16 provides an overlook of all baffles implanted into the Inter-HT Module.

Figure 15. Reduced-geometry supercell models: (a) full-order vs. (b) coarse-mesh.

Figure 16. Inter-HT Module sample mesh model

3.3 Neutron Diffusion Module
The objective of the neutron diffusion module is to determine the power distribution for the T/H module. The neutronic solution relies on a traditional steady-state multi-group diffusion equation under $P_1$ approximation:

$$-\nabla \cdot D_i \nabla \phi_i + \Sigma a_i \phi_i + S_{sink_i} = \frac{\chi_i}{k_{eff}} S_{fission_i} + S_{scct_i}$$  \hspace{1cm} (50)

where:

- $D_i$ Neutron diffusion coefficient (m)
- $k_{eff}$ Effective multiplication factor
- $S_{fission}$ Explicit fission source ($\frac{1}{m^3s}$)
- $S_{scct}$ Explicit scattering source ($\frac{1}{m^3s}$)
- $S_{sink}$ Scattering sink ($\frac{1}{m^3s}$)
- $\phi_i$ Neutron flux for energy group $i$ ($\frac{1}{m^2s}$)
- $\chi_i$ Neutron yield for energy group $i$
- $\nu$ Average number of neutrons per fission
- $\Sigma_f$ Fission cross-section
- $\Sigma_{s_i \rightarrow j}$ Scattering cross-section from energy group $i$ to $j$

The sink term $S_{sink_i}$, as well as the fission $S_{fission_i}$ and scattering $S_{scct_i}$ source terms can be further expanded as:

(Scattering Sink) \hspace{1cm} S_{sink_i} = \sum_{j \neq i} \Sigma_{s_i \rightarrow j} \phi_i  \hspace{1cm} (51)

(Explicit fission source) \hspace{1cm} S_{fission_i} = \sum_{j \neq i} \nu \Sigma_f \phi_j \hspace{1cm} (52)
(Explicit scattering source) \[ S_{\text{scit}} = \sum_{j \neq i} \Sigma_{s_{j-i}}(\phi_j) \] (53)

The solution approach relies on the power iteration technique. During the iterations \( n \), the effective multiplication factor \( (k_{\text{eff}}) \) is updated using the ratio of power between the absolute target/nominal power and the iterate calculated power given as:

\[
k_{\text{eff}}^n = \frac{P_{\text{total}}^n}{1 - k_{\text{eff}}^{n-1} P_{\text{target}}} = k_{\text{eff}}^{n-1} \frac{\sum_g \int \epsilon_g^n(r) \Sigma_{f_g}^n(r) \phi_g^n(r) dV}{P_{\text{target}}} \tag{54}\]

where \( P_{\text{target}} \) represents the volume integrated target power and \( P_{\text{total}} \) is the calculated total power overall volume \( (V) \) at the current iterative step. The subscript \( g \) represents the energy group and the superscript \( n \) represents the iteration index. The integration is performed for the source term that includes energy per fission \( (\epsilon_g) \), the fission macroscopic cross-section \( (\Sigma_{f_g}) \) and the flux \( (\phi_g) \) summed over all the groups \( g \).

The cross sections used by the neutron diffusion module can be pre-generated by any external code, such as the Monte Carlo-based, SERPENT, code. The current implementation also supports a duo reference-perturbed cross-section formalism for reactivity feedback calculations. This simple relation allows to interpolate cross sections based on a higher or a lower T/H condition \( (\text{e.g., fuel temperature and coolant density}) \) with respect to the nominal core state. In the implemented function, a linear interpolation scheme is used for coolant density feedback, and a square-root-based scheme is used for fuel temperature feedback. Eqs. (55) – (57) display the feedback coefficient \( (\alpha_i) \) and cross
section (Σ) interpolation scheme for fuel temperature (T) and coolant density (ρ) reactivity feedback calculations.

For fuel temperature feedback:

\[ \alpha_{fuel} = \frac{\Sigma(T_{ref}) - \Sigma(T_{pert})}{\sqrt{T_{ref}} - \sqrt{T_{pert}}} \]  \hspace{1cm} (55)

For coolant density feedback:

\[ \alpha_{cool} = \frac{\Sigma(\rho_{ref}) - \Sigma(\rho_{pert})}{\rho_{ref} - \rho_{pert}} \]  \hspace{1cm} (56)

The cross sections for the overall feedback when the actual perturbation (T, ρ) is known can be written as:

\[ \Sigma(T, \rho) = \alpha_{fuel}(\sqrt{T_{ref}} - \sqrt{T}) + \alpha_{cool} \cdot (\rho_{ref} - \rho) + \Sigma(T_{ref}, \rho_{ref}) \]  \hspace{1cm} (57)

3.3.1 Albedo Boundary Conditions

The current implementation of the neutron diffusion module includes a customized albedo boundary for each group. The boundary implementation is similar to the one embedded in GeN-Foam but does not account for the SP₃ correction [38]. The albedo coefficient \( \alpha_g \) for each group at the boundary is defined as:
\[ \alpha_g(r) = \frac{f_g^-(r)}{f_g^+(r)} \text{ for } r \in \text{Wall}_l \] (58)

Using the P₁ derivation for current and Fick’s Law [39], the neutron flux at albedo boundary can be determined by evaluating the following correlation:

\[ D_g(r) \nabla \phi_g(r) + \gamma(r) \phi(r) = 0 \text{ for } r \in \text{Wall}_l \] (59)

where \( \gamma(r) \) is defined as

\[ \gamma(r) = \frac{1 - \alpha(r)}{2 + \alpha(r)} \] (60)

In the current study, the albedo coefficients were used to replace the actual modeling of surrounding reflectors. This greatly simplifies the treatment of heterogeneous effects typically associated with generating the diffusion coefficient. If vacuum boundary conditions are required at the boundary, then the albedo will be set as \( \alpha = 0 \) (\( \gamma = 0.5 \)). In a case the boundary conditions rely on zero leakage, the albedo coefficients will be set to unity (\( \gamma = 0.0 \)).

### 3.4 Iterative Strategy in NTPSteadyFOAM

The NTPSteadyFOAM package consists of many modules designed to model and capture either single physics or multiphysics effects in a given NTP reactor-core. The main intention was to create a package with the ability to turn on/off any physics. This, however, requires the iterative strategy of each module to be dependent on the coupling situation.
This section will present the iterative strategy for the main T/H module, Inter-HT Module, and Neutronic Module. Finally, a coupling strategy that combines all the modules will also be discussed here.

3.4.1 Main T/H Module

As previously discussed, the Main T/H Module iterates upon simplified 1-D NS equations of mass, momentum, and energy with the assistance of various sub-functions (e.g., sub-structure finite-difference solver, Nusselt’s model for convective heat transfer, and temperature-dependent thermophysical properties. Figure 17 shows a simplified iterative strategy for a single sub-element analysis. The simulation starts with reading the input boundary conditions, element types, and sub-structure parameters for the finite-difference sub-functions. After reading the thermophysical properties, the solver will iterate on the NS equations for the FE and solve pressure, velocity, temperature, and density. For the ME region, the module will first solve the supply channel problem, where the solution will provide inlet velocity, temperature, pressure, and inner fuel surface temperature for the return channel. Then, the solver will model the return channel in the same manner as FE. The simulation will continue until the convergence criteria are satisfied. In NTPSteadyFOAM, the convergence criteria are categorized into local convergence and global convergence. The local convergence is reached when the maximum residual is below a certain value. The global convergence is satisfied when local convergence from all equation sets is reached.
3.4.2 Iterative Strategy of the Inter-elemental Heat Transfer Module

It should be noted that the Inter-HT Module is the only module that cannot be executed by itself. The purpose of this module is to supplement the main T/H module in predicting sub-element temperatures across different core regions. Therefore, it will not be sensible for the package to execute Inter-HT Module without updating the sub-structure fuel and coolant temperature. Figure 18 shows a simplified interaction diagram for solving two elements that are adjacent to each other. It is worth noting that NTPSteadyFOAM uses the OpenFOAM built-in mesh interpolation function to pass information between modules. For the illustrated case, the iterative procedure between Inter-HT Module and Main T/H
Module is based on the temperature and heat flux information generated using different B.Cs. The procedure starts with a zero-boundary-heat-flux \((q''_b)\) B.C., in which the T/H solver will update the sub-structure outer-edge temperature \((T_{f,\text{out}})\) and net volumetric heat \((Q_{\text{net}})\) as initial condition for Inter-HT Module. The Inter-HT Module will then solve for \(T_{f,\text{out}}\) and return the average outer-edge temperature at each sub-element to the main T/H module. At this point, the finite-difference sub-function will use the average temperature as fixed temperature B.C. and return \(Q_{\text{net}}\) back to the Inter-HT Module. Finally, the inter-elemental solver will once again solve for \(T_{f,\text{out}}\) and use Fourier heat equation \((q'_{b} = -k\nabla T)\) to calculate the total heat flux coming from six interface boundaries. The value of total heat flux will be used as the B.C. for finite-difference sub-function at the next iteration.

**Figure 18. Main T/H to Inter-HT modules iterative strategy overview.**
3.4.3 Neutron Diffusion Module Iterative Strategy

The Neutron Diffusion Module is executed in a separated mesh domain where extra components such as reflectors and reactor baffles can be modelled without the need to align with the T/H mesh domain. Figure 19 summarizes the iterative strategy for the Neutron Diffusion Module under single physics operation. The iteration will always start from reading the cross-section data from the reference (nominal) reactor state, where the cross-section set is provided (or assigned) for different zones and components. To account for the reactivity feedback at least two additional perturbed cross-section sets corresponding to a higher and lower reactor state (in terms of temperature or density) must be provided. The neutron diffusion module will then apply the cross-section data and solve for the neutron flux in each energy group. Finally, the solver will determine the power distribution and update $k_{eff}$ until the fission source is converged.

![Figure 19. Neutron diffusion module iterative strategy overview.](image-url)
3.4.4 Full Coupled Package

Figure 20 shows the full coupling scheme adopted for NTPSteadyFOAM. The simulation starts with an initial one-way coupling between the neutronic and T/H modules, where the neutron diffusion solution uses fixed cross-section values corresponding to the initially provided temperature and density distributions. Additionally, the main T/H module will first obtain the solution for individual elements without considering inter-elemental heat transfer. The purpose of this procedure is to provide a sensible initial guess for the full coupling iteration and avoid numerical instabilities if too many parameters are updated simultaneously (e.g., cross-sections and thermal properties). The coupling scheme continues with updating T/H properties and cross sections. The latter are used by the neutron diffusion solver to update the power distribution. The solver will then go through the iterative strategy between the main T/H and Inter-HT Modules with the iterative strategy introduced in Figure 18. The full coupling scheme is executed until both neutronic (e.g., power and $k_{\text{eff}}$) and T/H parameters (e.g., temperature and velocity fields) satisfy the global convergence criteria.
Figure 20. NTPSteadyFOAM full coupling scheme.
CHAPTER 4.  CHT MODELS VERIFICATION AND VALIDATION

This chapter will perform series of sensitivity studies and benchmark the high-resolution model against experimental data to verify and validate that the higher-order models are able to generate reference solutions for reduced-order models. The benchmark case will be based on data acquired from samples placed within a FE from the NRX-A6 experiment. Mesh dependency sensitivities studies are performed here for both axial and radial directions. The main purpose of this study is to validate the high-resolution model against the reference solution extracted from the NRX-A6 report and demonstrate the fidelity of the CHT method.

Among all the experiments conducted during the NERVA program, the NRX-A6 experiment is the most documented. The primary objective of the NRX-A6 test was to achieve a 60-minute full-power operation (1120 MW), while measuring various reactivity effects. However, additional objectives, such as the evaluation of FEs thermal performance and flow characterization, were also achieved during the experiment [2]. The NRX-A6 core consists of repeating clusters; each contains six FEs surrounding a central unfueled element where thermocouples are mostly placed inside the unfueled elements. Figure 22 shows the configuration and the radial location of the “Station 1” thermocouple inside the NRX-A6 FE cluster. Several additional thermocouples were placed inside the FE embedded 1 inch near the entrance of the channel inlet [40]. The validation work presented in this section focuses on the experimental data acquired during the NRX-A6 operation EP-IIIA at 17800 seconds control room time [41]. The control drums’ position was
measured to be 115.3 degree with a total core power of 1167 MW. The corresponding steady-state core temperature was recorded using multiple thermocouples and thermal capsules at various locations of the core. A series of additional measurements such as exit gas temperature, pressure drop, and mass flow rate were also performed. Finally, several post-experiment calculations to predict the axial fuel and bulk temperature profiles were performed. The final report, which was also used in our analysis, stated that a very good agreement was achieved between the measured and calculated results [41].

![Figure 21. Typical NRX-A6 fuel cluster configuration.](image)

### 4.1 Mesh Structure for the CHT Model

The mesh adopted for the CHT FE and ME models in OpenFOAM use hybrid grids that consist of structured hexahedron cells and unstructured tetrahedron cells. The structured mesh can be found near the solid-fluid interface boundary, while the
unstructured mesh is used in the remaining of the solid and coolant domains. The goal of generating a hybrid grid is to gain better grid size control near the solid-fluid interface while preserving the simplicity of grid generation with complex geometry. Additionally, the hybrid grid design can decrease the number of mesh cells that contain high degree of non-orthogonality, which can lead to numerical instability in FVM [42].

The mesh in the current study is generated using Gmsh-4.0. Figure 22 shows the mesh for an NRX-A6 FE, which will be used to verify and validate the CHT solver. This figure shows mesh structure near the flow channel, in which the mesh is sub-divided into four different layers: (a) freestream layer, (b) fluid boundary layer, (c) solid fine mesh layer, and (d) solid layer. The freestream layer is relatively distant from the wall where turbulent flow can be modeled without near-wall treatment. To capture the turbulent wall effect, the fluid sublayer uses finer mesh with the size of the first interface cell center estimated to maintain a $y^+$ less than unity. Layers of fine mesh cell are introduced at the solid domain near the solid-fluid interface to mitigate the potential heat flux discontinuity at the interface when OpenFOAM CHT boundary condition is used [20]. Lastly, the solid layer is relatively coarse as the physics is only governed by thermal conduction.

**Figure 22. NRX-A6 FE High-resolution Mesh Model.**
4.2 Input and Boundary Conditions for the NRX-A6 Sample FE

The presented study models fluid flow as incompressible with temperature-dependent thermophysical properties. To analyze the flow in a more realistic manner, the thermophysical properties for gaseous $H_2$ are directly taken from data reported by NASA [43]. However, for simplicity in the implementation, the fluid thermophysical properties are assumed to be only temperature dependent. As the propellant experience different operational pressure in the different elements (i.e., ME and FE), the temperature-dependent sets are generated for average pressure values in each element. Again, it must be pointed out that the variation of properties in each unique element due to pressure variation is not accounted for. This is merely a simplification that was adopted to ease the database implementation and integration. Yet, as the pressure losses within the FE are indeed small, the pressure variation effects have negligible impact (i.e., second order) on the thermophysical properties of the gaseous $H_2$ [43].

The NRX-A6 utilizes $UC_2$ as its primary fuel material, in which the thermal conductivity of $UC_2$ is estimated using multiple sources [44] [45]. The volumetric power profile presented in Figure 23 relies on the NRX-A6 operation EP-IIIA and was obtained from the data recorded in the ELM Program [46]. The total core power level was measured to be 1167 MW [41] and the thermal power per FE is estimated to be 69.1 kW.

Table 3 to Table 5 present OpenFOAM’s numerical solution scheme, FE model general parameters, and CHT solver’s boundary conditions, respectively. In this simulation, the coolant flow is assumed to be fully developed at the entrance of each
channel. For a typical steady-state pressure-linked CFD problem with internal flow, the velocity and temperature are usually fixed at the inlet while the pressure is fixed at the outlet.

![Graph](image)

**Figure 23.** Axial power profile for the sample FE model.

**Table 3.** Control parameters within the solution scheme.

<table>
<thead>
<tr>
<th>Description</th>
<th>Settings</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>chtMultiRegionSimpleFoam</td>
</tr>
<tr>
<td>Algorithm</td>
<td>SIMPLE</td>
</tr>
<tr>
<td>Relaxation factor</td>
<td>$U: 0.1 \mid h, k, \epsilon: 0.3$</td>
</tr>
<tr>
<td>Turbulence model</td>
<td>Standard $k - \epsilon$</td>
</tr>
<tr>
<td>Simulation Type</td>
<td>Steady-State</td>
</tr>
<tr>
<td>Gradient Scheme</td>
<td>Gauss linear</td>
</tr>
<tr>
<td>Divergence Scheme</td>
<td>Gauss limited linear</td>
</tr>
<tr>
<td>Laplacian Scheme</td>
<td>Gauss linear orthogonal</td>
</tr>
<tr>
<td>Interpolation Scheme</td>
<td>Linear</td>
</tr>
<tr>
<td>Residual criteria for all fields</td>
<td>1.00E-07</td>
</tr>
</tbody>
</table>

**Table 4.** FE General Parameter.

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parameter</td>
<td>Value</td>
<td></td>
</tr>
<tr>
<td>-----------</td>
<td>-----------</td>
<td></td>
</tr>
<tr>
<td>Inlet Bulk coolant temperature ($T_b$)</td>
<td>127.8 K</td>
<td></td>
</tr>
<tr>
<td>Mass flow rate per FE ($\dot{m}$)</td>
<td>0.019 kg/s</td>
<td></td>
</tr>
<tr>
<td>Inlet Pressure (P)</td>
<td>5.111 MPa</td>
<td></td>
</tr>
<tr>
<td>Number of flow channels</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>Flow channel radius ($R_{flow}$)</td>
<td>0.117 cm</td>
<td></td>
</tr>
<tr>
<td>Fuel flat-to-flat distance</td>
<td>1.902 cm</td>
<td></td>
</tr>
<tr>
<td>Fuel height</td>
<td>132 cm</td>
<td></td>
</tr>
</tbody>
</table>

Table 5. CHT solver boundary conditions.

<table>
<thead>
<tr>
<th>Fields</th>
<th>Fluid Domain</th>
<th>Solid Domain</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>T</strong> (Temperature)</td>
<td>Inlet</td>
<td>Outlet</td>
</tr>
<tr>
<td>fixedValue 127.8 K</td>
<td>zeroGradient</td>
<td>turbulentTemperature CoupledBaffleMixed</td>
</tr>
<tr>
<td>mapped (avg. 24.978 m/s)</td>
<td>zeroGradient</td>
<td>no slip</td>
</tr>
<tr>
<td>calculated</td>
<td>calculated</td>
<td>calculated</td>
</tr>
<tr>
<td>$P_{rgh}$ (Dynamic pressure)</td>
<td>zeroGradient</td>
<td>fixedMean 4.13 MPa zeroGradient</td>
</tr>
<tr>
<td>mapped setAverage false</td>
<td>zeroGradient</td>
<td>kqRWallFunction</td>
</tr>
<tr>
<td>turbulentMixingLength</td>
<td>zeroGradient</td>
<td>epsilonWallFunction</td>
</tr>
<tr>
<td>DissipationRateInlet</td>
<td>zeroGradient</td>
<td>nutkWallFunction</td>
</tr>
<tr>
<td>mapped setAverage false</td>
<td>zeroGradient</td>
<td>alphatJayatillekeWallFunction</td>
</tr>
<tr>
<td>$\nu_t$ (Turbulent viscosity)</td>
<td>calculated</td>
<td>calculated</td>
</tr>
<tr>
<td>$\alpha_t$ (Turbulent thermal diffusivity)</td>
<td>calculated</td>
<td>calculated</td>
</tr>
<tr>
<td>$\rho$ (Fluid density)</td>
<td>fixedValue 9.319 kg/m$^3$ calculated calculated</td>
<td></td>
</tr>
</tbody>
</table>

4.3 CHT Solver Mesh Sensitivity Study

The current section presents only a selected sample of sensitivity studies conducted to identify the mesh requirements to achieve accurate and converged results in both axial
and radial directions. Here, the number of axial layers was varied from 66 to 528 equal height layers. The verification process is based on the equivalent model as both full and equivalent models share the same channel flow parameters. Figure 24 shows the schematics of OpenFOAM’s equivalent model generated for the verification work. The inlet boundary conditions as well as all thermophysical properties for the verified model are identical to the full FE model. The results for the axial mesh sensitivity study are shown in Table 6. The radial mesh sensitivity study is primarily focused on perturbing the value of $y^+$ in the center of the first interface cell. All the examined cases rely on identical boundary conditions (e.g., inlet velocity and boundary wall functions). The performance in respect to the axial mesh dependence is monitored through the outlet Reynolds number, outlet fluid temperature, inlet fluid pressure, and maximum fuel temperature. The mesh sensitivity results for the radial direction are presented in Table 7. The red-color-highlighted rows in both Table 6 and 7 denote the mesh parameters that are adopted for the remainder of the high-resolution OpenFOAM simulations.

Figure 24. Equivalent FE model generated for CHT solver mesh sensitivity study.
Table 6. Mesh sensitivity study for FE in axial direction.

<table>
<thead>
<tr>
<th>Axial cell size (m)</th>
<th>No. of axial layers</th>
<th>Inlet P (MPa)</th>
<th>Outlet mean Reynolds number, Re ($\times 10^4$)</th>
<th>Outlet mean fluid T (K)</th>
<th>Max fuel T (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.00E-02</td>
<td>66</td>
<td>5.111</td>
<td>1.402</td>
<td>2521</td>
<td>2605</td>
</tr>
<tr>
<td>1.00E-02</td>
<td>132</td>
<td>5.111</td>
<td>1.404</td>
<td>2521</td>
<td>2606</td>
</tr>
<tr>
<td><strong>5.00E-03</strong></td>
<td><strong>264</strong></td>
<td><strong>5.111</strong></td>
<td><strong>1.413</strong></td>
<td><strong>2534</strong></td>
<td><strong>2615</strong></td>
</tr>
<tr>
<td>3.33E-03</td>
<td>396</td>
<td>5.111</td>
<td>1.412</td>
<td>2533</td>
<td>2614</td>
</tr>
<tr>
<td>2.50E-03</td>
<td>528</td>
<td>5.111</td>
<td>1.411</td>
<td>2531</td>
<td>2614</td>
</tr>
</tbody>
</table>

Table 7. Mesh sensitivity study at FE flow channel boundary.

<table>
<thead>
<tr>
<th>First cell $y^+$ at inlet</th>
<th>Inlet fluid P (MPa)</th>
<th>Outlet mean Reynolds number, Re ($\times 10^4$)</th>
<th>Outlet mean fluid T (K)</th>
<th>Outlet fluid surface $T_s$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.294</td>
<td>5.645</td>
<td>1.5292</td>
<td>2400</td>
<td>2427</td>
</tr>
<tr>
<td><strong>0.823</strong></td>
<td><strong>5.620</strong></td>
<td><strong>1.5284</strong></td>
<td><strong>2402</strong></td>
<td><strong>2430</strong></td>
</tr>
<tr>
<td>1.177</td>
<td>5.606</td>
<td>1.5279</td>
<td>2403</td>
<td>2431</td>
</tr>
<tr>
<td>2.349</td>
<td>5.593</td>
<td>1.5280</td>
<td>2403</td>
<td>2431</td>
</tr>
<tr>
<td>4.698</td>
<td>5.583</td>
<td>1.5278</td>
<td>2403</td>
<td>2431</td>
</tr>
</tbody>
</table>

4.4 Validation of the CHT Solver

The validation work for the current study compares OpenFOAM CHT solutions to a post-calculated experimental data set reported by the NRX-A6 experiment. In this section, the numerical model is validated against steady-state fluid exit temperature and average axial fuel temperature data obtained from the Station 1 (See Figure 21)
thermocouple measurements. The channel exit and Station 1 temperature data were directly collected by thermocouples and the axial fuel temperature data was the result of a post-experimental calculation effort [47]. Table 8 presents the comparison between numerical predictions and thermocouple measurements, in which the core Station 1 data represents the average temperature recorded by multiple thermocouples inside the NRX core. Figure 25 and Table 9 present the results of the axial fuel hotspot temperature comparison between CHT and the experimental calculations. The validation results show good agreement in the propellant’s exit temperature with about 1.5% difference in channel inlet-to-outlet temperature gradient. For core Station 1 temperature comparison, the CHT model shows an over-prediction around 50 K over the measured data average. Finally, the comparison in average axial fuel temperature shows generally good agreement between experimental calculations and the adopted numerical models with a maximum difference of 7.3%.

Table 8. Comparison between CHT and experimental measurements.

<table>
<thead>
<tr>
<th></th>
<th>OpenFOAM CHT</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Channel Exit Temp. (K)</td>
<td>2536 (avg.)</td>
<td>2500 ± 28</td>
</tr>
<tr>
<td>Station 1 Temp. (K)</td>
<td>381</td>
<td>332 ± 22</td>
</tr>
</tbody>
</table>
Figure 25. Comparison of CHT and experimental average axial fuel temperature.

Table 9. Average fuel temperature distribution along the axial length predicted by OpenFOAM CHT and the experimental calculation.

<table>
<thead>
<tr>
<th>Axial position (m)</th>
<th>CHT (K)</th>
<th>Experiment (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>271</td>
<td>278</td>
</tr>
<tr>
<td>0.1</td>
<td>596</td>
<td>601</td>
</tr>
<tr>
<td>0.2</td>
<td>865</td>
<td>896</td>
</tr>
<tr>
<td>0.3</td>
<td>1090</td>
<td>1163</td>
</tr>
<tr>
<td>0.4</td>
<td>1304</td>
<td>1403</td>
</tr>
<tr>
<td>0.5</td>
<td>1563</td>
<td>1628</td>
</tr>
<tr>
<td>0.6</td>
<td>1804</td>
<td>1845</td>
</tr>
<tr>
<td>0.7</td>
<td>1997</td>
<td>2060</td>
</tr>
<tr>
<td>0.8</td>
<td>2166</td>
<td>2240</td>
</tr>
<tr>
<td>0.9</td>
<td>2319</td>
<td>2398</td>
</tr>
<tr>
<td>1.0</td>
<td>2439</td>
<td>2529</td>
</tr>
<tr>
<td>1.1</td>
<td>2521</td>
<td>2580</td>
</tr>
<tr>
<td>1.2</td>
<td>2567</td>
<td>2604</td>
</tr>
<tr>
<td>1.3</td>
<td>2589</td>
<td>2509</td>
</tr>
</tbody>
</table>
Overall, the OpenFOAM CHT’s validation work has demonstrated good agreement between the experimental data and the numerical model. The results from this study have also demonstrated the CHT method’s ability to produce a high-resolution model that can complement the experimental effort. Therefore, in the following chapters the CHT method will be used to generate reference solutions for the analysis for which experimental measurements are not available.
CHAPTER 5. RESULTS

This chapter presents the preliminary validation and verification (V&V) effort of the T/H and neutronic sub-modules within the NTPSteadyFOAM package. All the analyzed models rely on a modern HALEU NTP core investigated in the CoRE group at Georgia Institute of Technology [12]. The reference solutions for the T/H part are generated using the high-resolution CHT method, and the reference for the neutronic solutions are obtained using the Monte Carlo, SERPENT 2, code. The chapter begins with the description of the selected FE and ME models, followed by the V&V demonstration for each sub-module. The end goal of this chapter is to confirm the proper implementation of the sub-modules in the NTPSteadyFOAM package before applying the package to large-scale multiphysics demonstration (Chapter 6).

5.1 Description of Selected Models

The benchmarked NTP model had adopted some modifications of the FE and tie-tube configurations from the NERVA KIWI-B4E program [2]. Figure 26 describes the configuration for the adapted FE and ME models, respectively. The presented FE design consists of 37 flow channels, each containing a cladded layer to separate the fuel meat and the propellant hydrogen. The ME design contains two solid layers at the inner region and three solid layers at the outer region. The two regions are separated by the return channel. The T/H solutions in this study focused only on the active fuel height (1 m) for both elements. Table 10 and Figure 26 present schematics and detailed description of materials and dimensions.
The study uses the hydrogen gas thermophysical properties suggested by NASA [32], in which the hydrogen properties is, once again, assumed independent of pressure under sub-sonic flow conditions. The material properties for all regions can be found in Appendix A. Table 11 presents the inlet and the boundary conditions for both FE and ME. The benchmark model assumes power is only generated in the fuel meat, ZrH$_2$ layer, and the YSZ layer (See Figure 26 and Table 10 for layers’ locations), where the axial power profile is detailed in Figure 27.

![Figure 26. Benchmarked FE & ME Model Configurations.](image)

<table>
<thead>
<tr>
<th>Location index</th>
<th>Dimensions (cm)</th>
<th>Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>FE1</td>
<td>0.389</td>
<td></td>
</tr>
<tr>
<td>FE2</td>
<td>0.132</td>
<td></td>
</tr>
<tr>
<td>FE3</td>
<td>0.147</td>
<td></td>
</tr>
<tr>
<td>(1)</td>
<td>[0, 0.200]</td>
<td>$Mo30W - UN$</td>
</tr>
<tr>
<td>(2)</td>
<td>[0.200, 0.257]</td>
<td>$Mo30W$</td>
</tr>
<tr>
<td>(3)</td>
<td></td>
<td>$H_2$ (Gaseous)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Location index</th>
<th>Dimensions (cm)</th>
<th>Material Specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>[0, 0.200]</td>
<td>Supply $H_2$ (Gaseous)</td>
</tr>
<tr>
<td>(b)</td>
<td>[0.200, 0.257]</td>
<td>Zircaloy – 4</td>
</tr>
</tbody>
</table>
Table 11. FE & ME Operating Conditions.

<table>
<thead>
<tr>
<th>Fuel Element</th>
<th>Moderating Element (supply channel inlet)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Temperature</td>
<td>300 K</td>
</tr>
<tr>
<td>Inlet Pressure</td>
<td>7.0 MPa</td>
</tr>
<tr>
<td>Mass Flow Rate</td>
<td>0.054042 kg/s</td>
</tr>
</tbody>
</table>

Figure 27. Benchmark Elements Power Profile.

5.1.1 High-resolution CHT Model Setup
Both the main T/H and Inter-elemental-HT modules were compared against the higher-order CHT models that were considered as the reference solution. The CHT model follows the discretization mechanism introduced in the previous chapter. Figure 28 presents snapshots of the hybrid mesh structures utilized by the FE and ME models. Figure 28(A) also shows the sub-division of the FE mesh structure into four different layers: (a) freestream layer, (b) fluid boundary layer, (c) solid fine mesh layer, and (d) solid layer. A similar representation is shown for the mesh structure adopted for the ME. The CHT solver simulates both models using the same solution scheme and boundary types described in the previous chapter (See Table 3 and 5). However, the input and boundary values rely on unique operating conditions described in Table 11. The propellant conditions (i.e., pressure, temperature, and mass flow rate) are continues. More specifically, the exit conditions from the supply channel are identical to the inlet conditions to the return channel. Form losses are not accounted for in the current NTPSteadyFOAM package.
5.2 Single Element Benchmark Study

This section focuses on validating the main T/H solution against the reference model. Section 5.2.1 begins with sensitivity studies for both FE and ME, in which the axial mesh-independency analyses are conducted in the finite volume, while the radial mesh-independency study uses the finite-difference domain. The results from the sensitivity studies will determine the mesh requirements for the remainder of the coarse-mesh T/H simulations. Finally, Section 5.2.2 compares NTPSteadyFOAM against the CHT model by modeling both the FE and ME under adiabatic boundary conditions.

5.2.1 Mesh Sensitivity Studies
Table 12-15 present the results of the mesh-independency study for the coarse-mesh model in the axial and radial direction, where the red-color-highlighted row indicates the selected mesh values for the subsequent simulations. The sensitivity studies vary the number of axial layers from 30 to 200 using equal height layers, and 10 to 25 layers in the radial direction. The sensitivity studies relied on the most limiting location (radially and axially) exhibiting the highest power peaking value. These analyses are reported in Table 12-15, and they set the axial and radial layers to be used in the subsequent comparisons. Mesh dependency studies for the reference CHT model followed considerations described in Section 4.3 and these can be found in Appendix B.

Table 12. Coarse-mesh FE model sensitivity study in axial direction.

<table>
<thead>
<tr>
<th>Axial cell size (m)</th>
<th>No. of axial layers</th>
<th>Outlet mean Reynolds number</th>
<th>Outlet mean fluid $T_b$ (K)</th>
<th>Max fuel T (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.33E-02</td>
<td>30</td>
<td>129374</td>
<td>153.561</td>
<td>236.174</td>
</tr>
<tr>
<td><strong>2.00E-02</strong></td>
<td>50</td>
<td><strong>129377</strong></td>
<td><strong>236.487</strong></td>
<td></td>
</tr>
<tr>
<td>1.00E-02</td>
<td>100</td>
<td>129383</td>
<td>153.526</td>
<td>236.174</td>
</tr>
<tr>
<td>5.00E-03</td>
<td>200</td>
<td>129397</td>
<td>153.489</td>
<td>236.216</td>
</tr>
</tbody>
</table>

Table 13. Coarse-mesh ME model sensitivity study in axial direction.

<table>
<thead>
<tr>
<th>Axial cell size (m)</th>
<th>No. of axial layers</th>
<th>Outlet mean Reynolds number</th>
<th>Supply ch. outlet $T_b$ (K)</th>
<th>Return ch. outlet $T_b$ (K)</th>
<th>Max fuel T (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.33E-02</td>
<td>30</td>
<td>129374</td>
<td>153.561</td>
<td>236.174</td>
<td></td>
</tr>
<tr>
<td><strong>2.00E-02</strong></td>
<td>50</td>
<td><strong>129377</strong></td>
<td><strong>236.487</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.00E-02</td>
<td>100</td>
<td>129383</td>
<td>153.526</td>
<td>236.174</td>
<td></td>
</tr>
<tr>
<td>5.00E-03</td>
<td>200</td>
<td>129397</td>
<td>153.489</td>
<td>236.216</td>
<td></td>
</tr>
</tbody>
</table>
Table 14. FE model sensitivity study in radial direction (at fuel meat layer).

<table>
<thead>
<tr>
<th>Radial grid size (m) (1 \cdot 10^{-5})</th>
<th>No. of radial layers</th>
<th>Channel interface (T_s) (K)</th>
<th>Clad-to-fuel interface (T_{int}) (K)</th>
<th>Fuel outer-edge (T) (K)</th>
<th>Fuel average (T) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.4473</td>
<td>10</td>
<td>2036.38</td>
<td>2050.17</td>
<td>2097.07</td>
<td>2083.3</td>
</tr>
<tr>
<td><strong>4.2982</strong></td>
<td><strong>15</strong></td>
<td><strong>2036.38</strong></td>
<td><strong>2050.17</strong></td>
<td><strong>2097.11</strong></td>
<td><strong>2083.36</strong></td>
</tr>
<tr>
<td>3.22365</td>
<td>20</td>
<td>2036.38</td>
<td>2050.17</td>
<td>2097.12</td>
<td>2083.38</td>
</tr>
<tr>
<td>2.57892</td>
<td>25</td>
<td>2036.38</td>
<td>2050.17</td>
<td>2097.13</td>
<td>2083.39</td>
</tr>
</tbody>
</table>

Table 15. ME model sensitivity study in radial direction (at ZrH_2 layer).

<table>
<thead>
<tr>
<th>Radial grid size (m) (1 \cdot 10^{-4})</th>
<th>No. of radial layers</th>
<th>Channel interface (T_s) (K)</th>
<th>Clad-to-fuel interface (T_{int}) (K)</th>
<th>Fuel outer-edge (T) (K)</th>
<th>Fuel average (T) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.250</td>
<td>10</td>
<td>92.0838</td>
<td>112.865</td>
<td>149.442</td>
<td>149.428</td>
</tr>
<tr>
<td>0.833</td>
<td>15</td>
<td>91.9826</td>
<td>112.727</td>
<td>149.4e41</td>
<td>149.566</td>
</tr>
<tr>
<td><strong>0.625</strong></td>
<td><strong>20</strong></td>
<td><strong>91.9498</strong></td>
<td><strong>112.682</strong></td>
<td><strong>149.453</strong></td>
<td><strong>149.61</strong></td>
</tr>
<tr>
<td>0.500</td>
<td>25</td>
<td>91.9353</td>
<td>112.662</td>
<td>149.44</td>
<td>149.63</td>
</tr>
</tbody>
</table>

5.2.2 Single Element V&V

The code-to-code verification between NTPSteadyFOAM main T/H module and CHT focuses on comparing the T/H conditions that are important in determining the NTP’s engine performance. For example, exit temperature and velocity impact the engine’s specific impulse and thrust, while ME’s outlet temperature affects the expander cycle performance [12]. This section presents the T/H results obtained for individual FE and ME using both fine and coarse-mesh simulations.

To ensure the finite-difference sub-solver is implemented correctly, the analysis begins by comparing the numerical finite-difference 1-D solution against an analytically derived one. Figure 29 shows the radial temperature profile within an annular pin
containing two layers with different materials and thus properties. The result of the comparison shows a very good agreement between the numerical and analytical models.

![Graph showing radial fuel temperature comparison](image)

**Figure 29. Comparison between the finite-difference and analytical solutions in FE.**

Figure 30 presents the verification analysis conducted for a single FE under adiabatic conditions. In this study, the convective heat transfer modeling relied on Gnielinski’s Nusselt model with a smooth sub-substructure surface assumption. Both simulations use identical input and boundary values taken from Section 5.1. The bulk coolant temperature ($T_b$) and mean velocity ($U$) distribution in Figure 30(a) and 30(b) indicate excellent agreement between the two methods. However, the results presented in Figure 30(a), (b), and (c) show a consistent over-prediction in the surface and average fuel temperature distributions. Such a deviation in fuel temperature could result from the geometric difference between the equivalent and the explicit configuration of FE. Finally,
Table 16 presents the percentage difference between NTPSteadyFOAM’s T/H and the reference solution taken at various locations of interest.
Figure 30. Code-to-code comparison in FE axial distributions: (a) coolant ($T_b$) and surface ($T_s$) temperatures, (b) mean velocity, (c) fuel outer-edge temperature, and (d) fuel temperature.
Table 16. Percentage difference between codes taken at FE location of interest.

<table>
<thead>
<tr>
<th></th>
<th>% Difference</th>
<th>Magnitude difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlet temperature</td>
<td>0.25</td>
<td>6.91 K</td>
</tr>
<tr>
<td>Outlet velocity</td>
<td>0.024</td>
<td>0.11 m/s</td>
</tr>
<tr>
<td>Surface temperature</td>
<td>8.46</td>
<td>57.70 K</td>
</tr>
<tr>
<td>Peak Fuel temperature</td>
<td>3.04</td>
<td>87.66 K</td>
</tr>
<tr>
<td>Maximum average fuel</td>
<td>12.15</td>
<td>98.60 K</td>
</tr>
<tr>
<td>Temperature deviation</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The following part of the study presents benchmark results for a single ME under adiabatic conditions. Figure 31 presents the average axial T/H profiles. The convective heat transfer relied on Taylor’s Nusselt number. The $T_s$ inner/outer notation in Figure 31(c) refers to the inner and outer surface temperature within the ME return channel and the $T_s$ supply denotes the supply channel surface temperature. The results presented here show a generally good agreement. Table 17 presents the percentage difference taken at the supply and return channel outlet as well as at the outer-edge temperature.
Figure 31. Code-to-code comparison of average axial: (a) coolant ($T_b$) temperature, (b) mean velocity magnitude, (c) flow channel surface ($T_s$) temperature, and (d) ME YSZ outer-edge temperature.
Table 17. Percentage difference between codes taken at ME location of interest.

<table>
<thead>
<tr>
<th></th>
<th>% Difference</th>
<th>Magnitude difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Supply channel outlet temperature</td>
<td>0.911</td>
<td>0.742 K</td>
</tr>
<tr>
<td>Supply channel outlet velocity</td>
<td>0.905</td>
<td>0.466 m/s</td>
</tr>
<tr>
<td>Return channel outlet temperature</td>
<td>1.540</td>
<td>2.40 K</td>
</tr>
<tr>
<td>Return channel outlet velocity</td>
<td>1.497</td>
<td>0.312 m/s</td>
</tr>
<tr>
<td>Maximum ME outer-edge temperature discrepancy</td>
<td>1.944</td>
<td>4.692 K</td>
</tr>
</tbody>
</table>

5.3 Verification of Two Adjacent Elements

This section details the computational efforts focused on inter-elemental heat transfer enabled by coupling the main T/H and inter-elemental HT modules. This section will demonstrate the importance and effects of the heat transfer occurring between the fuel and moderating elements. The simulations containing two different elements will be performed using both NTPSteadyFOAM and CHT solvers. The latter will be treated as the high-resolution reference solution.

The studies reported here begin with a simple FE-to-FE 1-D heat transfer problem to validate that the implemented finite-difference module predicts the correct radial temperature distribution across two conjugated sub-structures. The bottom part of Figure 32 demonstrates two connected equivalent FEs containing different volumetric power ($q_1'' = 5 \cdot 10^9 \frac{W}{m^3}$ and $q_2'' = 4 \cdot 10^9 \frac{W}{m^3}$). Given the inner edge fuel temperature on both
sides, Figure 32 compares the radial temperature distributions predicted by the finite-difference models against the analytical derived solutions in each region. As shown in this figure, a good agreement is obtained with a maximum error of 0.1%.

Figure 32. Comparison between the finite-difference sub-solver and analytical solution over two conjugated equivalent FE models.

Next, we proceed with analyzing the FE-to-ME heat transfer with both the NTPSteadyFOAM package and the CHT solver. The first analyzed case relies on a two-elements configuration that consists of a single FE adjacent to a single ME. To decrease the computational burden for the CHT model, the high-resolution mesh model uses one-twelfth of a full-order model with symmetry boundary conditions to simulate heat transfer across sub-elements. Figure 33 presents the reduced-geometry high-resolution model
adopted by the CHT solver. The inlet boundary conditions (e.g., temperatures) are set as fixed values. In reality, the inlet conditions to FE will depend on the outlet conditions of the ME, however this requires integrating the core T/H analysis with the complete system analysis package, which was not the focus of the current dissertation.

Figure 33. Reduced-geometry high-resolution mesh model for single FE-ME heat transfer analysis.

Figure 34 and 35 present the result of the FE-to-ME heat transfer simulation. The bulk coolant temperature and mean velocity show good agreement between the two codes. However, NTPSteadyFOAM slightly overpredicts the surface temperature near the inlet of ME supply and return channel (See Figure 34(c)). In addition to the geometrical treatment, the deviation can be attributed to the use of empirical convective correlation. This discrepancy is consistent with similar work recently performed on the subject [48]. Similarly, NTPSteadyFOAM’s prediction of the surface and fuel average temperatures in the FE shown in Figure 35 also shows conservative overprediction. In general, however, the FE-to-ME heat transfer demonstrate that the NTPSteadyFOAM package is a reliable
and efficient package that is able to capture the T/H effects as well as the inter-elemental heat transfer between different adjacent elements.
Figure 34. Comparison of ME’s axial profiles in FE-to-ME configuration: (a) coolant ($T_b$) temperature, (b) mean velocity magnitude, and (c) flow channel surface ($T_s$) temperature.
Figure 35. Comparison of FE’s axial profiles in FE-to-ME configuration: (a) coolant ($T_b$) and surface ($T_s$) temperature, and (b) FE-ME interface temperature.
In addition to comparing the axial temperature profile within FE and ME, the study also compares the radial temperature distribution within ME’s ZrH$_2$ moderator layer. Figure 36 details the radial temperature distribution taken at several axial locations with respect to the ME supply flow inlet. The radial temperature distribution within the ZrH$_2$ layer is well predicted by NTPSteadyFOAM. The latter indicates that the partial heat fluxes to the return and supply hydrogen regions are well predicted.

Figure 36. Radial temperature distribution in ZrH$_2$ compared at different axial layers. The green dash-line represents the boundary between the ZrH$_2$ inner edge and zircaloy-4 cladding outer-edge.
5.4 Supercell Analysis

The final verification step is to apply the coupled T/H-inter-elemental HT sequence to supercells configurations. The supercell simulations rely on multiple elements that can be found in a general NTP core. The results obtained with NTPSteadyFOAM will be compared against those obtained by the CHT solvers. The following section presents the simulations and results carried out for three types of ME-centered supercell configurations denoted as 6F0M, 4F2M, and 2F4M. The letters “F” and “M” denote the FE and ME respectively, while the number before the letter indicates the number of FE/ME that surround a central ME. Figure 37 presents the three supercell configurations used here.

Figure 37. Supercell configurations.

The main objective of this analysis is focused on comparing the results within the central ME as it is affected by the neighboring elements. To reduce the computational burden, the supercell configurations are modeled via a simplified reduced geometry. The latter relies on reducing the scale of the geometry into a single ME connected to six neighboring “chips”. Each chip represents a reduced-geometry sub-element with symmetry boundary conditions at the non-connected boundaries. For the simplicity of the demonstration, both the CHT and NTPSteadyFOAM assume no heat transfer between the
chips. Figure 38 details an example of the high-resolution reduced-geometry supercell used by the CHT solver compared to NTPSteadyFOAM’s coarse-mesh representation.

![Reduced-geometry supercell mesh models generated with: (left) high-resolution full-order mesh, and (right) NTPSteadyFOAM coarse-mesh.](image)

**Figure 38.** Reduced-geometry supercell mesh models generated with: (left) high-resolution full-order mesh, and (right) NTPSteadyFOAM coarse-mesh.

Figure 39 to Figure 42 present the benchmark results for the 4F2M and 2F4M supercells in a respective order. It should be noted that the 6F0M results will not be presented here because the simulation case is effectively identical to the single FE-to-ME analysis presented in Section 5.3. The results demonstrate that NTPSteadyFOAM has accurately predicted the thermal performance when compared to the CHT model’s prediction. As the number of fuel elements surrounding the central ME increases so does the total heat flux. NTPSteadyFOAM was able to accurately predict such an increase. As expected, there are some differences as our method relies on reduced-scale and reduced-order analysis, *e.g.*, the ME outlet temperature is underpredicted by 16 K in 4F2M and 21 K in 2F4M. Mostly, these discrepancies could be attributed to the heat transfer correlation...
applied within the NTPSteadyFOAM. The latter challenge can be mitigated if the CHT model is used to generate updated set of heat transfer correlations. This, however, was not included in the current research and should be pursued in future studies. Overall, Figure 39-42 and Table 18 show that accurate results can be obtained by the NTPSteadyFOAM package.

Figure 39. Propellant temperature distributions for 4F2M and 2F4M supercell configurations.
Figure 40. Propellant velocity distributions for 4F2M and 2F4M supercell configurations.

Figure 41. Surface temperature distributions for 4F2M and 2F4M supercell configurations.
Figure 42. Interface FE-ME surface temperature distributions for 4F2M and 2F4M supercell configurations.

Table 18. Summary of Supercell Analysis.

<table>
<thead>
<tr>
<th>Supercell models</th>
<th>CHT prediction</th>
<th>NTPSteadyFOAM prediction</th>
<th>Percentage difference (%)</th>
<th>Difference in magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>ME outlet temperature (K)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6F0M</td>
<td>476.4</td>
<td>459.2</td>
<td>3.666</td>
<td>17.1</td>
</tr>
<tr>
<td>4F2M</td>
<td>393.2</td>
<td>377.2</td>
<td>4.163</td>
<td>16.0</td>
</tr>
<tr>
<td>2F4M</td>
<td>298.9</td>
<td>277.8</td>
<td>7.328</td>
<td>21.1</td>
</tr>
<tr>
<td>ME outlet velocity (m/s)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6F0M</td>
<td>61.4</td>
<td>59.2</td>
<td>3.586</td>
<td>2.2</td>
</tr>
<tr>
<td>4F2M</td>
<td>49.3</td>
<td>49.0</td>
<td>0.596</td>
<td>0.3</td>
</tr>
<tr>
<td>2F4M</td>
<td>36.1</td>
<td>36.4</td>
<td>0.925</td>
<td>0.3</td>
</tr>
<tr>
<td>Maximum ME outer-edge temperature (K)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6F0M</td>
<td>2617.0</td>
<td>2766.0</td>
<td>5.533</td>
<td>148.9</td>
</tr>
<tr>
<td>4F2M</td>
<td>1944.3</td>
<td>2075.1</td>
<td>6.511</td>
<td>130.9</td>
</tr>
<tr>
<td>2F4M</td>
<td>1135.6</td>
<td>1211.2</td>
<td>6.440</td>
<td>75.6</td>
</tr>
</tbody>
</table>
5.5 Neutronic Verification

This section presents the code-to-code comparison between the diffusion module implemented in NTPSteadyFOAM and the Monet Carlo-based, SERPENT 2, code. In addition to providing the reference solution, SERPENT 2 was also used to generate two-group homogenized group constants. An explicit supercell model was used in SERPENT 2 for cross-section generation to preserve a realistic neutron spectrum.

Figure 43 demonstrates the explicit model and the full 3-D vertical stack modeled by both NTPSteadyFOAM and SERPENT 2. The figure depicts the axial and radial cross-section views. The full 3-D model (the physics is really modeled in 1-D) contains three regions: a central active core, an axial upper reflector, and a lower support plate. The homogenized active core region assumes an FE-centered supercell surrounded by six MEs (Figure 43). In order to obtain the macroscopic group-wise diffusion, fission, absorption, energy production, and scattering matrix, a 2-dimensional SERPENT 2 simulation was applied. The homogenized group constants for the axial reflector and support plate were obtained using a 3-dimensional SERPENT 2 simulation. These group constants are provided in Appendix C. For the benchmark simulation, NTPSteadyFOAM applies vacuum boundary conditions in the upper- and bottom-most axial boundaries and assumes no leakage (symmetry) conditions at the radial boundaries.
Similarly to the T/H results section, the neutronic analysis also begins with mesh sensitivity studies. Assuming an evenly distributed axial mesh size in each axial region, the sensitivity study focuses on the mesh dependency in $k_{\text{eff}}$, maximum neutron flux, and the maximum power peaking ratio. Table 19 details the results of the axial mesh sensitivity analysis. It must be pointed out that the statistical uncertainty on reactivity from SERPENT 2 was around 30 pcm.

**Table 19. Neutronic model axial mesh independency study (Red-color-highlighted row indicates selected mesh parameter).**

<table>
<thead>
<tr>
<th>Number of axial layers</th>
<th>Number of axial layer in each region [upper, active, lower]</th>
<th>$k_{\text{eff}}$</th>
<th>Reactivity (pcm)</th>
<th>Max. fast flux ($\phi_1$) $\frac{n}{m^2s}$</th>
<th>Max. thermal flux ($\phi_2$) $\frac{n}{m^2s}$</th>
<th>Max. power peaking</th>
</tr>
</thead>
<tbody>
<tr>
<td>22</td>
<td>[1 20 1]</td>
<td>1.20846</td>
<td>17250.3</td>
<td>1.55E+20</td>
<td>2.36E+19</td>
<td>1.83</td>
</tr>
<tr>
<td>27</td>
<td>[2 20 5]</td>
<td>1.21188</td>
<td>17483.7</td>
<td>1.51E+20</td>
<td>1.71E+19</td>
<td>1.79</td>
</tr>
<tr>
<td><strong>117</strong></td>
<td>[2 100 15]</td>
<td><strong>1.21365</strong></td>
<td><strong>17604.2</strong></td>
<td><strong>1.36E+20</strong></td>
<td><strong>1.57E+19</strong></td>
<td><strong>1.62</strong></td>
</tr>
<tr>
<td>234</td>
<td>[4 200 30]</td>
<td>1.21393</td>
<td>17623</td>
<td>1.36E+20</td>
<td>1.58E+19</td>
<td>1.61</td>
</tr>
<tr>
<td>468</td>
<td>[8 400 60]</td>
<td>1.21406</td>
<td>17631.9</td>
<td>1.36E+20</td>
<td>1.59E+19</td>
<td>1.61</td>
</tr>
</tbody>
</table>

For the benchmark comparison, the calculations assume that the 2 MW power is only generated within the active core region and not the axial reflector regions. Figure 44 and 45 present the results of neutronic simulations conducted using the two-group diffusion...
solver implemented in NTPSteadyFOAM. The results are then compared against SERPENT 2. The flux distribution reported in Figure 44 shows good agreement in both fast and thermal groups. Moreover, the fast-to-thermal flux ratio and the volumetric power profiles are both well predicted with a maximum error of 2.07% in flux ratio and 4.10% in power. Finally,

Table 20 compares the effective multiplication factor and the reactivity between two modes. In general, the neutronic benchmark study has shown good agreement between NTPSteadyFOAM and SERPENT 2 simulations.

Figure 44. Two-group axial flux distribution for single physics neutronic analysis.
Figure 45. Neutronic benchmark analysis with: (a) thermal-to-fast flux ratio, and (b) axial power distribution.

<table>
<thead>
<tr>
<th>$k_{\text{eff}}$</th>
<th>Reactivity (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SERPENT 2</td>
<td>1.21321</td>
</tr>
<tr>
<td>NTPSteadyFOAM</td>
<td>1.21365</td>
</tr>
<tr>
<td>pcm difference</td>
<td>-29.86</td>
</tr>
</tbody>
</table>
CHAPTER 6. DEMONSTRATION OF NTPSTEADYFOAM

The previous chapter has demonstrated NTPSteadyFOAM’s ability to accurately model heat transfer and neutron diffusion within sub-elements. The package was developed with a specific end-objective to apply this package on full core level analysis. This chapter focuses on demonstrating the coupled capability of all the sub-modules. An arbitrary sample miniature NTP core is used to demonstrate the full multiphysics capabilities of the package. Again, it must be pointed out that only neutronic and T/H feedback are included. However, future research could focus on adding other important feedback, such as the thermo-mechanics. The presented simulation begins with a simple one-way coupling T/H-neutronic model (referred as nominal state model) with no reactivity feedback calculation. The results for the nominal state model are compared against a simulation that decouples Inter-HT module to examine the importance of element-to-element heat transfer. Moreover, a coupled T/H-neutronic model is applied to investigate the reactivity feedback effects.

The chapter then presents additional core patterns to demonstrate the capability and versatility of NTPSteadyFOAM to perform coupled multiphysics analysis applied on a full-core level. The final section will compare the general computational performance between NTPSteadyFOAM and the higher-order modeling approaches.

6.1 Sample Miniature Core Description

The adopted active core relies on a NERVA-type NTP reactor model that includes 127 elements producing 110 MW. The core consists of 55 FEs and 72 MEs, where the loading pattern was adopted directly from a design investigated by Krecicki et al. [49]. Figure 46 presents the cross-section view of the active core configuration and Table 21.
lists the operating/boundary conditions. For the simplicity of the demonstration, the sample core will use the thermophysical properties, structural materials, and sub-element input conditions provided in Chapter 5. The two-group homogenized cross sections for both the nominal and perturbed cases can be found in Appendix C. Neutronic simulations relied on generating cross sections for supercells rather than individual FE and ME. Therefore, the neutron flux resolution treats each supercell as unique entity characterized by unique thermal and fast fluxes. The latter described approach is deemed to be acceptable as it is analogous to cross sections generating for Light Water Reactors fuel assemblies, where the generation process is focused on the fuel assembly as a whole rather than decomposing it to fuel pins and guide tubes. Having said that, the cross-section generation was outside the scope of the current study.

The power split between the FE and ME relied on a pre-determined constant that describes the fraction of power generated in FE compared to the power generated in ME due to elastic scattering and radiative capture reactions. This pre-determined power split constant is applied to determine the sub-element volumetric heat source in FE fuel meat, ME ZrH₂, and ME YSZ. The constant is directly deducted from Monte Carlo simulations reported in Table 21.
Figure 46. Sample core configuration.
Table 21. Input and boundary conditions for the subsequent sample reactor models.

<table>
<thead>
<tr>
<th>Neutronic albedo coefficients</th>
<th>Fast group</th>
<th>Thermal group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top axial plate</td>
<td>0.0551</td>
<td>0.1951</td>
</tr>
<tr>
<td>Bottom plate</td>
<td>0.3599</td>
<td>0.3968</td>
</tr>
<tr>
<td>Radial albedo conditions</td>
<td>0.0360</td>
<td>0.0250</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>T/H boundary conditions</th>
<th>FE</th>
<th>ME</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power split fraction</td>
<td>0.97796</td>
<td>ZrH₂: 0.015</td>
</tr>
<tr>
<td>Inlet temperature</td>
<td>300 K</td>
<td>YSZ: 0.007</td>
</tr>
<tr>
<td>Inlet mass flow rate</td>
<td>0.054042 kg/s</td>
<td>0.02393 kg/s</td>
</tr>
<tr>
<td>Inlet pressure</td>
<td>7.0 MPa</td>
<td>14.0 MPa</td>
</tr>
</tbody>
</table>

6.2 Multiphysics Modeling

Figure 47 demonstrates the multiphysics simulation performed by NTPSteadyFOAM. It depicts only a sample of results distributions (e.g., bulk temperature of the propellant) within the core. The solution approach relied only on one-way T/H-neutronic coupling with no reactivity feedback calculations reapplied to the neutron diffusion solution. This one-way T/H-neutronic coupling will be referred to as the nominal state model. The subsequent studies will couple or decouple specific functions from the simulation to examine the physical impact imposed on the nominal state model.

Table 22 presents the comparison between the nominal state model where inter-elemental HT is considered and a case in which the heat transfer between elements is ignored (i.e., adiabatic conditions are used instead). The results indicate the importance of considering the heat transfer effects between the different elements. The simplified solution with no inter-elemental heat transfer produces artificially higher T/H condition in FEs and
lower MEs compared to the nominal state. To conclude, the multiphysics results reported here emphasize the need to properly model the FE-to-ME heat transfer in NTP cores.

![Figure 47](image_url)

**Figure 47.** Selected solutions from a one-way multiphysics analysis: (a) Average fuel temperature distribution, (b) bulk coolant temperature distribution taken at ME return channels, and (c) volumetric power \( (q''') \) distribution.

**Table 22. Impact summary of inter-elemental HT in the multiphysics simulations.**

| Inter-HT coupling | Avg. \( T_b \) at FE outlet (K) | Avg. \( T_b \) at ME outlet (K) | Avg. \( |U| \) at FE outlet (m/s) | Avg. \( |U| \) at ME outlet (m/s) | Max. \( T_{fuel} \) (K) |
|-------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|----------------------|
| Yes (nominal)     | 2455.9                        | 306.8                         | 394.4                         | 40.1                          | 2756.8               |
| No                | 2499.7                        | 114.1                         | 401.5                         | 15.4                          | 2880.2               |
| Absolute difference | 43.8                         | 192.8                         | 7.1                           | 24.7                          | 123.4               |

Next, we include the reactivity feedback and investigate the importance of its inclusion for the analyzed NTP core. The previously simulated nominal state model uses
the cross-section data generated with nominal fuel temperature and coolant density condition taken at some averaged T/H conditions (e.g., 1500K for fuel temperature, 400K for ZrH₂ temperature, and \(2 \frac{kg}{m^3}\) for coolant density). Two additional cross-sections sets are generated at low and high reactor T/H states with respect to the nominal condition (See Appendix C for specific reference conditions). The latter is required to create the dependency of cross sections on actual operational conditions. For this demonstration, the feedback calculation will only consider the reactivity feedback due to temperature change in FE fuel meat, temperature in the ZrH₂ moderator, and propellant density. Table 23 compares the solutions between the loosely coupled and fully coupled models. The results demonstrate:

- A decrease in the overall reactivity due to thermal feedback.
- Shift of the power towards the propellant’s inlet point due to the non-uniform propellant density that is higher near the inlet point as well as a non-uniform temperature distribution. It is important to note that the location of fuel temperature peak is located closer to the exit point of the propellant. In addition, the elevated fuel temperature near the peak tends to saturate the Doppler coefficient. As such, the local Doppler effect in regions closer to the peak temperature has a negligible impact on the power shape.

Figure 48 presents the power distribution with and without the feedback. As shown by the figure, the feedback has a relatively small effect on the power distribution. The main reason for the lack of strong variation, as typically seen in LWR systems, is associated with the temperature reactivity coefficients that are much smaller specifically as the NTP cores
are typically under-moderated. Another reason that the results are not varying strongly is associated to the fact that truly average conditions were applied in the nominal case, rather than just some arbitrary T/H conditions. The percentage change indicates that the power varies the most near the axial edge of the active core. Finally, Figure 49 shows the power variation in radial direction taken at 0.15 m (top figure) and 0.5 m (bottom figure) above the FE inlet boundary.

Table 23. Sample core model nominal vs. feedback simulations

<table>
<thead>
<tr>
<th></th>
<th>$k_{\text{eff}}$</th>
<th>Power at FE inlet ($\frac{W}{m^3}$)</th>
<th>Power at FE outlet ($\frac{W}{m^3}$)</th>
<th>Peak Power ($\frac{W}{m^3}$)</th>
<th>Peak $T_{\text{fuel}}$ (K)</th>
<th>Avg. $T_{b}$ at FE outlet (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal (No feedback)</td>
<td>1.00056</td>
<td>3.61E+09</td>
<td>7.54E+08</td>
<td>1.05E+10</td>
<td>2756.8</td>
<td>2455.9</td>
</tr>
<tr>
<td>Feedback</td>
<td>0.99844</td>
<td>3.80E+09</td>
<td>7.26E+08</td>
<td>1.05E+10</td>
<td>2748.</td>
<td>2454.3</td>
</tr>
<tr>
<td>Variations due to feedback</td>
<td>-212.01 (pcm change)</td>
<td>5.27%</td>
<td>-3.77%</td>
<td>0.003%</td>
<td>-8.4 K</td>
<td>-1.7 K</td>
</tr>
</tbody>
</table>
Figure 48. Axial power distribution with and without the reactivity feedback obtained for the center-most FE.
Finally, the multiphysics package was applied to different reactor-core loading patterns. Figure 50 details three selected design patterns, all containing an identical ME-to-FE ratio. It should be noted that these design patterns are only used for demonstration purposes and do not represent final or optimal core designs. NTPSteadyFOAM was applied to all three patterns to predict trends and compare results variation. Ideally, the results should have been verified against other higher-fidelity tools. Unfortunately, such coupled computational tools are not readily available. The latter, again, emphasizes the need to develop tools applicable for NTP analysis, such as presented in this dissertation. Therefore, we can only investigate trends in the current demonstration section.

The loading patterns presented here were proposed in recent studies [49]. The idea behind these patterns is to create different level of power peaking variation inside the core. For example, Design III experiences its highest power peaking in the center due to the high

![Figure 49. Radial power distributions with and without the reactivity feedback.](image)
concentration of MEs in that region. At the same time, the neutron leakage of that pattern is the lowest. Design I and II, on the other hand, are alternative designs that flatten the power distribution, but increase the total neutron leakage.

![Design I, Design II, Design III](image)

**Figure 50. Selected reactor pattern designs.**

Table 23 compares different T/H parameters obtained at arbitrary selected locations. As expected, the results demonstrate that Design III experiences the highest outlet T/H condition in FE. In contrast, Designs I & II report considerably lower outlet T/H conditions in FE. Figure 51 presents the average radial fuel temperature distribution for each design. The samples are taken at the axial location where the maximum fuel temperature occurs. As expected, the general power trends follow the loading pattern configurations, but more rigorous verification will be needed in the future. Overall, the showcases presented here serve to demonstrate the capabilities of NTPSteadyFOAM to perform multiphysics simulations.
Table 24. NTPSteadyFOAM solution summary for different reactor pattern designs.

| Models   | Avg $T_b$ at FE outlet (K) | Max/min $T_b$ at FE outlet (K) | Avg $|U|$ at FE outlet (m/s) | Max/min $|U|$ at FE outlet (m/s) | Maximum $T_{fuel}$ (K) |
|----------|---------------------------|--------------------------------|---------------------------|-------------------------------|----------------------|
| Design I | 2454                      | 2565/2302 (263)                 | 394.2                     | 412.6/369.6                   | 2740                 |
| Design II| 2445                      | 2591/2367 (224)                 | 392.6                     | 416.3/380.0                   | 2768                 |
| Design III| 2469                     | 2582/2440 (142)                | 396.5                     | 414.8/391.8                   | 2769                 |

| Models   | Avg $T_b$ at ME outlet (K) | Max/Min $T_b$ at ME outlet (K) | Avg $|U|$ at ME outlet (m/s) | Max/Min $|U|$ at ME outlet (m/s) |
|----------|---------------------------|--------------------------------|---------------------------|-------------------------------|
| Design I | 308                       | 362/245 (117)                  | 40.3                      | 47.1/32.3                     |
| Design II| 305                       | 365/250 (115)                  | 39.9                      | 47.5/33.0                     |
| Design III| 288                      | 378/220 (158)                 | 37.8                      | 49.1/29.1                     |

*Red* indicates maximum and *Blue* indicates minimum out of three designs.

![Avg. $T_{fuel}$ (K)](image)

**Figure 51** Radial core fuel temperature distributions in the different loading patterns.
6.3 Summary of NTPSteadyFOAM Computational Performance

The nature of NTPSteadyFOAM’s coarse-mesh-based approach has enabled a relatively robust computational performance compared to the high-resolution simulation technique. This section summarizes NTPSteadyFOAM’s computational performance. Table 25 presents the execution time for all the analyzed cases. These calculations were carried out through the PACE research cluster using Intel® Xeon Gold 6266 “Cascade Lake” @ 2.7Hgz processor, with 24 processors per node. It is worth noting that not all simulations are based on single CPU calculations, in fact, it is not feasible to execute some higher-order CHT models without the assistance of parallel computing. The intention of Table 25 is to provide a general performance comparison between high-resolution and higher-order modeling approach against the reduced-order approach applied in NTPSteadyFOAM.
Table 25. Computational performance results for different models executed using different numerical solvers.

<table>
<thead>
<tr>
<th>Modeling method</th>
<th>Single Fuel Element analysis</th>
<th>Wall clock time / CPU utilization</th>
<th>Estimated single CPU time</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Axial cell number</td>
<td>Number of mesh</td>
<td></td>
</tr>
<tr>
<td>Full-order CHT</td>
<td>200</td>
<td>2,780,000</td>
<td>6 hrs / 14 CPUs</td>
</tr>
<tr>
<td>Reduced-geometry CHT (1/12 reduction)</td>
<td>200</td>
<td>345,000</td>
<td>1.8 hrs / 6 CPUs</td>
</tr>
<tr>
<td>NTPSteadyFOAM Main T/H module</td>
<td>50</td>
<td>300</td>
<td>~6 seconds / 1 CPU</td>
</tr>
<tr>
<td>Full-order CHT</td>
<td>200</td>
<td>808,800</td>
<td>~6 hrs / 8 CPUs</td>
</tr>
<tr>
<td>Reduced-geometry CHT (1/12 reduction)</td>
<td>200</td>
<td>67,400</td>
<td>~2.8 hrs / 4 CPUs</td>
</tr>
<tr>
<td>NTPSteadyFOAM Main T/H module</td>
<td>50</td>
<td>300</td>
<td>~14 seconds / 1 CPU</td>
</tr>
<tr>
<td>Neutronic analysis</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SERPENT 2</td>
<td></td>
<td></td>
<td>~5 min / 24 CPU</td>
</tr>
<tr>
<td>NTPSteadyFOAM Neutron diffusion mod.</td>
<td>117</td>
<td>702</td>
<td>&lt; 1 second / 1 CPU</td>
</tr>
<tr>
<td>127-elements core multiphysics analysis</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NTPSteadyFOAM full-multiphysics</td>
<td>100</td>
<td>76,200</td>
<td>45 min / 5 CPU</td>
</tr>
</tbody>
</table>

115
CHAPTER 7. CONCLUSIONS

NTP is a promising technology that is heavily investigated in recent years, specifically in the context of crewed mission to Mars. There are, however, some challenges in designing a HALEU-base engine. To alleviate some uncertainties and challenges associated with the NTP reactor-core design, heavy experimental as well as computational work are required. The latter, which is the focus of this dissertation, requires to enable high-resolution and high-fidelity capabilities. In addition, there is a real need to have the ability to model the entire core and capture multiphysics effects. This dissertation introduced a numerical package for NTP multiphysics analysis. This chapter summarizes the theory and work performed for the proposed NTPSteadyFOAM package. Additional discussion regarding potential future improvements is also addressed.

7.1 Summary of NTPSteadyFOAM Package

The objective of the thesis was to develop a steady-state OpenFOAM-based numerical tool tailored for NERVA-type NTP reactor multiphysics simulations. The proposed package, NTPSteadyFOAM, is built upon multiple custom-made OpenFOAM modules; each module is designed to model a certain physics within a NTP reactor-core. The multi-module foundation and the coupling strategy of NTPSteadyFOAM are inspired by the GeN-Foam reactor multiphysics solver, initially developed for both coarse and fine-mesh modeling of fast reactors. The current NTPSteadyFOAM version contains three sub-modules that consider sub-elements fuel-to-coolant heat transfer, inter-elemental heat transfer, and neutron diffusion for flux and power distribution calculations. The inclusion of these modules is based on the knowledge acquired from previous observations and
research that focused on solving the T/H and heat transfer problems inherent to the expander-cycle-based NTP engine. More specifically, previous studies identified the gaps in the computational approach (e.g., lack of proper treatment of the inter-elemental heat transfer), and the current dissertation addressed these computational issues.

There are three major modules embedded within the package. The first module within the NTPSteadyFOAM package, the Main T/H module, is a 1.5-D subchannel solver that models T/H conditions within each sub-element. The solver relies on the equivalent modeling assumption that treats sub-elements as annular cylinders with radially symmetric conditions. Such an assumption allows this module to iterate upon a simplified 1-D NS equations of mass, momentum, and energy with the assistance of a 1-D multi-region finite-difference sub-function that calculates the sub-structure radial temperature distribution within each axial layer. Moreover, the module can also model T/H conditions within an ME, which contains a more complex twice-through counterflow configuration.

The second module in the NTPSteadyFOAM package models the element-to-element heat transfer across the active core. The Inter-elemental Heat Transfer module (Inter-HT module) is a 2-D conduction heat transfer solver that models thermal conduction heat transfer between elements at each axial layer. The Inter-HT module’s solution scheme is equipped with several interface conditions and mesh baffles to emulate the actual contact situations between full-order sub-element models when, in fact, the previously assumed equivalent sub-element models are in contact with each other.

The third module implemented in NTPSteadyFOAM is a $P_1$-based multi-group neutron diffusion solver that calculates the neutron flux and power distribution. This
neutronic module relies on user-provided cross-section library that can be distributed into different mesh zones. The current implementation includes only a duo-point reactivity feedback calculation capability that perturbs the cross-section set based on the reference data generated at a higher and lower reactor state. The perturbation is performed in respect to temperature (fuel or other such as ZrH$_2$) and coolant density. Finally, the neutronic model allows to apply albedo boundary conditions for each energy group to simulate reflective boundaries.

The package is modular and allows the user to switch solvers/modules on and off. The main T/H module and the neutron diffusion module can be executed individually to obtain single physics simulations. However, the Inter-HT module must be coupled with the main T/H module if multi-element T/H calculation is desired as the Inter-HT module relies on the 1.5-D model to update T/H conditions for each sub-element. The package allows flexibility in defining mesh domains for each physics. In the case that full coupling is required, each module will be executed using a unique mesh domain, and the data will be transferred in-between domains through OpenFOAM’s built-in mesh interpolation sub-function. Finally, parallel computation mode is also available through the built-in domain decompositions routines embedded within OpenFOAM.

7.2 Summary of The Work Performed

As opposed to the NERVA program which accumulated a lot of measured and computational data, the newly proposed HALEU-based programs have not yet gathered and published enough data supporting this technology. As a matter of fact, the technology is constantly evolving, and a final design has not yet been obtained. This dissertation has
focused on designing a computational framework to allow the support of current and future NTP-related design work.

However, any computational framework must be heavily validated and verified to increase the confidence and reliability of such computational packages. Thus, the first objective was to develop a high-fidelity computational route to model the heat transfer within NTP systems. In the current study, the high-order solutions relied on the Conjugate Heat Transfer (CHT) approach. It was assumed that the CHT can generate reference solutions for reduced-order T/H models carried out by the NTPSteadyFOAM package.

The CHT methodology is a widely used numerical approach designed to model convective heat transfer problems by substituting the empirical convective models with CHT interface condition that assumes continuity of heat flux and temperature. OpenFOAM’s multi-region CHT solver iterates upon 3-D NS equations for the fluid domain and the 3-D thermal conduction equation for the solid domain. At the solid-fluid domain interface, where the effect of fluid convection is relatively minor compared to conduction, the solver utilizes the CHT interface condition to model heat transfer across two domains.

The first objective was to qualify the CHT as the best available reference solution to solve heat transfer problems. Chapter 4 of this thesis compared CHT’s solution against the empirical measured data obtained from NASA’s historical NERVA NRX-A6 experiment. The results demonstrated very good agreement between the applied CHT model and the experiment, and therefore indicates that CHT models can be used as reference solutions to complement future experimental efforts.
The next step was to compare the heat transfer capabilities implemented in NTPSteadyFOAM against the CHT models (Chapter 5). Extensive analytic validation and code-to-code verification work was carried out. The benchmark cases focused on modeling a single FE, single ME, single FE-to-ME bundle, and two additional supercell models with different sub-element configurations. The fuel materials, configurations, and boundary conditions of the benchmark models are based on modern HALEU core designs. The sensitivity studies applied to the main T/H module were necessary to determine the mesh requirements. Analytic validation work was then applied to the implemented finite-difference sub-function. The numeric results were compared against the analytically derived solution, and a perfect agreement was obtained. The verification work had multiple stages where the complexity of the analyzed problems was gradually increased. First, the FE and ME were modeled using adiabatic conditions. There was generally a good agreement with the CHT model, however, a small and consistent discrepancy was identified. To remedy the geometric effect imposed by the equivalent modeling assumptions a geometric correction technique can be implemented in future studies (Section 7.3.1). The Inter-HT capabilities were benchmarked using supercell models having different FE-ME configurations. NTPSteadyFOAM was shown to produce fairly accurate results with relatively small differences attributed to the heat transfer correlations and coarse geometry that might require additional correction.

The final verification work focused on comparing the neutron diffusion solver applied to model 3D supercell elements against a reference solution obtained using SERPENT. The homogenized 2-group constants were also generated with SERPENT. The comparison demonstrated very good agreement between NTPSteadyFOAM and
SERPENT, with a maximum difference of 30 pcm between NTPSteadyFOAM and SERPENT.

Finally, full core multiphysics capabilities were demonstrated using the NTPSteadyFOAM package. Chapter 6 performed selected sensitivity studies to emphasize the importance of each feedback in the multiphysics analysis, e.g., the effects of inter-elemental heat transfer. The main purpose of Chapter 6 was to show the versatility and capability of the newly developed package to perform multiphysics calculations applied to full core analysis – a capability not readily available elsewhere. Various loading pattern designs were investigated, and the results indicate that correct trends were obtained using the NTPSteadyFOAM package.

This dissertation has demonstrated the fidelity and the multiphysics capabilities through series of extensive simulations performed on different NTP sub-element and full core models. The ultimate outcome is a multiphysics package that can be applied to obtain full core solutions in a timely-efficient manner.

7.3 Future work

This section discusses potential improvements that can be adopted by NTPSteadyFOAM.

7.3.1 Geometric weighting

The analysis reported in Chapter 5 demonstrated consistent difference between NTPSteadyFOAM and the high-resolution CHT solver. The main suspect was assumed to be the heat flux treatment using an inconsistent geometry. The CHT approach relies on the
explicit geometry and distributes the heat flux correctly and unevenly over the different flow channels. Whereas the reduced-order approach adopted in our package treats the heat flux as equally distributed over all the flow channels within the hexagonal element using an equivalent cylinder. Overall, such an approach is successful in capturing the average conditions within a single element for a given heat flux, as the energy is preserved. However, when modelling a supercell (e.g., a central ME surrounded by FEs), the heat flux is not known in advance and is determined by the local rather than average boundary conditions. In other words, local flow conditions (i.e., mainly temperature), within the surrounding FEs dictate the FE-ME heat flux. To be even more specific, the main local flow channels that contribute to the heat flux are located on the periphery of the FE hexagon. Therefore, the use of a single equivalent model must be corrected to include such local effects. Here, we propose a geometric weighting mechanism to improve the local heat flux prediction while still relying on the simple and time-efficient equivalent cylinder assumption. This section only applies post-analysis techniques to present the benefits of the geometric weighting technique, but rigorous formulation and analysis are required in future studies. The main idea is to divide the FE hexagon to radial hexagon-shaped rings as shown in Figure 52. Each ring will then be represented by unique equivalent annular pins. Table 26 presents the parametric calculation applied to a known solution within the FE using a four-rings decomposition.
Figure 52. Schematic of decomposition methods for FE geometric weighting calculations.

Table 26. Parametric calculations for each ring.

<table>
<thead>
<tr>
<th>Geometric name</th>
<th>Number of flow channel</th>
<th>Fuel area per channel (m²)</th>
<th>Effective equivalent ( R_{fuel} ) (m)</th>
<th>Occupied areal fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unweighted equivalent</td>
<td>37</td>
<td>7.260E-06</td>
<td>0.00211</td>
<td>1</td>
</tr>
<tr>
<td>Ring 1</td>
<td>1</td>
<td>1.333E-06</td>
<td>0.00161</td>
<td>0.005</td>
</tr>
<tr>
<td>Ring 2</td>
<td>6</td>
<td>4.041E-06</td>
<td>0.00186</td>
<td>0.090</td>
</tr>
<tr>
<td>Ring 3</td>
<td>12</td>
<td>4.041E-06</td>
<td>0.00186</td>
<td>0.180</td>
</tr>
<tr>
<td>Ring 4</td>
<td>18</td>
<td>1.080E-05</td>
<td>0.00237</td>
<td>0.725</td>
</tr>
</tbody>
</table>

Eq. (61) presents a simple weighted function for the average bulk coolant temperature and the average cladding surface temperature. In this equation, the average temperature is estimated by weighting the number of channels distributed in each ring.

\[
T_{\phi,wt} = \frac{1}{N_{total}} \sum_{i=1}^{4} N_i T_{\phi_i}
\]  

(61)
where \( T_{ϕ,wt}, i, N_{total}, N_i \), and \( T_{ϕ_i} \) represents the weighted average temperature, ring number index, total number of channels, number of channels in ring \( i \), and the corresponding equivalent temperature at each ring \( i \), respectively.

Similarly, the weighted average fuel temperature is estimated using the fuel area occupied in each ring \( i \), as shown in Eq. (62):

\[
T_{fuel,wt} = \frac{1}{A_{total}} \sum_{i=1}^{4} N_i A_i T_{fuel_i}
\]

where \( T_{fuel,wt}, A_i, A_{total}, \) and \( T_{fuel_i} \) are the weighted overall average fuel temperature, equivalent fuel area in each ring, total fuel area in FE, and local average fuel temperature, respectively.

Finally, the overall outer-edge fuel temperature is directly taken from the local outer-edge fuel temperature value at the outer-most ring; in this case, ring number four.

Figure 53 compares the preliminary solutions for the proposed weighting technique and compares the results against a CHT full-order model. The results show definite improvements, specifically in the treatment for the outer edge, which is the most important for determining the heat flux from the FE to the ME. However, some discrepancies are still present and could be attributed to both the heat flux correlation and the heat flux in-between the rings that are treated using the equivalent channel approximation.
Figure 53 Axial thermal distributions following the application of the geometric weighting technique: (a) coolant temperature, (c) fuel temperature, and (d) outer-surface temperature.

Future work should focus on implementing an automatic procedure that includes the geometric weighting mechanism directly to the NTPSteadyFOAM package.

7.3.2 Neutron Diffusion Module

The neutron diffusion module implemented in this dissertation relies on a very simple technique that was merely used to provide a realistic reactivity feedback and obtain the power distribution without requiring third-party code. This module should be heavily expanded and include a general interface and treatment of multi-dimensional cross sections.
In addition, the solution procedure must account for the discontinuity of the homogeneous flux by including the so-called assembly discontinuity factors.

7.3.2.1 Cross section treatment and interface

The current implementation allows perturbations only in temperatures and coolant density. In addition, the evaluation process of cross sections when the package is executed relies on linearly perturbing the cross sections by using either a higher or lower temperature/density than the nominal. The main objective in the current thesis was to build the skeleton to enable neutron diffusion calculations applied to full core problems. However, to account for more realistic dependence of cross sections, additional dependencies must be included. In the operation of NTP systems, the xenon concentration will be play an important role and must be tabulated as well. The latter is analogous to burnup dependency typically considered when generating few-group constants. In addition, the rotational angle of the control drums must be included as well to enable transient calculations and study shutdown margins. Finally, the cross sections must be tabulated using arbitrary selected points for each dependency.

7.3.3 Discontinuity Factors

Discontinuity factors are known to be important in regions with higher level of heterogeneity. In our simulations, interface between the active core and reflectors was modelled via the use of albedo coefficients, but future realistic calculations would require generating few-group cross sections. These will need to be complemented by the discontinuity factors to maintain the continuity of the heterogeneous flux. Therefore, the neutron diffusion equations require adjustment to include the discontinuity factors in the
formulation and maintain the flux continuity. In fact, GeN-Foam’s multi-group neutron diffusion sub-solver has suggested a procedure to automatically generate and adjust discontinuity factors in each region [50]. Future study will focus on implementing discontinuity factors to enable improved diffusion calculations.
APPENDIX A. THERMOPHYSICAL PROPERTIES FOR T/H SIMULATION

This appendix presents the thermophysical properties used by the T/H simulation in Chapter 5, 6, and 7. The properties for the FE and ME solid material are taken from multiple references [51] [52] [53] [54] [55] [56], while the hydrogen working fluid properties are fitted using the data provided by NASA [43]. Figure 54 recasts the configuration from the HALEU-based NTP core FE and ME presented in Section 5.1. Table 27 details the solid material thermophysical properties corresponded to the label presented in Figure 54. Eqs. (63) – (67) then presents the fitted correlation for gaseous hydrogen thermophysical properties.

![Diagram of NTP fuel element and moderating element configurations with material labels.](image-url)
### Table 27. FE and ME Solid Material Definitions.

<table>
<thead>
<tr>
<th>Material label</th>
<th>Material description</th>
<th>Thermal conduction ( \frac{W}{mK} )</th>
<th>Specific heat capacity ( \frac{J}{kg \ K} )</th>
<th>Density ( \frac{kg}{m^3} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Mo30W</td>
<td>90</td>
<td>215</td>
<td>11268</td>
</tr>
<tr>
<td>2</td>
<td>Mo30W-UN</td>
<td>50</td>
<td>215</td>
<td>12784</td>
</tr>
<tr>
<td>3</td>
<td>Zircaloy-4</td>
<td>30</td>
<td>1.41E+04</td>
<td>6363</td>
</tr>
<tr>
<td>4</td>
<td>ZrH(_{1.89})</td>
<td>20</td>
<td>5.68E+03</td>
<td>5433</td>
</tr>
<tr>
<td>5</td>
<td>ZrC</td>
<td>3</td>
<td>5.68E+03</td>
<td>3298</td>
</tr>
<tr>
<td>6</td>
<td>YSZ</td>
<td>2</td>
<td>5.68E+03</td>
<td>6000</td>
</tr>
</tbody>
</table>

Gaseous hydrogen thermophysical properties:

\[
\rho \left[ \frac{kg}{m^3} \right] = \begin{cases} 1733 \cdot T^{-1.0054}, & 300 \leq T \leq 3000 \ (for \ FE) \\ 2589.6 \cdot T^{-0.9657}, & 40 \leq T \leq 400 \ (for \ ME) \end{cases}
\]

(63)

\[
\mu [Pa - s] = -4.1592 \times 10^{-13}T^2 + 1.2616 \times 10^{-8}T + 8.8844 \times 10^{-6}
\]

(64)

\[
300 \leq T \leq 3000 \ (for \ FE)
\]

\[
\mu [Pa - s] = -3.8960 \times 10^{-12}T^2 + 2.0918 \times 10^{-8}T + 3.2457 \times 10^{-6}
\]

(65)

\[
40 \leq T \leq 400 \ (for \ ME)
\]

\[
k \left[ \frac{W}{mK} \right] = 3.7196 \times 10^{-14}T^4 - 1.3154 \times 10^{-10}T^3 + 1.4265 \times 10^{-7}T^2 + 3.0284 \times 10^{-4}T + 9.5793 \times 10^{-2}
\]

(66)

\[
300 \leq T \leq 3000 \ (for \ FE)
\]

\[
k \left[ \frac{W}{mK} \right] = 9.990 \times 10^{-12}T^4 - 1.3369 \times 10^{-8}T^3 + 5.9688 \times 10^{-6}T^2 - 6.3625 \times 10^{-4}T + 1.3759 \times 10^{-1}
\]

(67)

\[
40 \leq T \leq 400 \ (for \ ME)
\]

\[
C_p \left[ \frac{J}{kg \ K} \right] = \begin{cases} 15010, & 300 \leq T \leq 3000 \ (for \ FE) \\ 12140, & 40 \leq T \leq 400 \ (for \ ME) \end{cases}
\]

(68)
APPENDIX B. CHT MESH SENSITIVITY STUDIES

This appendix presents the results of CHT models’ mesh dependency study for the high-resolution FE and ME presented in Chapter 5. To reduce the computational requirements, the study will use three equivalent models to represent FE, ME supply channel (SC), and ME return channel (RC). All equivalent models contain adiabatic boundary conditions with the input and material properties taken from Section 5.1. Figure 55 shows schematics of the equivalent models for the mesh dependency study. The results of the sensitivity studies are presented in Table 28-32, where the highlighted row denotes CHT model’s mesh parameter selected for the benchmark analysis presented in Chapter 5.

Figure 55. Equivalent sub-element models for mesh dependency study: (a) FE, (b) ME supply channel, and (c) ME return channel.

Table 28. Mesh sensitivity study for high-resolution FE model in axial direction.

<table>
<thead>
<tr>
<th>Axial cell size (m)</th>
<th>No. of axial layers</th>
<th>Inlet P (MPa)</th>
<th>Outlet mean Reynolds number, Re ($\times 10^4$)</th>
<th>Outlet mean fluid T (K)</th>
<th>Maximum fuel T (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.00E-02</td>
<td>50</td>
<td>7.758</td>
<td>1.962</td>
<td>2701</td>
<td>2942</td>
</tr>
<tr>
<td>1.00E-02</td>
<td>100</td>
<td>7.757</td>
<td>1.964</td>
<td>2701</td>
<td>2943</td>
</tr>
<tr>
<td>5.00E-03 (highlighted)</td>
<td>200</td>
<td>7.757</td>
<td>1.971</td>
<td>2712</td>
<td>2954</td>
</tr>
<tr>
<td>3.33E-03</td>
<td>300</td>
<td>7.757</td>
<td>1.970</td>
<td>2711</td>
<td>2954</td>
</tr>
<tr>
<td>2.50E-03</td>
<td>400</td>
<td>7.757</td>
<td>1.470</td>
<td>2711</td>
<td>2955</td>
</tr>
</tbody>
</table>
Table 29. Mesh sensitivity study for high-resolution ME model in axial direction.

<table>
<thead>
<tr>
<th>Axial cell size (m)</th>
<th>No. of axial layers</th>
<th>SC Inlet P (MPa)</th>
<th>RC outlet mean Reynolds number, ( \text{Re} \times 10^5 )</th>
<th>RC outlet mean fluid T (K)</th>
<th>YSZ layer maximum fuel T (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.00E-02</td>
<td>50</td>
<td>13.383</td>
<td>1.274</td>
<td>153</td>
<td>297</td>
</tr>
<tr>
<td>1.00E-02</td>
<td>100</td>
<td>13.382</td>
<td>1.279</td>
<td>153</td>
<td>297</td>
</tr>
<tr>
<td>5.00E-03</td>
<td>200</td>
<td><strong>13.382</strong></td>
<td><strong>1.285</strong></td>
<td><strong>156</strong></td>
<td><strong>303</strong></td>
</tr>
<tr>
<td>3.33E-03</td>
<td>300</td>
<td>13.382</td>
<td>1.284</td>
<td>156</td>
<td>303</td>
</tr>
<tr>
<td>2.50E-03</td>
<td>400</td>
<td>13.382</td>
<td>1.282</td>
<td>155</td>
<td>303</td>
</tr>
</tbody>
</table>

Table 30. Mesh sensitivity study for high-resolution FE model in radial direction taken at the coolant channel solid-fluid domain interface.

<table>
<thead>
<tr>
<th>Maximum first cell ( y^+ ) at inlet</th>
<th>Inlet fluid P (MPa)</th>
<th>Outlet mean Reynolds number, ( \text{Re} \times 10^4 )</th>
<th>Outlet mean fluid T (K)</th>
<th>Outlet fluid surface ( T_s ) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.893</td>
<td>7.760</td>
<td>1.9721</td>
<td>2712</td>
<td>2726</td>
</tr>
<tr>
<td>1.283</td>
<td>7.757</td>
<td>1.9712</td>
<td>2712</td>
<td>2728</td>
</tr>
<tr>
<td>1.755</td>
<td>7.745</td>
<td>1.9709</td>
<td>2712</td>
<td>2729</td>
</tr>
<tr>
<td><strong>2.936</strong></td>
<td><strong>7.723</strong></td>
<td><strong>1.9705</strong></td>
<td><strong>2712</strong></td>
<td><strong>2729</strong></td>
</tr>
<tr>
<td>4.998</td>
<td>7.702</td>
<td>1.9703</td>
<td>2711</td>
<td>2729</td>
</tr>
</tbody>
</table>

Table 31. Mesh sensitivity study for high-resolution ME model in radial direction taken at the supply channel solid-fluid domain interface.

<table>
<thead>
<tr>
<th>Maximum first cell ( y^+ ) at inlet</th>
<th>Inlet fluid P (MPa)</th>
<th>Outlet mean Reynolds number, ( \text{Re} \times 10^6 )</th>
<th>Outlet mean fluid T (K)</th>
<th>Outlet fluid surface ( T_s ) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.322</td>
<td>14.212</td>
<td>1.3463</td>
<td>118</td>
<td>150</td>
</tr>
<tr>
<td>0.666</td>
<td>14.260</td>
<td>1.3464</td>
<td>118</td>
<td>149</td>
</tr>
<tr>
<td>0.997</td>
<td>14.268</td>
<td>1.3467</td>
<td>118</td>
<td>149</td>
</tr>
<tr>
<td><strong>1.334</strong></td>
<td><strong>14.264</strong></td>
<td><strong>1.3470</strong></td>
<td><strong>118</strong></td>
<td><strong>148</strong></td>
</tr>
<tr>
<td>1.669</td>
<td>14.254</td>
<td>1.3473</td>
<td>118</td>
<td>148</td>
</tr>
</tbody>
</table>
Table 32. Mesh sensitivity study for high-resolution ME model in radial direction taken at the return channel (RC) solid-fluid domain interface.

<table>
<thead>
<tr>
<th>RC inner surface max. first cell $y^+$ at inlet</th>
<th>RC outer surface max. first cell $y^+$ at inlet</th>
<th>Inlet fluid P (MPa)</th>
<th>Outlet mean Reynolds number, $Re \times 10^6$</th>
<th>Outlet mean fluid $T$ (K)</th>
<th>Outlet fluid surface $T_s$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.262</td>
<td>0.180</td>
<td>13.765</td>
<td>0.1193</td>
<td>181</td>
<td>190</td>
</tr>
<tr>
<td>0.448</td>
<td>0.289</td>
<td>13.806</td>
<td>0.1193</td>
<td>181</td>
<td>187</td>
</tr>
<tr>
<td><strong>0.726</strong></td>
<td><strong>0.523</strong></td>
<td><strong>13.816</strong></td>
<td><strong>0.1193</strong></td>
<td><strong>181</strong></td>
<td><strong>187</strong></td>
</tr>
<tr>
<td>1.837</td>
<td>1.028</td>
<td>13.760</td>
<td>0.1192</td>
<td>181</td>
<td>189</td>
</tr>
</tbody>
</table>
APPENDIX C. FEW-GROUP CROSS-SECTION DATA

This appendix presents the homogenized cross-section data sets utilized by the neutron diffusion module as part of the code demonstration in Chapter 5 and 6. The following data is extracted using SERPENT 2 with the ENDF/B-VII.0 evaluated data library [57]. Table 33 presents the cross-section data for the nominal NTP reactor condition and Table 34-39 presents the reference data at different reactor states.

Table 33. Cross-section data for nominal NTP reactor conditions.

<table>
<thead>
<tr>
<th>Cross-section type</th>
<th>Fast group</th>
<th>Thermal group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion Coeff. $[m]$</td>
<td>0.015127</td>
<td>0.004985</td>
</tr>
<tr>
<td>$\nu \Sigma_f \left[ \frac{1}{m} \right]$</td>
<td>0.889526</td>
<td>18.060200</td>
</tr>
<tr>
<td>$\epsilon \Sigma_f \left[ \frac{W}{m} \right] \times 10^{-10}$</td>
<td>0.1167</td>
<td>2.4033</td>
</tr>
<tr>
<td>$\Sigma_{scatter} \left[ \frac{1}{m} \right]$</td>
<td>1.184840 (down scatter)</td>
<td>0.147040 (up scatter)</td>
</tr>
<tr>
<td>$\Sigma_{reduced.abs} \left[ \frac{1}{m} \right]$</td>
<td>1.027170</td>
<td>10.391100</td>
</tr>
<tr>
<td>$\chi$</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>
### Table 34. Cross-section data at higher FE fuel meat temperature condition.

Operating Conditions: $T_{fuel} = 2700K \mid T_{ZrH2} = 400K \mid \rho_{FE.cool} = 2\frac{kg}{m^3}$

<table>
<thead>
<tr>
<th>Cross-section type</th>
<th>Fast group</th>
<th>Thermal group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion Coeff. [m]</td>
<td>0.015133</td>
<td>0.004983</td>
</tr>
<tr>
<td>$\nu \Sigma_f \left[ \frac{1}{m} \right]$</td>
<td>0.888066</td>
<td>17.961200</td>
</tr>
<tr>
<td>$\epsilon \Sigma_f \left[ \frac{W}{m} \right] \times 10^{-10}$</td>
<td>0.1169</td>
<td>2.3885</td>
</tr>
<tr>
<td>$\Sigma_{scatter} \left[ \frac{1}{m} \right]$</td>
<td>1.173510</td>
<td>0.180146</td>
</tr>
<tr>
<td>$\Sigma_{reduced.abs} \left[ \frac{1}{m} \right]$</td>
<td>1.047180</td>
<td>10.341300</td>
</tr>
<tr>
<td>$\chi$</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

### Table 35. Cross-section data at lower FE fuel meat temperature condition.

Operating Conditions: $T_{fuel} = 500K \mid T_{ZrH2} = 400K \mid \rho_{FE.cool} = 2\frac{kg}{m^3}$

<table>
<thead>
<tr>
<th>Cross-section type</th>
<th>Fast group</th>
<th>Thermal group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion Coeff. [m]</td>
<td>0.015118</td>
<td>0.004986</td>
</tr>
<tr>
<td>$\nu \Sigma_f \left[ \frac{1}{m} \right]$</td>
<td>0.885694</td>
<td>18.168400</td>
</tr>
<tr>
<td>$\epsilon \Sigma_f \left[ \frac{W}{m} \right] \times 10^{-10}$</td>
<td>0.1163</td>
<td>2.4161</td>
</tr>
<tr>
<td>$\Sigma_{scatter} \left[ \frac{1}{m} \right]$</td>
<td>1.199820</td>
<td>0.118155</td>
</tr>
<tr>
<td>$\Sigma_{reduced.abs} \left[ \frac{1}{m} \right]$</td>
<td>0.999812</td>
<td>10.445300</td>
</tr>
<tr>
<td>$\chi$</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>
### Table 36. Cross-section data at higher ME ZrH₂ temperature condition.

Operating Conditions: $T_{fuel} = 1500K \mid T_{ZrH2} = 500K \mid \rho_{FE.cool} = 2^{kg/m^3}$

<table>
<thead>
<tr>
<th>Cross-section type</th>
<th>Fast group</th>
<th>Thermal group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion Coeff. $[m]$</td>
<td>0.015117</td>
<td>0.004942</td>
</tr>
<tr>
<td>$\nu \Sigma_f [1/m]$</td>
<td>0.890735</td>
<td>17.551300</td>
</tr>
<tr>
<td>$\epsilon \Sigma_f \left[\frac{W}{m}\right] \times 10^{-10}$</td>
<td>0.1168</td>
<td>2.3340</td>
</tr>
<tr>
<td>$\Sigma_{scatter} [1/m]$ (down scatter)</td>
<td>1.186910</td>
<td>0.172606</td>
</tr>
<tr>
<td>$\Sigma_{reduced.abs} [1/m]$</td>
<td>1.028700</td>
<td>10.248500</td>
</tr>
<tr>
<td>$\chi$</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

### Table 37. Cross-section data at lower ME ZrH₂ temperature condition.

Operating Conditions: $T_{fuel} = 1500K \mid T_{ZrH2} = 300K \mid \rho_{FE.cool} = 2^{kg/m^3}$

<table>
<thead>
<tr>
<th>Cross-section type</th>
<th>Fast group</th>
<th>Thermal group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion Coeff. $[m]$</td>
<td>0.015130</td>
<td>0.005045</td>
</tr>
<tr>
<td>$\nu \Sigma_f [1/m]$</td>
<td>0.887355</td>
<td>18.655300</td>
</tr>
<tr>
<td>$\epsilon \Sigma_f \left[\frac{W}{m}\right] \times 10^{-10}$</td>
<td>0.1163</td>
<td>2.4808</td>
</tr>
<tr>
<td>$\Sigma_{scatter} [1/m]$ (down scatter)</td>
<td>1.184540</td>
<td>0.130479</td>
</tr>
<tr>
<td>$\Sigma_{reduced.abs} [1/m]$</td>
<td>1.025980</td>
<td>10.908800</td>
</tr>
<tr>
<td>$\chi$</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

### Table 38. Cross-section data at lower FE coolant density condition.

Operating Conditions: $T_{fuel} = 1500K \mid T_{ZrH2} = 300K \mid \rho_{FE.cool} = 0.5^{kg/m^3}$

135
<table>
<thead>
<tr>
<th>Cross-section type</th>
<th>Fast group</th>
<th>Thermal group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion Coeff. [m]</td>
<td>0.015141</td>
<td>0.004987</td>
</tr>
<tr>
<td>$\nu \Sigma_f \left[ \frac{1}{m} \right]$</td>
<td>0.888281</td>
<td>18.036900</td>
</tr>
<tr>
<td>$\epsilon \Sigma_f \left[ \frac{W}{m} \right] \times 10^{-10}$</td>
<td>0.1168</td>
<td>2.3986</td>
</tr>
<tr>
<td>$\Sigma_{scatter} \left[ \frac{1}{m} \right]$ (down scatter)</td>
<td>1.178920</td>
<td>0.148054 (up scatter)</td>
</tr>
<tr>
<td>$\Sigma_{reduced.abs} \left[ \frac{1}{m} \right]$</td>
<td>1.025110</td>
<td>10.378000</td>
</tr>
<tr>
<td>$\chi$</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 39. Cross-section data at higher FE coolant density condition.

Operating Conditions: $T_{fuel} = 1500K \mid T_{ZRH2} = 300K \mid \rho_{FE.cool} = 7 \frac{kg}{m^3}$

<table>
<thead>
<tr>
<th>Cross-section type</th>
<th>Fast group</th>
<th>Thermal group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion Coeff. [m]</td>
<td>0.015087</td>
<td>0.004969</td>
</tr>
<tr>
<td>$\nu \Sigma_f \left[ \frac{1}{m} \right]$</td>
<td>0.891244</td>
<td>18.130900</td>
</tr>
<tr>
<td>$\epsilon \Sigma_f \left[ \frac{W}{m} \right] \times 10^{-10}$</td>
<td>0.1168</td>
<td>2.4111</td>
</tr>
<tr>
<td>$\Sigma_{scatter} \left[ \frac{1}{m} \right]$ (down scatter)</td>
<td>1.198950</td>
<td>0.147669 (up scatter)</td>
</tr>
<tr>
<td>$\Sigma_{reduced.abs} \left[ \frac{1}{m} \right]$</td>
<td>1.034900</td>
<td>10.430400</td>
</tr>
<tr>
<td>$\chi$</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>
REFERENCES


VITA

Jim Wang was born in Taichung, Taiwan, a city famous for its Museum of Natural Science. Jim’s parents, David and Wendy, would bring him to the museum every week since he was three. It was the time Jim began to develop his interest in science. Jim moved to Cary, NC, USA with his family at the age of 15; and graduated from Panther Creek High School in May 2010. Following graduation, Jim began his journey in studying Nuclear Engineering at North Carolina State University. After receiving his bachelor’s degree in 2016, Jim attended the Georgia Institute of Technology for graduate school. During his free time, Jim likes to try out different recipes for Bolognese sauce. In addition to his passion for Nuclear Engineering and Italian cuisine, Jim is also on a quest to find the perfect formula for whiskey old-fashioned.