Analysis of Natural Convection Flow in a Detector Using Computational Fluid Dynamics

Weston Christensen
South Dakota State University

Follow this and additional works at: https://openprairie.sdstate.edu/etd

Part of the Mechanical Engineering Commons

Recommended Citation
https://openprairie.sdstate.edu/etd/3667

This Thesis - Open Access is brought to you for free and open access by Open PRAIRIE: Open Public Research Access Institutional Repository and Information Exchange. It has been accepted for inclusion in Electronic Theses and Dissertations by an authorized administrator of Open PRAIRIE: Open Public Research Access Institutional Repository and Information Exchange. For more information, please contact michael.biondo@sdstate.edu.
ANALYSIS OF NATURAL CONVECTION FLOW IN A DETECTOR USING COMPUTATIONAL FLUID DYNAMICS

BY

WESTON CHRISTENSEN

A thesis submitted in partial fulfillment of the requirements for the

Master of Science

Major in Mechanical Engineering

South Dakota State University

2019
This thesis is approved as a creditable and independent investigation by a candidate for the master’s degree and is acceptable for meeting the thesis requirements for this degree. Acceptance of this does not imply that the conclusions reached by the candidate are necessarily the conclusions of the major department.

Gregory Michna
Advisor

Kurt Bassett
Department Head

Dean, Graduate School

Date

Date

Date
ACKNOWLEDGEMENTS

I would like to thank my thesis advisors Dr. Stephen Gent and Dr. Gregory Michna from the Mechanical Engineering Department at South Dakota State University for all their help and expertise in this research.

I would also like thank the SDSU High Performance Computing Cluster (HPC) team whose knowledge and support were invaluable. This research would not have possible without using the SDSU HPC.
CONTENTS

LIST OF FIGURES ........................................................................................................... ix

LIST OF TABLES ................................................................................................................. xiii

NOMENCLATURE ................................................................................................................. xiv

LIST OF SYMBOLS .............................................................................................................. xvi

ABSTRACT .......................................................................................................................... xvii

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

1.1 Dune Project .................................................................................................................. 1

1.1.1 How to Detect Neutrinos Traveling Long Distances ............................................ 2

1.1.2 Engineering the Long-Range Detectors ................................................................. 4

1.1.3 SDSU’s Involvement in DUNE ............................................................................... 7

1.2 Previous Work .............................................................................................................. 7

1.3 Focus of this Thesis ..................................................................................................... 11

1.4 Research Goals .......................................................................................................... 15

2. LITERATURE REVIEW ............................................................................................... 17

2.1 Grid Refinement ......................................................................................................... 17

2.2 Mesh Refinement in Critical Areas ........................................................................... 18

2.3 Boundary Conditions ............................................................................................... 22
2.4 Shear Stress Specification .......................................................... 22
  2.4.1 Shear Stress Specification for Fluid-Fluid Interfaces ................. 24
2.5 Passive Scalar ............................................................................. 27
  2.5.1 Turbulent Schmidt Number of the Passive Scalar .................... 28
2.6 Key Findings and Conclusions ..................................................... 31
3. METHODOLOGY .......................................................................... 33
  3.1 Far Detector Simulation ............................................................... 33
  3.2 Simplifying Assumptions ............................................................. 38
    3.2.1 Steady-State Conditions ....................................................... 38
    3.2.2 Liquid Argon Properties ..................................................... 39
    3.2.3 Liquid Argon Flow ............................................................. 39
    3.2.4 Boussinesq Approximation ............................................... 41
    3.2.5 Atmospheric Conditions .................................................... 43
    3.2.6 Liquid-Ullage Interface Conditions ..................................... 43
  3.3 Geometry CAD Modeling ............................................................ 43
    3.3.1 Insulation ........................................................................ 44
    3.3.2 Features Modeled as Porous Media ...................................... 45
    3.3.3 Impermeable Features ....................................................... 46
  3.4 CFD Settings ........................................................................... 47
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4.1</td>
<td>Mesh Settings</td>
</tr>
<tr>
<td>3.4.2</td>
<td>Mesh Sensitivity Study</td>
</tr>
<tr>
<td>3.4.3</td>
<td>Mesh Refinement in Critical Areas</td>
</tr>
<tr>
<td>3.5</td>
<td>Custom Controls</td>
</tr>
<tr>
<td>3.5.1</td>
<td>Volume Controls</td>
</tr>
<tr>
<td>3.5.2</td>
<td>Surface Controls</td>
</tr>
<tr>
<td>3.6</td>
<td>Remeshing Discontinuous Regions</td>
</tr>
<tr>
<td>3.6.1</td>
<td>Threshold Values</td>
</tr>
<tr>
<td>3.7</td>
<td>Physics Models</td>
</tr>
<tr>
<td>3.7.1</td>
<td>Turbulence Models</td>
</tr>
<tr>
<td>3.7.2</td>
<td>Heat Transfer Properties</td>
</tr>
<tr>
<td>3.7.3</td>
<td>Physics Settings</td>
</tr>
<tr>
<td>3.8</td>
<td>Liquid-Ullage Interface Conditions</td>
</tr>
<tr>
<td>3.9</td>
<td>Using Passive Scalars to Model Impurities</td>
</tr>
<tr>
<td>3.9.1</td>
<td>Passive Scalar Definition</td>
</tr>
<tr>
<td>3.9.2</td>
<td>Turbulent Schmidt Number Study</td>
</tr>
<tr>
<td>3.9.3</td>
<td>Electron Lifetime</td>
</tr>
<tr>
<td>3.9.4</td>
<td>Normalizing Impurity</td>
</tr>
<tr>
<td>4.</td>
<td>RESULTS AND DISCUSSION</td>
</tr>
</tbody>
</table>
4.1  Mesh Refinement Study ............................................................... 68
  4.1.1  Temperature Comparison ......................................................... 68
  4.1.2  Impurity Comparison .............................................................. 77
  4.1.3  Summary of Mesh Refinement Study ........................................... 86
4.2  Passive Scalar Turbulent Schmidt Number .................................... 88
  4.2.1  Temperature Comparison .......................................................... 88
  4.2.2  Scaled Impurity Comparison .................................................... 90
  4.2.3  Summary of Results for Varying the Turbulent Schmidt Number ........ 94
4.3  Slip vs No-Slip Boundary Condition ........................................... 95
  4.3.1  Temperature Comparison .......................................................... 95
  4.3.2  Scaled Impurity Comparison .................................................... 99
  4.3.3  Slip vs. No-Slip Summary ........................................................ 102
  4.3.4  Comparison to ProtoDUNE Slip vs. No-Slip .................................. 103
  4.3.5  Slip vs. No-Slip Conclusions ................................................... 106
4.4  Comparison to ProtoDUNE Detectors .......................................... 106
4.5  Comparison to Previous Far Detector Simulations .......................... 108

5. CONCLUSIONS AND FUTURE WORK ............................................ 111
  5.1  Conclusions ................................................................................. 111
  5.1.1  Limitations ............................................................................. 113
5.2 Future Work .............................................................................................................. 113

6. BIBLIOGRAPHY ........................................................................................................ 115
LIST OF FIGURES

Figure 1.1 Path neutrinos will travel to the Far Detector at SURF [4]. ......................... 2
Figure 1.2 Far Detector depiction [5]. ................................................................. 3
Figure 1.3 Diagram of excavation for LBNF [5]. ................................................. 4
Figure 1.4 End view of elements within the TPC [6]. ............................................. 5
Figure 1.5 Time Projection Chamber in the Far Detector. ....................................... 5
Figure 1.6 Geometry scene of the 35-ton prototype in Star-CCM+. ......................... 8
Figure 1.7 Comparison of Proto-DUNE experimental and simulation data [9]. .......... 10
Figure 1.8 Liquid-ullage boundary highlighted for the ProtoDUNE simulations [9].... 10
Figure 1.9 Internal features within the cryostat. .................................................... 14
Figure 1.10 Exploded view demonstrating complex flow features in Far Detector ....... 14
Figure 3.1 Exploded view of simplified geometry ............................................... 35
Figure 3.2 Shows four outer pipes used for inlets, surrounding the initial filling pipes... 36
Figure 3.3 Shows a close up of piping system, with filling pipes shown in red and inlet pipes from filtration system shown in blue......................................................... 37
Figure 3.4 Diagram showing ports in the ullage region (top view) [37]. ................. 37
Figure 3.5 Exploded view of ullage model, with gaseous region shown below insulation (isometric view) ................................................................. 38
Figure 3.6 Diagram of model showing the inlet and outlet locations (top view). ........ 41
Figure 3.7 3D CAD model of the liquid region of the Far Detector......................... 44
Figure 3.8 Solid features of the Far Detector as modelled in Star-CCM.................... 45
Figure 3.9 Cross-sectional view of computational mesh ......................................... 48
Figure 3.10 Wall y+ values for inner features of the cryostat. ............................ 53
Figure 3.11 Volumetric control area highlighted

Figure 3.12 Surface controlled areas in the CFD model highlighted.

Figure 3.13 Cell set highlighting areas containing discontinuous solution of initial mesh.

Figure 4.1 Plot of the residuals on Mesh 4 (60.7 million cells) from 95,000 to 100,000 iterations.

Figure 4.2 Geometry scene of surface slices in the Z direction, with field cage front and back planes shown in yellow.

Figure 4.3 Geometry scene of surface slices in the X direction.

Figure 4.4 Temperature comparison at cross-section Z = 20 m.

Figure 4.5 Temperature comparison at cross-section Z = 0 m.

Figure 4.6 Temperature comparison at cross-section Z = -20 m.

Figure 4.7 Temperature comparison at cross-section Z = -28 m.

Figure 4.8 Temperature comparison at cross-section X = -1 m.

Figure 4.9 Temperature comparison at cross-section X = 1 m.

Figure 4.10 Temperature comparison at cross-section X = 4 m.

Figure 4.11 Plot of volume average temperature within the detector by mesh size.

Figure 4.12 Scaled impurity comparison at cross-section Z = 20 m.

Figure 4.13 Scaled impurity comparison at cross-section Z = 0 m.

Figure 4.14 Scaled impurity comparison at cross-section Z = -20 m.

Figure 4.15 Scaled impurity comparison at cross-section Z = -28 m.

Figure 4.16 Scaled impurity comparison at cross-section X = -1 m.

Figure 4.17 Scaled impurity comparison at cross-section X = 1 m.
Figure 4.18 Scaled impurity at cross-section X = 4 m

Figure 4.19 Comparison of impurity concentration to number of cells in the mesh.

Figure 4.20 Plot of volume average temperature relative to the turbulent Schmidt number.

Figure 4.21 Scaled Impurity comparison at z = 20 m (0.5-left, 0.9-center, 2-right).

Figure 4.22 Scaled Impurity comparison at z = 0 m (0.5-left, 0.9-center, 2-right).

Figure 4.23 Scaled Impurity comparison at z = -20 m (0.5-left, 0.9-center, 2-right).

Figure 4.24 Scaled Impurity comparison at z = -28 m (0.5-left, 0.9-center, 2-right).

Figure 4.25 Scaled Impurity comparison at x = -1 m (0.5-top, 0.9-center, 2-bottom).

Figure 4.26 Scaled Impurity comparison at x = 1 m (0.5-top, 0.9-center, 2-bottom).

Figure 4.27 Scaled Impurity comparison at x = 4 m (0.5-top, 0.9-center, 2-bottom).

Figure 4.28 Comparison of No-Slip and Slip Boundary condition at liquid-ullage interface at z = 20 m (slip, left and no-slip, right).

Figure 4.29 Comparison of No-Slip and Slip Boundary condition at liquid-ullage interface at z = 0 m (slip, left and no-slip, right).

Figure 4.30 Comparison of No-Slip and Slip Boundary condition at liquid-ullage interface at z = -20 m (slip, left and no-slip, right).

Figure 4.31 Comparison of No-Slip and Slip Boundary condition at liquid-ullage interface at z = -28 m (slip, left and no-slip, right).

Figure 4.32 Temperature comparison at x = -1 m (slip, top and no-slip, bottom).

Figure 4.33 Temperature comparison at x = 1 m (slip, top and no-slip, bottom).

Figure 4.34 Temperature comparison at x = 4 m (slip, top and no-slip, bottom).

Figure 4.35 Scaled Impurity comparison at z = 20 m (slip, left and no-slip, right).
Figure 4.36 Scaled Impurity comparison at z = 0 m (slip, left and no-slip, right)........... 99
Figure 4.37 Scaled Impurity comparison at z = -20 m (slip, left and no-slip, right)........ 99
Figure 4.38 Scaled Impurity comparison at z = -28 m (slip, left and no-slip, right)..... 100
Figure 4.39 Scaled Impurity comparison at x = -1 m (slip, top and no-slip, bottom).... 100
Figure 4.40 Scaled Impurity comparison at x = 1 m (slip, top and no-slip, bottom)..... 101
Figure 4.41 Scaled Impurity comparison at x = 4 m (slip, top and no-slip, bottom)..... 101
Figure 4.42 Surface Temperature, Slip, CFD Vs Experimental, Static Temperature Probe, Pumps On.......................................................... 104
Figure 4.43 Surface Temperature, No-Slip, CFD Vs Experimental, Static Temperature Probe, Pumps On .......................................................... 104
Figure 4.44 Comparison of ProtoDUNE (left) and Far Detector (right) temperatures near center.......................................................... 107
Figure 4.45 Comparison of ProtoDUNE (left) and Far Detector (right) scaled impurities near center.......................................................... 108
Figure 4.46 Shows a comparison of the temperature distribution for previous simulations at SDSU [7] and the most recent simulations for the plane at Z = 0m. ......................... 109
Figure 4.47 Shows a comparison of the impurity distribution for previous simulations at SDSU [7] and the most recent simulations for the plane at Z = 0m. .......................... 110
LIST OF TABLES

Table 2.1 Summary of Shear Stress Specification Boundary Condition ............................................ 27
Table 2.2 Summary of Studies on Optimal Turbulent Schmidt Values. .............................................. 30
Table 3.1 Properties of Porous Model Features. ............................................................................. 46
Table 3.2 Levels of mesh density for mesh refinement study. .......................................................... 49
Table 3.3 Physics settings used in Star-CCM+ model. ..................................................................... 61
Table 3.4 Properties of liquid argon for Star-CCM+ model. .............................................................. 61
Table 3.5 Properties of solid features used in Star-CCM+ model. .................................................... 62
Table 4.1 Temperatures within the detector for differing levels of mesh refinement. .......... 76
Table 4.2 Comparison of impurities at differing levels of mesh refinement. ............................... 85
Table 4.3 Temperatures within the detector for varying turbulent Schmidt numbers. ............ 89
Table 4.4 Comparison of scaled impurities for differing levels of the turbulent Schmidt number. ........................................................................................................................................ 94
Table 4.5 Shows the temperature results for the slip and no-slip conditions. .............................. 98
Table 4.6 Summary of results for the impurity for the slip and no-slip conditions. ................. 101
Table 4.7 Temperature correction adjustment for ProtoDUNE simulations. ............................... 105
Table 4.8 Mean squared error *10^6 based on probe type and boundary conditions after correcting. ........................................................................................................................................ 106
Table 4.9 Design differences between the ProtoDUNE and Far Detectors. ................................. 107
# NOMENCLATURE

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Complete Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>APA</td>
<td>Anode Plane Array</td>
</tr>
<tr>
<td>CAD</td>
<td>Computer-Aided Design</td>
</tr>
<tr>
<td>CERN</td>
<td>European Organization for Nuclear Research</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CISC</td>
<td>Cryogenic Instrumentation and Slow Controls</td>
</tr>
<tr>
<td>CPA</td>
<td>Cathode Plane Array</td>
</tr>
<tr>
<td>DP</td>
<td>Dual-Phase</td>
</tr>
<tr>
<td>DUNE</td>
<td>Deep Underground Neutrino Experiment</td>
</tr>
<tr>
<td>FC</td>
<td>Field Cage</td>
</tr>
<tr>
<td>Fermilab</td>
<td>Fermi National Accelerator Laboratory</td>
</tr>
<tr>
<td>GAr</td>
<td>Gaseous Argon</td>
</tr>
<tr>
<td>GP</td>
<td>Ground Plane</td>
</tr>
<tr>
<td>LAr</td>
<td>Liquid Argon</td>
</tr>
<tr>
<td>LBNF</td>
<td>Long Baseline Neutrino Facility</td>
</tr>
<tr>
<td>PPB</td>
<td>Parts Per Billion</td>
</tr>
<tr>
<td>PPM</td>
<td>Parts Per Million</td>
</tr>
<tr>
<td>PPT</td>
<td>Parts Per Trillion</td>
</tr>
<tr>
<td>SDSU</td>
<td>South Dakota State University</td>
</tr>
<tr>
<td>SP</td>
<td>Single-Phase</td>
</tr>
<tr>
<td>SST k-ω</td>
<td>Shear Stress Transport k-ω</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Full Form</td>
</tr>
<tr>
<td>--------------</td>
<td>---------------------------</td>
</tr>
<tr>
<td>SURF</td>
<td>Sanford Underground Research Facility</td>
</tr>
<tr>
<td>TPC</td>
<td>Time Projection Chamber</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------------------------</td>
</tr>
<tr>
<td>h</td>
<td>heat transfer coefficient</td>
</tr>
<tr>
<td>k-omega</td>
<td>Two-equation turbulence model</td>
</tr>
<tr>
<td>k-epsilon</td>
<td>Two-equation turbulence model</td>
</tr>
<tr>
<td>kg</td>
<td>Kilogram</td>
</tr>
<tr>
<td>ρ</td>
<td>Density</td>
</tr>
<tr>
<td>ω</td>
<td>Specific Rate of Dissipation</td>
</tr>
</tbody>
</table>
ABSTRACT

ANALYSIS OF NATURAL CONVECTION FLOW IN A DETECTOR USING COMPUTATIONAL FLUID DYNAMICS

WESTON CHRISTENSEN

2019

The goal of this research was to simulate the flow, temperature, and impurity concentration within the Deep Underground Neutrino Experiment (DUNE) Single Phase Far Detector using a commercially available computational fluid dynamics (CFD) solver. DUNE is a research collaborative investigating properties of neutrinos in an effort to better understand the origins of matter and behavior of subatomic particles. The Far Detector is a geometrically complex neutrino detector containing: anode plane arrays and cathode plane arrays which induce an electric field within the detection region that causes electrons to drift to the sensing equipment, field cage planes to enclose the neutrino detection region, inlets and outlets for liquid argon flow, ground planes to ground the electric field outside the detection region, a service floor, and other smaller features. High-fidelity models are required to accurately simulate the flow patterns within the detector. This research investigated the effects of: 1) mesh refinement, 2) turbulent Schmidt number, and 3) the boundary condition employed at the liquid-ullage interface, i.e. slip vs. no slip. The effect of mesh refinement was analyzed by comparing the results of six levels of mesh refinement, ranging from 40.8 to 151.6 million cells. The simulation was also completed for turbulent Schmidt numbers of 0.5, 0.9, and 2.0 to determine how this property, which is difficult to quantify, impacted the results. Finally, the results of the simulation were compared for using a slip boundary condition at the liquid-ullage
interface to the simulations using a no-slip boundary condition. It was expected that these factors would significantly impact the flow, temperature and impurity concentration within the cryostat and that by comparing the simulation results to experimental data the ideal simulation parameters could be identified and implemented. The computationally generated results of this research are validated using the results of the prototype experimental and simulation data.

This thesis research led to three distinct findings. First, appropriate mesh refinement in critical areas, such as near walls or surrounding inlets and outlets led to the outcome that all levels of mesh refinement investigated in this work are able to appropriately capture the movement of liquid argon within the detector. By capturing the complex flow features with local mesh refinements, the impact of global mesh refinement was minimized. Second, the effect of changing the turbulent Schmidt number was negligible, with the impurity concentrations varying less than 0.17% for all turbulent Schmidt numbers in this study. This contradicted the hypothesis that lower turbulent Schmidt numbers would results in greater impurity variance within the detector. This may be due to the extreme purity conditions of the detector but confirms that greater study is necessary to determine to optimum turbulent Schmidt guidelines. Third, the selection of a slip vs. no-slip boundary condition at the ullage-liquid interface yields significantly different flow and consequently different thermal profiles. The no-slip boundary condition leads to the predictions of significantly warmer temperatures in the liquid volume. The slip condition provided results much more consistent with those seen in experiments than the no-slip condition. This is most likely due to the reduced mixing between the warmer gaseous argon and cooler liquid argon caused by forcing the fluid
along the interface to remain stationary. The slip condition allows the simulated fluid to move along this interface, which is consistent with conditions in the actual detector.
1.1 Dune Project

The Deep Underground Neutrino Experiment (DUNE) is an international study of neutrinos and proton decay [1]. The DUNE project is directed by Fermi National Accelerator Laboratory, hereafter referred to as Fermilab, part of the United States Department of Energy and involves collaborators from around the world. Contributors include the European Organization for Nuclear Research (CERN) and over 175 research institutions from more than 30 countries.

The research goals for the DUNE project include discovering the role of neutrinos in the origins of matter, developing a unifying theory of forces, and learning how black holes form [1]. Investigators are hoping that the experiment will demonstrate evidence of proton decay and detect neutrinos from supernovas, which could lead to discoveries providing new insight on these research goals.

Neutrinos are subatomic particles that are a fundamental particle of matter, which means they are not made up of smaller parts. Neutrinos are abundant, with billions of neutrinos one millionth the mass of an electron passing through each square centimeter of Earth every second [2], emitted even by commonplace objects such as bananas. Scientists are able to emit large quantities of neutrinos from particle accelerators and other power sources.

Physicists desire to find out more about how the actions of neutrinos and the antimatter mirror of neutrinos, known as antineutrinos, are related. If neutrino oscillations, which refer to the changing properties of neutrinos as they travel, are
elementally dissimilar from those of antineutrinos, it would be evidence of the charge-parity violation, indicating that matter and antimatter do not receive mirror treatment by the universe. Further evidence of the charge-parity violation could provide insight into why the universe is made of matter.

1.1.1 How to Detect Neutrinos Traveling Long Distances

DUNE will utilize a particle accelerator at the Fermi National Accelerator Laboratory [1] in Batavia, Illinois to send neutrinos to the detectors planned for construction at the Sanford Underground Research Facility (SURF) in Lead, South Dakota. The Fermilab particle accelerator will fire neutrinos 800 miles underground to SURF [3]. The neutrinos will travel through the Near Detector in Illinois and the Far Detector in South Dakota. Figure 1.1 shows the path of the neutrinos from acceleration to detection.

![Figure 1.1 Path neutrinos will travel to the Far Detector at SURF](image)

Detecting the presence and behavior of a neutrino is very difficult due to its size, infrequency of interaction, and the tendency of neutrinos to change flavor as they travel. Therefore, neutrinos must be detected by their interactions within the detector [2]. The most common form of neutrino interaction takes place when a neutrino strikes another
particle and emits radiation in the form of photons or electrons. These emissions are detected in the attempt to learn more about neutrinos, rather than directly detecting the neutrinos.

Long-term neutrino detection for the Deep Underground Neutrino Experiment will be achieved by the four Far Detectors. The Far Detectors will be located 4,850 feet underground at the Sanford Underground Research Facility in Lead, South Dakota. The detectors will consist of four separate chambers, with two design variations, as shown in Figure 1.2.

![Figure 1.2 Far Detector depiction [5].](image)

Excavation for the Long Baseline Neutrino Facility (LBNF) began in 2019, with installation of the first DUNE detector set for 2022. A diagram of the excavation location is shown in Figure 1.3. With construction for LBNF beginning, and experimental and CFD results from ProtoDUNE-SP under study, the final design plans for the SP and DP Far Detectors are currently under review.
1.1.2 Engineering the Long-Range Detectors

The two design variations are the single-phase (SP) and dual-phase (DP) designs. Single-phase indicates that the detection area is completely within the liquid argon region of the chamber, while dual-phase indicates detection in both the liquid and gaseous argon regions. Each chamber will keep 68,000 tons of liquid argon at approximately 88 Kelvin, making them the largest neutrino detection chambers in the world.

Holding the temperature of the liquid argon at 88 K will require state-of-the-art exterior insulation. The insulation consists of a polystyrene synthetic foam, surrounding the detector with 800 mm thick insulation to prevent large thermal gradients within the detector. Accurately modelling the heat transfer properties of the detector will be vital for the simulation.

The detection area within each single-phase detector is the Time Projection Chamber (TPC). The TPC is formed mainly by three elements: the field-cage planes, Anode Plane Arrays (APA), and Cathode Plane Arrays (CPA). The APA and CPA planes
are parallel wire mesh assemblies that alternate along the width of the cryostat, APA, CPA, APA, CPA, APA. The four remaining sides between the APA and CPA planes are enclosed by the field-cage planes. Figure 1.4. shows an end view of the APA, CPA, and field cage planes. The area enclosed by the elements is the TPC, highlighted in the Star-CCM+ model shown in Figure 1.5.

Figure 1.4 End view of elements within the TPC [6].

Figure 1.5 Time Projection Chamber in the Far Detector.
The intended operation of the TPC is as follows. A voltage is applied to the Anode Plane Arrays and Cathode Plane Arrays to create a uniform electric field between the APA and CPA planes [6]. This electric field directs the electrons created by neutrino interactions toward the APA planes, which leaves a trail of ionization in the liquid argon. This induces currents in the electronic sensing equipment placed within the cryostat detection chamber. This equipment transmits the signals through cables to the data acquisition system outside the cryostat.

These signals are used to calculate where the neutrino interaction occurred within the TPC. It is important to pinpoint as many of these locations as possible. To successfully map the location of neutrino interactions, free electrons must be able to drift from the interaction location to the APA planes. Argon is used within the TPC since, as a noble gas element, the free electrons created by the neutrino interactions will not attach to the argon atoms.

Impurities in the form of electronegative particles, such as water and oxygen, can attract the free electrons, which will not allow these electrons to drift to the APA planes for sensing. Therefore, the impurity levels within the TPC must be kept extremely low, on the order of parts per trillion, for proper neutrino detection. Any areas with relatively high levels of contamination would decrease the chances of detecting neutrino interactions in these areas.

The total size of the chambers is 19m wide, 18m high, and 66m long. The active area of the TPC producing the data of importance is 14.5m wide, 12m high, and 58m long [6]. The APA and CPA planes have a vertical orientation, with the electric field applied perpendicularly to the planes. The APA planes are 2.3m by 6m, stacked two in
height for a total height of 12m. The CPA planes are similar width, but only half the height of the APA planes, requiring a stack of four CPA planes to reach the 12m height.

1.1.3 SDSU’s Involvement in DUNE

The current design of the Far Detector is based on the operation and success of previous prototype models. Detectors have been constructed and experimental data has been collected for a single-phase detector containing 35 tons of liquid argon at Fermilab in Illinois and a single-phase detector containing 800 tons of liquid argon at CERN on the border of Switzerland and France. These prototype detectors have also been modelled with Star-CCM+ CFD simulations at South Dakota State University with a high level of accuracy [7].

1.2 Previous Work

Work on the DUNE project, then called the Long Baseline Neutrino Experiment (LBNE), began in the United States only, but in 2015 over 700 scientists formed the original DUNE international collaboration. The first DUNE prototype was the 35-ton detector built at Fermilab and coming online in 2016. Separate CFD simulations were also completed both at South Dakota State University and Fermilab to predict flow characteristics, offer design insights, and validate the methods to be used to simulate future detector versions.
These simulations included simulations at Fermilab to determine the porous and viscous resistances through the APA and field cage planes to enable the simplified modelling of these planes as porous media [8]. Erik Voirin at Fermilab also completed simulations to study the effect of varying inlet locations on the flow characteristics, temperature and impurity distributions.

Work at SDSU examined the effect of mesh types, boundary conditions, different inlet locations on the flow throughout the cryostat, settings required to accurately model the impurities as passive scalars, the APA and field cage planes as porous media, and the effect of different boundary conditions on the solution [7]. This work established a baseline for future work, but after the study on the effect of mesh types on the solution, further analysis of the effect of varying mesh sizes was also desired. In addition, the time required for convergence of the passive scalars was not optimized, and further study of the passive scalars settings was indicated.

The CFD model of the 35-ton prototype is shown in Figure 1.6.
The next step in preparing for the construction of the full-scale models at the SURF was the construction of two 400-ton detectors at CERN. The models at CERN are referred to as the ProtoDUNE detectors, one testing the single-phase design and another the dual-phase design. CFD simulations were also completed for the ProtoDUNE models at South Dakota State University and Fermilab, building upon the methods used to successfully simulate the 35-ton prototype.

Accurately modelling the interface between the liquid and ullage regions was an important objective for the ProtoDUNE simulations. This was completed by creating separate models for the liquid and ullage regions and using the results of the liquid region as a boundary condition for the ullage simulation [9]. Liquid argon is vaporized at the surface of the liquid and travels into the ullage region. The amount of argon vaporized varies, however, so a location map of the mass flux from the liquid region was used as the boundary condition for the mass flux of the liquid argon entering the ullage region.

Another important aspect of the liquid-ullage interface is the shear stress-specification boundary condition. This can be a slip condition, which allows fluid next to the boundary to move relative to the boundary, or the no-slip condition, indicating the fluid stationary relative to the boundary surface. The ProtoDUNE simulations generally agreed closer to the experimental data using the slip condition, but some discrepancies indicate a need for further study on this condition, which will be examined in this thesis.

The results of the ProtoDUNE simulations agreed with the results from the experimental testing conducted at CERN with a high level of precision, as shown in Figure 1.7. Figure 1.7 displays a comparison of the ProtoDUNE experimental data (red) and simulation data (blue) from SDSU. The simulation data lie well within the error bars.
for nearly all points of experimental data. The level of precision is in the range of several milli-Kelvin. Figure 1.8 shows the Star-CCM+ models of the liquid and ullage regions.

![Graph showing temperature and height](image1.png)

**Figure 1.7** Comparison of Proto-DUNE experimental and simulation data [9].

![3D model with liquid-ullage boundary highlighted](image2.png)

**Figure 1.8** Liquid-ullage boundary highlighted for the ProtoDUNE simulations [9].

Work completed to model these prototype versions of the detector was critical in determining proper techniques for simulating the full-scale Far Detector, which has not been constructed at the time of this analysis. With no available experimental results for
the Far Detector, previous simulations were important in validating the methods used to
model the Far Detector. Knowledge used from previous work includes proper boundary
conditions, physics settings, mesh settings, and turbulence models. The use of previous
results in modeling the Far Detector will be discussed in further sections of this analysis.

1.3 **Focus of this Thesis**

Aspects of the Far Detector required to accurately simulate its conditions include
natural convection-driven flow, cryogenic temperatures, complex geometry, and extreme
purity conditions. These circumstances are difficult to resolve, but critical to achieving an
accurate solution. Accurately resolving these features required a variety of CFD
techniques and this thesis will focus on the effects of:

1) Varying the mesh size
2) Setting proper boundary conditions at the liquid-ullage interface
3) Diffusivity of the passive scalar

The mesh size refers to the discretized computational cells within the model. CFD
simulations estimate the solutions to the Navier-Stokes equations for discrete spaces,
referred to as cells, and solve the equations numerically for each cell. Theoretically,
decreasing the cell size should improve the simulation’s accuracy, as approaching
infinitely small cells should approach the exact analytical solution for the flow. The goal
of CFD simulations, however, is often to maximize mesh efficiency.

Maximizing the mesh efficiency means creates the simplest mesh that produces a
solution at or above the desired accuracy and precision. This would indicate mesh
independence, meaning that a small change in mesh size would not produce significantly
different results. This thesis will analyze the results of the Far Detector for three different mesh sizes, to determine whether the model produces a mesh independent solution.

The effect of changing the shear stress specification at the liquid-ullage interface will also be examined. The shear stress setting specifies whether the fluid is allowed to move relative to the boundary surface. A slip condition allows the fluid to move, while the no-slip condition forces the fluid to remain stationary, relative to the boundary surface. This condition significantly influences the heat transfer characteristics occurring at the surface. While the slip condition was observed to provide results more similar to the experimental results than the no-slip condition for most simulations of the Proto-DUNE model [9], this boundary condition will also be further investigated for the Far Detector.

Diffusivity affects the rate at which particles spread throughout the fluid. A higher diffusivity indicates that particles to spread more quickly through the fluid, while a lower diffusivity means particles will take longer to propagate. The turbulent Schmidt number within Star-CCM+ controls the diffusivity of the passive scalar for turbulent flow. The meaning of this value will be further discussed in the literature review section of this report. Most recent CFD studies have assumed an ideal value of 0.7-0.9 for near wall turbulence [10]. The effect of changing the turbulent Schmidt number will be examined in this analysis.

Though there is a small amount of mechanically driven flow, 10 kg/s, used to send liquid argon through the filtration system, this flow is relatively insignificant for the 70,000 tons of liquid argon contained by the cryostat. To verify that natural convection is important for a given flow, a comparison of the Grashof number and the Reynolds
number must be considered. If the Grashof number, which compares buoyant forces to viscous forces, is on the same order or much greater than the square of the Reynolds number, which compares inertial force to viscous forces, natural convection may not be neglected in an accurate simulation of the Far Detector [11].

Based on previous calculations completed at SDSU, the Grashof number is much greater than the square of the Reynolds number, and natural convection dominates the flow within the cryostat [7]. Natural convection flows are driven by differences in temperature rather than mechanical means. Warmer fluid expands, and this less dense fluid rises due to gravitational forces, while colder, denser fluid sinks. Since subtle temperature differences drive the flow, accurate simulation of natural convection flows requires precise modelling of the temperature gradients.

This necessitates closely modelling the heat transfer characteristics. The heat transfer from the surroundings to the insulation and the heat transfer from the solid regions to the fluid regions are of great importance. Much of the previous work completed at SDSU was to determine the ideal boundary conditions, which heavily influence proper heat transfer calculations within the cryostat.

The intricate geometry of the Far Detector is another factor that necessitates careful modelling consideration. Flow is more difficult to model near walls and relatively small gaps between solid features can complicate the turbulence modelling. Figure 1.9 displays some of the complex internal geometry of the Far Detector. This requires careful simplifying assumptions of the geometry and meticulous meshing to maintain the integrity of the system for accurate flow simulation. An exploded view demonstrating the complex internal features of the cryostat is shown in Figure 1.10. Custom mesh controls
were used in this analysis to accurately represent these areas and will be further discussed in the methodology section of this thesis.

Figure 1.9 Internal features within the cryostat.

Figure 1.10 Exploded view demonstrating complex flow features in Far Detector.
The extreme purity conditions required in the Far Detector, less than 5 parts per trillion (ppt) or less, also present unique modelling challenges. Modelling a mesh resolution that could detect such impurities would require more computational resources than is feasible and modelling the effect of impurity on fluid flow and properties also increases computational expense. With impurity levels in the ppt, the effect of impurities on the flow characteristics and fluid properties is assumed to be negligible, therefore a passive scalar can be used to model the impurities within the fluid. A passive scalar is an inert, user-defined particle used in CFD simulations like a marker particle to track fluid properties without affecting the physical properties of the fluid flow. This approach will be further explored in the methodology section of this report.

1.4 **Research Goals**

This thesis will examine how certain various CFD parameters affect the simulation results. This thesis will study how the predicted results of the Far Detector are impacted by varying the base size and total number of cells in the computational domain, the boundary conditions, particularly the shear stress specification at the liquid-ullage interface, and the diffusivity of the passive scalar.

Examining the effect of mesh refinement on the accuracy of the solution has many industrial applications. Developing methods to minimize computational costs will help to maximize the efficiency of CFD and result in increased use of CFD and maximized profitability for many industries involving fluid flows. The study of shear stress specification will further the shear stress behavior at the fluid-fluid interface, which has yet to be ideally modelled. Furthermore, previous literature recommendations on the
optimum turbulent Schmidt number have produced varying optimum ranges for CFD simulations, and it is hoped that this work will provide more insight on this topic.

The main goal of the long-term CFD research on DUNE is to validate the design plan for the LBNF Far Detector. This research will use simulation methods validated by comparison of experimental data and simulations on the prototype detectors to predict conditions in the current design of the Far Detector. The predicted temperature gradients and impurity distribution within the TPC will be of key concern. Ideally, temperature and impurity distributions will be very similar to those seen in the prototype detectors.

Any significant differences in geometry, flow velocities, temperature, and impurity distributions predicted by the CFD simulation and those seen in the prototype detectors must be examined to ensure that these differences will not negatively impact neutrino detection. The temperature gradient within the TPC must kept relatively small to ensure proper function of neutrino detection equipment. The desired impurity condition is a low, uniform level of impurities, less than 5 parts per trillion (ppt) throughout the TPC. Higher concentration areas of impurities may hide neutrino interactions from detection, resulting in inaccurate mapping of neutrino interaction locations.
2. LITERATURE REVIEW

This section will focus on a review of literature relevant to this thesis. Important topics will include grid refinement, passive scalar diffusivity, and the shear stress specification boundary condition. The goal of the literature review will be to examine research on these conditions to determine how these settings and techniques will affect the simulation and which will produce the most accurate solution.

2.1 Grid Refinement

One of the most important factors in developing an accurate CFD simulation is producing an accurate mesh. The finite volume approach to CFD, which is used by Star-CCM+, approximates a numerical solution to the fluid flow by breaking the fluid domain into a number of discrete cells, which make up the mesh. The accuracy of the CFD solution is highly dependent on the number of cells in the mesh. Many studies have shown that the higher resolution the mesh, the more accurate the solution, but the increase in cells also results in a higher computational cost, and more time before the CFD solver is able to converge to a solution. This makes ideal CFD simulations a balance between enough resolution to produce the most accurate solution feasible and limiting the number of cells to maintain an acceptable computational cost.

Wendt discusses the importance of adequate mesh refinement in his book, Computational Fluid Dynamics an Introduction [12]. This book discusses basic numerical techniques and their background, to illustrate the applications of CFD and provides guidance on CFD best practices. They stress that the boundary layer is of special interest and must be accurately resolved by the mesh to ensure an adequate solution.
Furthermore, he states that relatively small boundary layers require mesh refinement beyond the usual levels to yield an accurate solution.

2.2 Mesh Refinement in Critical Areas

Finding the proper mesh resolution is a problem that must be confronted each time a CFD user seeks to estimate fluid flow using CFD software. A proper mesh contains a balance, with sufficient mesh resolution to resolve flow conditions, while simple enough to allow for practicable computation time to convergence. One method often used to obtain the most accurate CFD solution with the simplest mesh is to isolate areas of high refinement only to regions that are difficult to resolve. Near boundary walls, geometrically complex regions, regions with significant heat transfer, phase change interfaces, inlets, and outlets are among the other foremost areas requiring additional mesh refinement. High velocity gradients within the near wall boundary layer is one factor that makes flow near walls difficult to resolve. Failure to converge may also indicate that a model requires further mesh refinement.

Yakkundi and Mantha studied the effect of mesh refinement and turbulence models on the aerodynamics properties of car using CFD and wind tunnel experiments [13]. They studied the effect of reducing the global mesh size as well as creating local mesh refinements at 10% of the global cell size on a car of frontal area 1.51 m². They studied global meshes of 1000 mm, 500 mm, 256 mm, and 500 mm with a local refinement up to 50 mm. They determined that while increasing the global refinement results in a continually decreasing simulated drag force, local mesh refinement had a larger effect on the calculated drag force than the global refinement. It should be noted,
however, that this study strictly limited the overall mesh refinement for the sake of computational costs.

Natural convection flows are driven by buoyancy differences, caused by a temperature induced density gradient. This makes natural convection flows, in particular, require a relatively higher resolution mesh to resolve flow features, as it is critical to calculate subtle temperature differences within the fluid [14]. This can make it difficult to maintain the required level of mesh resolution while staying within feasible bounds for computation for natural convection flows, especially those with large and complex geometries. By isolating these areas, mesh refinement can be increased in areas significant to driving the fluid flow. Areas without complex geometry or temperature differences, however, may be maintained at a coarser base mesh to reduce computational cost, as will be shown in the following studies.

A 2006 study by Omri and Galanis examined the effect of grid refinements on the results of a numerical solution for a two-dimensional heated cavity with turbulent natural convection using the K-ω SST model and compared this solution to an experimental benchmark [15]. To create the K-ω SST model, Menter added blending functions to the K-ω model, providing his new model with a combination of the advantages of both the K-ω and K-ε models [16]. Omri and Galanis examined a 0.75m by 0.75m cavity, with 1.5m depth. The study assumed the vertical walls were maintained at a constant temperature of 50 °C and 10 °C while the horizontal walls were insulated from an ambient temperature of 30 °C.
They found that grid independent results can be obtained with fewer nodes than those required for Large Eddy Simulations if the distribution of nodes within the boundary layer is sufficient. This study found that for the geometry considered, 80% of the nodes for the cavity should be contained within the boundary layers. The mesh sizes examined in this study were four non-uniform grids varying 30×30 to 150×150. For the 80% of cells within the 300 mm boundary layer established in this study, this equates to an approximate cell size ranging from 4.5 mm to 22.5 mm per cell side for the grids. They found that the 30×30 and 150×150 cell grids produced similar results. They concluded that maintaining enough cells within the boundary layer was more significant to the solution than the cell size.

Another factor that makes near wall grid resolution important is heat transfer at the boundaries. It is important to accurately resolve the heat transfer characteristics between regions to obtain an accurate solution, especially in natural convection flows where temperature gradients drive the flow. The heat transfer boundary conditions will be further discussed in the methodology section of this report.

For instance, a 2005 study completed by Zitzmann et al. studied the influence of near wall mesh density on the flow and heat transfer calculations air flow driven by natural convection over a heated vertical plate in a differentially heated cavity [14]. The flow was studied for three different geometries. The Boussinesq approximation was utilized to model the buoyancy of the fluid flow. The study examined the effect of the first prism layer thickness, core prism size, and prism inflation.

The first prism layer value represents the thickness of the first layer from the wall to the end of the first layer. The effect of the first prism layer was evaluated by varying
the thickness from 0.1 to 2mm. The core prism size varied from 1.33 – 4mm. Finally, the prism inflation, which is the growth rate of the prism layers from the first, smallest, layer was varied from 1.5-2.5. The results of the numerical solution were compared to analytical, where possible, and experimental benchmarks. They concluded that results were most sensitive the first prism size, and that small inflation factors produced best results, but that the inflation factor of 1.5 was still too large for the geometry considered. The study admitted that future work would be required for a more definitive conclusion regarding the optimum inflation size.

Newer techniques to control the overall mesh size, while achieving high resolution areas have been studied, and include programs to automatically refine areas meeting certain criteria indicating further refinement is required. This saves the CFD engineer time by reducing the time spent manually examining the mesh and determining which regions need to be refined. These techniques may be useful for future consideration in the DUNE simulations.

Gao studied the techniques to automatically refine the mesh for numerical simulations of turbulent flow without increasing the overall computational costs beyond what is practicable [17]. The simulations were completed for aerodynamic geometries such as airfoils. He used criteria such as excessive y+ values and the size ratio of neighboring cells to flag cells for refinement. Specifically, his method called for refinement of cells with y+ values greater than 7 or cells that were more than twice the size of their neighbors. The study found that the local mesh refinements successfully improved the prediction of airfoil stall without significantly increasing the overall size of the computational mesh.
2.3 **Boundary Conditions**

Some of the most important parameters in a CFD model to obtaining an accurate solution are the boundary conditions. Boundary conditions are assumptions on fluid behavior at the bounds of the computational domain of the model. Boundary conditions set the fluid behavior characteristics such as flow through inlets and outlets, behavior near walls, and heat transfer properties, among others, which will be discussed in the methodology section of this report. This research investigated the shear stress specification’s effect on the simulation, and this section will focus on review of literature of that boundary condition.

The shear stress specification at the liquid-ullage interface determines the transport of the passive scalar, which enters the liquid region at this interface, since this boundary condition determines how the fluid flow at this interface, as will be discussed in the next section. The shear stress specification relates to the viscosity of the fluid, which describes a fluid’s resistance to deformation [28]. High viscosity fluids would be more resistant to deformation by shear stress and therefore more likely to fit the no-slip condition, while the opposite is true for low velocity fluids.

2.4 **Shear Stress Specification**

The shear stress specification allows the user to specify how the fluid flow is affected by shear forces along the wall. The no-slip condition maintains a traditional simplifying fluid mechanics assumption that the fluid adjacent to the wall has zero velocity, relative to the wall [29]. The slip condition assumes that the fluid slides along the wall without shear forces. The study of these assumptions predates CFD simulations,
and these conditions have been examined extensively in order to appropriately simplify the calculation of fluid flow characteristics.

The slip vs no-slip boundary conditions have been studied and debated with varying conclusions. In “The No-Slip Condition of Fluid Dynamics,” Day examines the historical acceptance of the no-slip idealization on the boundary condition of a fluid domain [29]. The no-slip condition is applicable for a solid-fluid boundary when the fluid molecules adhesions, attraction to solid molecules of boundary surface, is greater than the cohesion, attraction amongst the fluid particles. Day states that there have been four methods used to justify the no-slip assumption:

1) Experiments varying the surface
2) Comparing theoretical results using the no-slip assumption to experimental testing
3) Examining fluid behavior near solid surfaces
4) Justifications based on the physics interactions between fluids and solids.

He concludes that the no-slip condition is usually accepted for fluids that follow closely to the viscous theory of fluids but can often be rejected for fluids that can accurately be modelled by the ideal fluids assumption.

In his 2017 book Microfluidics: Modeling, Mechanics and Mathematics, Rapp discusses lab-based approaches to modeling, and includes a discussion on the slip vs no-slip boundary condition [30]. Rapp states that the no-slip boundary condition is a useful assumption for the boundary condition of most cases with a solid boundary and incompressible fluid. He further suggests that the slip condition must be used when the no-slip boundary condition is not appropriate.
NASA has successfully used the no-slip boundary condition to achieve accurate results for the fluid movement and heat transfer characteristics within a cryogenic fuel tank [31]. The NASA study considered the draining of a fuel tank containing ullage gases and liquid fuel. The purpose of the NASA simulation was to examine the heat transfer and velocity characteristics of a fluid within a fuel tank exposed to high heat fluxes to determine the optimum tank design.

2.4.1 Shear Stress Specification for Fluid-Fluid Interfaces

Most of the research completed on the shear stress specification boundary condition has been completed for solid-liquid interfaces. Limited research is available for the shear stress interactions between two differing fluids. Therefore, the liquid-gas interface in the DUNE detectors requires careful modeling consideration.

A study completed by Ta and Hague studied ozone contactor design and aimed to use CFD simulations to produce an accurate simulation of the experimental detector [32]. The contactors under consideration contained mixed flow conditions, with both natural and forced convection present. The study cited a lack of past work on two-phase (liquid-gas) models in CFD as a difficulty in modelling the interaction between the gas and liquid. This study used a frictionless water surface with zero shear stress, and the slip condition. They determined that their approach was able to accurately model the flow distribution for this two-phase model.

Another study investigating the shear stress specification at fluid-fluid interfaces was completed by Ng et al [33]. They studied the shear effect on slip length for liquid-gas interactions and aimed to create an analytical liquid-gas coupled model to simulate this.
shear effect. The conditions studied in their analysis was a pressure-driven flow of viscous fluid through two parallel surfaces with gas filled grooves. They determined that slip occurs along the liquid gas interface, which would violate a no-slip assumption model, and that even small liquid to gas viscosity ratios can lead to a large effect on the slip length.

Studies have indicated that more refined models may be necessary to accurately the conditions of multiphase interfaces. Recent studies have investigated modifications on the traditional slip and no-slip boundary conditions to create more realistic models. These studies have indicated that more nuanced boundary conditions at the multiphase interface may resolve fluid interactions more accurately than the idealized slip and no-slip conditions.

Sibley et al. performed an analytical study in 2013 on a solid-liquid-gas system with a moving interface at the fluid-fluid boundary [34]. Their model used the viscosities of the fluids as general functions so that the model could be applied for fluids of the same or differing viscosity ratios. They determined that the no-slip condition can be used to accurately model the interface even in the case of a moving contact line if the sharp liquid-gas interface is relaxed. This is achieved by using the diffuse-interface method, which uses a continuous transition from liquid to gas or gas to liquid, rather than an instant property and phase change at the interface. They determined that these conditions resulted in an accurate solution of the stress, pressure, and fluid velocity. Table 2.2 summarizes the studies reviewed and the shear stress specification boundary condition used.
In addition to the shear forces and velocity profiles at the liquid-gas interface, it is important to properly model the heat transfer at the interface. At the interface between the liquid and gas, liquid is continuously evaporating into the gaseous region while gas condenses into the liquid region. This process of evaporating the warmer liquid argon as it circulates to the top of the detector and purging gaseous argon from the top of the ullage region is vital in maintaining the cryogenic temperatures within the detector. This results in significant heat transfer between the regions, and accurate modeling of heat transfer is critical to accurately resolving the liquid-gas interface.

Vinnichenko et al. studied the heat exchange near the liquid-gas interface for evaporating water and ethanol, comparing the evaporating structures of the two fluids [35]. They used thermal imaging to experimentally observe these processes and compared the results to numerical simulations. They discovered water exhibited slow heat transfer across the interface, while ethanol showed much faster heat transfer across the liquid-gas interface. This corresponded to the no-slip condition modelling the water interface accurately, but the no-slip condition was not appropriate to accurately model the liquid-gas interface of ethanol. They stated that the heat transfer near the surface of the interface is highly dependent on the motion boundary condition. Furthermore, they stated that this surface motion depends on the surface tension properties of the liquid, and that liquids with high surface tension are more likely to be accurately modelled by the no-slip condition.
Table 2.1 Summary of Shear Stress Specification Boundary Condition

<table>
<thead>
<tr>
<th>Interface Type</th>
<th>Study Topic</th>
<th>Condition Used/Finding</th>
<th>Study</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solid-Fluid</td>
<td>Historical acceptance of no-slip</td>
<td>No-slip appropriate for viscous fluids</td>
<td>Day [29]</td>
</tr>
<tr>
<td>Solid-Fluid</td>
<td>Modeling microfluids</td>
<td>No-slip useful for incompressible fluids</td>
<td>Rapp [30]</td>
</tr>
<tr>
<td>Solid-Fluid</td>
<td>Cryogenic fuel tank</td>
<td>No-slip</td>
<td>Greer [31]</td>
</tr>
<tr>
<td>Fluid-Fluid</td>
<td>Ozone contactors</td>
<td>Slip</td>
<td>Ta and Hague [32]</td>
</tr>
<tr>
<td>Fluid-Fluid</td>
<td>Shear effect on slip length of liquid-gas interactions</td>
<td>No-slip condition violated at fluid-fluid interface</td>
<td>Ng. et. Al [33]</td>
</tr>
<tr>
<td>Moving Fluid-Fluid</td>
<td>Appropriate boundary condition for moving interface</td>
<td>No-slip can be used under certain conditions, but more complex conditions are ideal</td>
<td>Sibley et. Al [34]</td>
</tr>
<tr>
<td>Fluid-Fluid</td>
<td>Heat transfer near liquid-gas interface</td>
<td>No-slip for liquids with high surface tension</td>
<td>Vinnichenko et. Al [35]</td>
</tr>
</tbody>
</table>

2.5 Passive Scalar

A passive scalar can be used to track concentrations within fluid flow simulations. A passive scalar is an arbitrary, user-defined variable that acts like a dye within the fluid [18]. That is, the passive scalar can be used to track the concentration of the particle without affecting the physical flow of the fluid. Much of the research done using passive scalars in CFD simulations has been completed on modeling air pollutant dispersion, such as studies [19-22]. Passive scalars can also be very useful to model extremely low concentrations, such as for the impurities seen in the DUNE detectors.

One advantage of using passive scalars to model low concentrations is the simplification of the required computational mesh. It is difficult to resolve the
computational mesh enough to accurately represent very low concentrations, but scaling concentrations to a higher level may affect the flow of the fluid, depending on the particle being modelled. Because the passive scalar is modelled by one-way coupling, however, the concentration can be scaled to a detectable level without impacting the flow of the fluid [18].

2.5.1 Turbulent Schmidt Number of the Passive Scalar

An important characteristic of the passive scalar is the turbulent Schmidt number. The turbulent Schmidt number is a descriptor of the diffusivity for turbulent flow. The turbulent Schmidt number represents the ratio of turbulent momentum diffusivity and mass diffusivity [10]. When the turbulent momentum diffusivity is greater than the mass diffusivity the Schmidt number is greater than one.

Many studies have been completed to determine the ideal value of the turbulent Schmidt number for different CFD scenarios. Historically, values of 0.7-0.9 have been assumed to best represent the value of the turbulent Schmidt number for near wall turbulence in CFD simulations. This section will discuss the varying turbulent Schmidt numbers used to model passive scalars and the situations where other values may be advantageous.

A study completed by Baik et al. in 2003 developed a 3D CFD model to examine urban airflow and pollutant dispersion [19]. This study used the Reynolds-averaged equations and Boussinesq approximation to simplify the calculation of fluid flow. They examined three cases: an infinitely long canyon, a long canyon of finite length, and orthogonally intersecting canyons, to approximate urban geometries. This study utilized a
Schmidt number of 0.9 and determined that the model reached reasonable agreement with wind and water tunnel testing.

Santiago et al. also used a turbulent Schmidt number of 0.9 to produce results comparable to wind tunnel testing [20]. This study examined air flow inside an array of cubes 0.15m per side with 0.15m between cubes. The passive scalar particles were more concentrated at the downstream end of the model and in similar concentration patterns to those seen in the wind tunnel experimental results. The results showed that the main features of the passive tracer particles used in the wind tunnel were reproduced in the CFD simulations.

A 2007 study by Tominaga and Stathopoulous, however, indicated that finding the optimum turbulent Schmidt number may be highly dependent on the geometry and local flow characteristics under consideration [10]. This study reviewed many sources of CFD studies on the turbulent Schmidt number. The review revealed that many studies, such as Delauney’s study of atmospheric dispersion [23] and Kim et al.’s study on urban pollutant dispersion [24], determined that a turbulent Schmidt number of 0.9 produced good results, while others, such as Lien et al.’s study on numerical models for prediction of pollutant dispersion [25] and Bzroska’s examination of plume capture by building wakes [26], determined optimum values ranging from 0.63 to 0.8.

By examining the flow and geometry characteristics, Tominaga and Stathopoulous determined that lower turbulent Schmidt value produced better results for simpler geometries such as flow around single buildings, due to the tendency of higher Schmidt numbers to underestimate the turbulent momentum diffusion in these cases [10]. They also determined that for situations without this tendency, the typical turbulent Schmidt
values produce better results. They further recommended that the specific geometric under consideration be evaluated to determine the appropriate turbulent Schmidt number.

Gauding et al., studied the effect of varying the Schmidt number in CFD simulations for both Direct Numerical Simulations and Large Eddy Simulations [27]. This study examined the turbulent mixing of a passive scalar in a cube, while varying the Schmidt number from 0.11 to 5.56, holding the velocity and Reynolds number constant. They also determined that the optimum Schmidt number varies based on the scenario, specifically on the length scale and dominant energy transport within the system. Furthermore, they concluded that the turbulent transport of the passive scalar is reduced for smaller Schmidt numbers. Table 2.1 shows a summary of the findings regarding the turbulent Schmidt numbers.

**Table 2.2 Summary of Studies on Optimal Turbulent Schmidt Values.**

<table>
<thead>
<tr>
<th>Turbulent Schmidt Range</th>
<th>Comments</th>
<th>Study</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.7-0.9</td>
<td>Reaches reasonable agreement for pollutant dispersion</td>
<td>Baik [19], Santiago [20], Delauney [23], Kim [24]</td>
</tr>
<tr>
<td>0.63-0.80</td>
<td>Provides better pollutant dispersion modeling, especially in building wakes</td>
<td>Lien [25], Bzroska [26]</td>
</tr>
<tr>
<td>0.2-1.3</td>
<td>Varies based on flow geometries and properties</td>
<td>Tominaga and Stathopoulus [10]</td>
</tr>
<tr>
<td>0.11-5.56</td>
<td>Varies based on length scale and dominant transport (laminar/turbulent)</td>
<td>Gauding et al. [27]</td>
</tr>
</tbody>
</table>

In the case of the DUNE simulations, however, the geometry is more complicated than flow around a single value, so the advantages found Tominaga Stathopoulous found
in lower turbulent Schmidt numbers for simple cases may be less applicable. The default value of 0.9 was used in previous simulations at SDSU that reached relatively high agreement with the experimental impurity distribution, as discussed previously [10]. This analysis will include a study on the effect of varying turbulent Schmidt numbers on the impurity distribution.

2.6 Key Findings and Conclusions

1) Local mesh refinements have been used to successfully achieve appropriate mesh resolutions while preventing excessive mesh sizes.

2) Determining critical areas of the computational domain and limiting the finest mesh to those areas decreases computation cost, while providing sufficient accuracy.

3) Proper prism layer settings are key to providing an accurate solution.

4) The optimum turbulent Schmidt number is highly dependent on geometric and flow conditions.

5) No-slip conditions have successfully been used to achieve accurate results in many numerical studies, but complicated conditions caused by fluid-fluid interfaces require careful investigation.

These findings will be used for the focus of this thesis. Using local meshing techniques to refine critical areas within the computational domain will be of high importance to maintain a computationally efficient mesh while resolving the large and complex features of the DUNE Far Detector. Though the literature provides a good starting point for choosing the turbulent Schmidt number, further investigation will be required in this thesis to determine an optimum value. Previous work and literature
review indicate that a no-slip condition may be appropriate at the liquid-ullage interface, but this thesis will examine both conditions to verify that the no-slip condition yields optimum results.
3. METHODOLOGY

This chapter will discuss the methodology used to perform the CFD simulations used in this thesis. The methods used to evaluate the effect of differing mesh refinements, the slip vs. no-slip boundary condition at the liquid-ullage interface, and varying values of the turbulent Schmidt number on the temperature and impurity distribution within the detector. It is anticipated that mesh will reach a level of refinement where increasing the number of cells will have negligible impact on the solution. Based on previous work at SDSU, it is expected that the no-slip condition will produce a higher overall temperature within the detector and greater concentration of impurities. The turbulent Schmidt number is expected to produce large differences in impurity concentrations but no change in the temperature distribution.

3.1 Far Detector Simulation

In this investigation, the DUNE Single Phase Far Detector was modeled and simulated. These simulations were completed on the South Dakota State High-Performance Computing Cluster (HPC). Creating an accurate CFD model of the Far Detector required several steps. First was building a 3D computer-aided design (CAD) model representative of the geometry inside the cryostat. It was important to simplify enough to provide computational efficiency, while maintaining enough detail to achieve retain accuracy. The assumptions made in this process will be covered in a later section.

Next, physics continua were set up to properly represent the properties of the materials present in the cryostat. This involves setting the CFD model assumptions for calculation of flow characteristics such as the Boussinesq approximation, constant
density assumption, segregated flow model, and other simplifying assumptions for the flow. The physics continua also determine the material properties, for example, the density, dynamic viscosity, and thermal conductivity, among other properties. Then boundary conditions were established to determine flow and heat transfer conditions. This determines how the model calculates the behavior at the outer surface of each region and the interaction between regions. These steps will be further explained in later sections of this chapter.

The Far Detector has a complex geometry to detect the presence and activity of neutrinos. The assembly consists of an outer insulation, three anode plane assemblies (APA), two cathode plane assemblies (CPA), field cage planes along the top, bottom, front, and back of the APA and CPA planes, grounding planes above and below these elements, a service floor, a system of pipes for incoming liquid argon, and many other less significant features. An exploded view of the simplified model of the cryostat geometry is shown in Figure 3.1.
The cryostat within the insulation contains a mixture of liquid and gaseous argon, with liquid argon filling approximately 95-95% of the cryostat by volume, with gas filling the remaining space (hereafter referred to as the ullage region). The liquid and gaseous regions were modelled separately, as in previous work on Proto-DUNE simulations [9], and the results the liquid region can be used as an input boundary condition at the liquid-ullage interface for the ullage region.

Within the cryostat, the region designed for the detection of neutrinos is referred to as the Time Projection Chamber (TPC). This region is enclosed by the outer APA planes and field cage planes and contains the CPA planes and the center APA plane. As discussed previously, the CPA and field cage planes enclose an electric field to drift electrons toward the APA planes. This region is where the focus of the DUNE data
collection will take place, making it critical to determine the impurity distribution within the TPC. This region is fully contained within the liquid portion of the cryostat.

The liquid argon enters the cryostat through 128 inlets, sized and spaced to create equal flow through each inlet, across the bottom of the cryostat. These outlets are placed in two separate U-shaped pipes within the cryostat, shown as the outer pipes in Figure 3.2, and blue pipes in Figure 3.3. The inner pipes in Figure 3.2, shown in red in Figure 3.3, will be used for filling the cryostat, before being closed. The LAr exits the cryostat and enters the filtration system through four equally spaced outlets at one end of the cryostat. The filtration system purifies the LAr by removing the impurities in the form of oxygen and water. Studies performed by Fermilab indicate that after the filtration process liquid argon returns to the cryostat 0.44 K warmer that it exits through the outlets [8].
Figure 3.3 Shows a close up of piping system, with filling pipes shown in red and inlet pipes from filtration system shown in blue.

The ullage region consists of many ports (shown in Figure 3.4) where gaseous argon exits the cryostat. The gas leaving the ullage region is condensed into liquid and sent through the filtration system with the liquid argon leaving the cryostat, before returning as purified liquid argon. The ullage region is used to cool the cryostat by allowing liquid argon to evaporate and the liquid-ullage interface. The liquid-gas interface has a constant pressure, and the temperature of the interface is set to the transition temperature of argon from liquid to gas at the given pressure.

Figure 3.4 Diagram showing ports in the ullage region (top view) [37].
Though some work has been completed to set up the ullage model, the design process of the ullage space is ongoing, with future changes still expected. An initial model of the ullage region is shown in Figure 3.5, with an exploded view separating the gaseous argon region from the insulation region. The pumping and filtration system is outside the scope of this analysis, and information about these processes has been determined by studies from Fermilab and other groups within the DUNE project [8]. These studies will provide inputs for the boundary conditions in the liquid region. Therefore, the focus of this thesis will be on proper modeling and simulation of the liquid region.

![Figure 3.5 Exploded view of ullage model, with gaseous region shown below insulation (isometric view).](image)

3.2 Simplifying Assumptions

3.2.1 Steady-State Conditions

The cryostat was assumed to reach steady-state conditions after the tank was filled and operating. The Far Detector is planned to remain closed and under constant operation for at least 20 years, justifying this assumption [4]. The cryostat will likely experience
small temperature fluctuations with time, but in the case of Proto-DUNE these fluctuations were within 3 mK and proved insignificant to the overall results and temperature distribution.

3.2.2 Liquid Argon Properties

The properties of the liquid argon were also assumed to remain constant with temperature. The temperature range within the cryostat was less than 0.5 K, so the variance in temperature-dependent properties is negligible. The mass flux of liquid argon evaporating from the liquid-ullage interface was also considered negligible relative to the liquid argon leaving the cryostat through the outlets. In the Proto-DUNE experiment, the boil off was approximately five to seven g/s compared to 1.67 kg/s through the outlet [9], or less than 0.3% of the flow through the outlets.

3.2.3 Liquid Argon Flow

The flow of liquid argon can enter the cryostat through either of two sets of 128 inlets. After initial filling, the mass flow of liquid argon to maintain purity is 10 kilograms per second. The piping system was determined to negligible geometrically, relative to other components in cryostat. The inlets were modeled as circular holes in space through which the liquid argon entered the cryostat. The boundary condition is specified as a mass flow inlet of 10 kg/s entering the cryostat upward. The liquid argon enters the cryostat 0.4418 K warmer than the liquid argon exiting the outlet to account for heat added by the filtration and pumping system, as determined by studies at CERN and Fermilab [8].
The liquid argon exits the cryostat through four outlets located at the end of the cryostat. At steady-state conditions the flow through the outlets will match the flow from the inlets, 10 kg/s or 2.5 kg/s from each outlet. The outlets are four 350 mm holes through the insulation thickness of 800 mm, with the center of each outlet approximately 550 mm above the cryostat floor. The flow into the filtration system was not modelled, as this was outside the scope of this analysis. The boundary condition for the outlets was flow split outlets with an equal split ratio for each outlet to ensure 2.5 kg/s flow through each outlet. A diagram of the Star-CCM+ model showing the location of the inlets and outlets is shown in Figure 3.6.
3.2.4 Boussinesq Approximation

Flow in fluids dominated by natural convection is driven by buoyancy differences due to variable density. The density differences are usually due a temperature gradient, warmer fluid being less dense than cooler. When the fluid warms it expands and rises, while cooling fluid contracts and sinks. Thus, temperature gradients within the fluid create circulation zones, where flow cycles throughout the fluid domain as the temperature changes.
Closure of the Navier-Stokes equations quickly becomes prohibitively complex when the density term is variable, however. The density term is repeated many times in the Navier-Stokes equations. Introducing this much variability requires vast computational costs to simulate. Therefore, a model simplifying the method to consider buoyancy and density effects on fluid flow is required to reduce computational costs.

The Boussinesq approximation is a model to simplify the calculation of fluid circulation due to density differences. The computational cost is reduced with the assumption that the density differences are only considered in the buoyancy term of the momentum equation, while the density term is considered constant elsewhere [38]. The Boussinesq approximation can be represented by Equation 3.1

\[ \rho_\infty - \rho = \rho \beta (T - T_\infty) \quad \text{Eq. 3.1} \]

This assumption limits the Boussinesq model’s accuracy to those models with small density differences within the fluid. The term small density difference is relative to the fluid and required precision of the model, but the previous work at South Dakota State University considered less than 1-degree Kelvin a sufficiently small range [7]. For models with larger temperature gradients, varying density differences must be considered throughout the Navier-Stokes equations to ensure accuracy as these larger differences have significant effect on more than just the buoyancy. However, it can be very effective at simplifying the computation of fluid flow due to buoyancy effects in models with small temperature differences.
3.2.5 Atmospheric Conditions

The DUNE Far Detectors will be located nearly a mile underground at SURF, which coincidentally means the detectors are at sea level, since SURF is one mile above sea level at ground surface. This led to atmospheric conditions surrounding the cryostat of about 104.5 kPa of atmospheric pressure and an ambient temperature of approximately 294.15 K. These values are assumed constant surrounding the cryostat. The cryostat is insulated and as will be demonstrated in the results section of this thesis, the results are expected to be robust against small fluctuations in atmospheric pressure and temperature. A drainage system has also been implemented at SURF to keep excessive groundwater from penetrating to the cavern containing the cryostat [6].

3.2.6 Liquid-Ullage Interface Conditions

The boundary conditions at the liquid-ullage interface are critical to the results of the simulations and were carefully chosen after research, discussion, and comparison of Proto-DUNE experimental and CFD results. The Proto-DUNE analysis determined that a constant temperature of 87.593 K and shear stress specification of slip condition yielded simulations most similar to results seen in the experimental model [9]. Similar conditions are expected in the Far Detector, and the temperature was also set to 87.593, and the results were compared for the shear stress specification using the slip and no-slip conditions.

3.3 Geometry CAD Modeling

Solidworks modeling software was used to create a 3D CAD model of the Far Detector. The cavity features created a liquid region that the filled the empty space within
the insulation and around the solid features, such as APA, CPA, ground, and field cage planes in the cryostat. This enabled the liquid regions to precisely align to the space within the cryostat. Figure 3.7 shows a view of the liquid model, with transparent insulation to show the inner features of the cryostat.

3D CAD model of the liquid region of the Far Detector.

![3D CAD model of the liquid region of the Far Detector.](image)

Figure 3.7 3D CAD model of the liquid region of the Far Detector.

### 3.3.1 Insulation

The insulation is modelled as 800-mm-thick polyurethane insulation surrounding the cryostat. The 12 mm corrugated stainless-steel plates that will be constructed around the insulation were neglected in this model. The focus of the insulation in the model is the effect of the heat transfer from the ambient air to the cryostat. The effect of the stainless steel on the heat transfer from the ambient air to the cryostat is considered negligible as the thermal conductivity of stainless steel is approximately 500 times higher than that of the insulation. The solid features as modelled in Star-CCM+ are shown in Figure 3.8.
3.3.2 Features Modeled as Porous Media

Many features within the cryostat are made of small, complex, geometric features such as wire arrays rather than solid planes. Accurately resolving these features within a CFD simulation would require an impracticable amount of time and computing power. Therefore, these regions were modelled as porous regions represented by solid features. This allows liquid argon flow through the planes as if these were not solid regions, without modelling the extensive wire mesh, which is a similar method to that used to model the Proto-DUNE cryostat, which compared favorably to the experimental results.

Modelling features as porous regions requires the calculation of certain properties such as: porosity, porous inertial resistance, and viscous inertial resistance. Previous studies were conducted at SDSU [7] and Fermilab [8] to determine resistances of the APA, field cage, and ground planes. These studies modelled a small section of the planes using the precise geometry and determined the pressure drop across the planes based on properties of the fluid. The calculations were performed at multiple velocities and a
quadratic regression line was used to model the relationship between the velocity and the pressure drop. Table 3.1 shows the properties of the porous features as modelled in Star-CCM+.

Table 3.1 Properties of Porous Model Features.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Porosity (% open)</th>
<th>Porous Inertial Resistance (kg/m$^4$)</th>
<th>Viscous Inertial Resistance (kg/m$^3$-s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>APA Planes</td>
<td>0.73</td>
<td>11,264.2</td>
<td>118.6</td>
</tr>
<tr>
<td>Field Cage</td>
<td>0.23</td>
<td>411,280</td>
<td>247.4</td>
</tr>
<tr>
<td>Ground</td>
<td>0.10</td>
<td>$2.373 \times 10^7$</td>
<td>4,007</td>
</tr>
</tbody>
</table>

3.3.3 Impermeable Features

Other features in the cryostat are impermeable, thus simplifying the model. Though the CPA planes also consist of smaller geometric features, they are impermeable which can be sufficiently modelled by solid planes. The service floor is also accurately represented by a solid plane. These features are completely immersed in the liquid argon, but block the flow, so that the liquid must flow around the boundaries of these features, which contributes greatly to the temperature gradient within the cryostat. Most significantly, the service floor is located directly above the liquid argon inlets, separating the flow of the warmer entering argon from the cooler liquid argon in the TPC, creating a warmer region below the service floor.
3.4 CFD Settings

3.4.1 Mesh Settings

The computational mesh in these simulations consisted of varying sizes. The mesh used for most simulations in this analysis consisted of a total of 60.6 million cells. The base size for mesh was 0.285 m for the solid regions and 0.185 m for the liquid regions. Custom controls, which will be discussed later in this analysis, were used to refine the mesh in critical areas of the simulation.

Polyhedral cells were used in the insulation region of the mesh to allow more customized shape control, while trimmed cell mesher was used in the other regions to reduce the computation cost by concentrating the refined mesh on areas of more complex geometry. The number of prism layers varied from 7-12 layers based on the geometry of the regions. For complex areas in the model, more prism layers were required to accurately capture the fluid flow. A section view of the mesh is shown in Figure 3.9, demonstrating the coarser mesh in the insulation region and increased cell refinement near areas of complex geometry.
A mesh sensitivity study was performed to determine the grid sensitivity of the solution. The goal was to create a robust model, where the solution was not significantly impacted by minor changes in the mesh. The model robustness was studied by analyzing the differences in the solution among four levels of mesh refinement. The cell meshes are summarized in table 3.2. The similarities and differences of the results from the differing mesh sizes will be discussed in the results section of this analysis.
Table 3.2 Levels of mesh density for mesh refinement study.

<table>
<thead>
<tr>
<th></th>
<th>Number of Cells (in millions)</th>
<th>Solid Region Base Size (m)</th>
<th>Liquid Region Base Size (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh 1</td>
<td>40.8</td>
<td>0.32</td>
<td>0.26</td>
</tr>
<tr>
<td>Mesh 2</td>
<td>56.0</td>
<td>0.30</td>
<td>0.20</td>
</tr>
<tr>
<td>Mesh 3</td>
<td>58.9</td>
<td>0.29</td>
<td>0.19</td>
</tr>
<tr>
<td>Mesh 4</td>
<td>60.7</td>
<td>0.285</td>
<td>0.185</td>
</tr>
<tr>
<td>Mesh 5</td>
<td>65.5</td>
<td>0.28</td>
<td>0.175</td>
</tr>
<tr>
<td>Mesh 6</td>
<td>151.6</td>
<td>0.25</td>
<td>0.15</td>
</tr>
</tbody>
</table>

3.4.3 Mesh Refinement in Critical Areas

Computational power and time constraints are the most significant limiting factors in the accuracy of CFD simulations. Natural convection driven flows require especially well resolved meshes since subtle differences in temperature will affect the flow of the fluid. To maximize the efficiency of available computational resources, the computational mesh of the model was concentrated on areas that required a particularly fine mesh to resolve flow characteristics. By focusing the refinement on critical areas, the total number of cells required for the model was reduced, decreasing the time required for the solution to reach convergence.

Several factors were considered when determining which regions of the model would require increased mesh refinement. The complexity of the geometry, relative turbulence of fluid flow, importance of results, and discontinuities in initial simulations were among the factors that determined which regions required mesh refinement. The coarsest mesh was used in relatively open areas with small temperature gradients, since
the flow in the areas was easiest to resolve. The area surrounding the inlets and outlets, for example, were deemed especially important to solution and were refined to a higher mesh resolution. Another region requiring careful refinement was near walls.

3.4.3.1 Wall Treatments

Proper mesh refinement and treatment is especially critical for fluid flows near the walls of the system under consideration. As seen in classical fluid dynamics problems, flow over a plate or past a boundary is affected by the boundary surface. The fluid affected by the boundary is contained within a layer known as the boundary layer. Fluid behavior within the boundary layer is complicated, with very high velocity gradients within the boundary layer, and therefore requires additional modeling considerations.

One additional feature required to accurately resolve the fluid flow in the boundary layer is prism layers. Prism layers are layers of cells orthogonal to a wall or boundary that provide additional mesh refinement and customization options in the boundary layer [18]. Layer thicknesses, the number of layers, and the size distribution amongst layers are a few of the characteristics that define the mesh in the prism layers. These characteristics determine the wall y+ values of the model, which are discussed in a later section. Prism layers are crucial in providing accurate near-wall characteristics including, heat transfer, flow separation, velocity, and temperature [14].

Prism layers also reduce error propagation in the model, by reducing what is called numerical diffusion [18]. Numerical diffusion is a discretization error that can propagate throughout a model, originating from discontinuities, which can be caused by a lack of resolution in the boundary layer. When cell sizes near the wall are too large, a solution discontinuity may be created, forcing an illogical solution for a characteristic
such as temperature or velocity, which can propagate throughout the entire model when the CFD software iterates to achieve a solution. Usually this results in model failure, which makes proper prism layer selection even more critical.

There are three common treatments to wall y+ values used to obtain accurate near wall turbulence in CFD simulations: low wall y+, high wall y+, and all y+. The y+ value relates the size of the cell and the distance of the centroid of the near wall cell to the wall with the relative velocity and shear stress within the cell. The equation used to calculate y+ values is given in Equation 3.2 [39].

\[ y^+ = \frac{y \mu}{u^* \rho} \text{ and } u^* = \sqrt{\frac{\tau_w}{\rho}} \]

Eq 3.2

Where: \( y^+ \) = dimensionless wall distance, \( u^* \) = friction velocity, \( y \) = distance to wall adjacent cell centroid, \( \mu \) = dynamic viscosity, \( \rho \) = density, and \( \tau_w \) = wall shear stress

It is important to verify that the prism layers are properly set up to achieve the wall y+ values assumed in the wall treatment setting. Reducing the thickness of the prism layers can be used to reduce wall y+ values as this decreases the distance to the centroid of the wall adjacent cell, as shown in Eq 3.2. Increasing the number of prism layers, while holding the total thickness constant, is another way to reduce the wall y+ values.

3.4.3.2 Low Wall Y+ Values

Low wall y+ treatment does not require special treatment near the walls but uses the fluid dynamics governing equations all the way through the fluid domain right up to the wall. This treatment assumes that the viscous sublayer of the boundary layer can be completely resolved by a fine mesh [18]. The fine mesh is required to resolve the
transition from laminar flow to turbulent flow that occurs within the viscous sublayer. The wall y+ values should be less than or equal to one for this treatment to maintain accuracy. This wall treatment is appropriate for models with low-Reynolds flow.

3.4.3.3 High Wall Y+ Values

High wall y+ treatments model the viscous sublayer of the boundary layer. This involves calculating the near wall shear stress, turbulent production and dissipation, which is more computationally expensive than the low wall y+ assumptions [39]. This increase in computational cost is introduced by assuming that the viscous sublayer is not completely resolved by the mesh and requires further calculations by the model to determine flow within this sublayer. The wall y+ values should be greater than 30 to meet the assumptions of the high wall y+ treatment, which is appropriate for high Reynolds number flows [18].

3.4.3.4 All Wall Y+ Values

The all wall y+ treatment method seeks to combine the low and high wall y+ treatments. This treatment is the most versatile treatment method and can be very useful for models where it is difficult to obtain a very fine or highly resolved mesh in all areas near the wall. This wall treatments can obtain accurate results for a wide range of y+ values but is best for values less than one or between 30 and 50 [39]. The versatility of this method is that it can obtain results similar to the high wall treatment for areas of coarse mesh, while getting results close to the low wall treatment for areas of finer mesh. Models with complex geometries may contain areas where the boundary layer and viscous sublayer is difficult to resolve. Customizing the mesh to obtain a narrow range of wall y+ value throughout the model can become difficult and
time-consuming for these cases. This makes the all wall y+ model appropriate for models with complex geometries.

Achieving the proper y+ values required some trial and error. Since the all y+ treatment was used in this analysis, the ideal wall y+ values were <1 or 30-50. The simulations were run until the residuals converged, and then the wall y+ values were examined for each region. Then, the number of prism layers and the overall thickness of the prism layers was adjusted to increase or decrease the wall y+ values into the proper range. This process was repeated until the wall y+ values were near the ideal ranges, with most values near or less than one for the internal features of the cryostat, as shown in Figure 3.10, for the all y+ treatment to ensure accurate calculation of the flow near the walls. Values in some areas exceeded this ideal range, but the advantage of the all y+ treatment is model robustness against varying wall y+ values.

![Figure 3.10 Wall y+ values for inner features of the cryostat.](image)

3.5 **Custom Controls**

Custom controls are used to tailor the mesh in model to achieve the desired refinement in each region of the model. Star-CCM+ contains several options for customizing the mesh. Surface controls, volume controls, part controls, and curve
controls are among these options. This analysis utilized parts-based meshing to create the computational mesh, which means that the base mesh setting was set for each part within the model, and surface and volume controls to refine the mesh in critical areas.

### 3.5.1 Volume Controls

Volume controls refine the mesh within a given volume of space. A volume control was used to refine the mesh surrounding the outlet region of the model in Star-CCM. This region contained complicated streamlines as flow moved into the outlets and heat transfer from the warmer insulation to the liquid argon as it travelled through the outlets. These factors complicated the computation in this region and required a higher mesh resolution to accurately resolve flow. The volumetric control refined the base size in this region to 0.03 meters, which equates to 10% of the base size in the liquid region.

Figure 3.11 shows the region where this volumetric control refined the model mesh.

![Figure 3.11 Volumetric control area highlighted.](image)
3.5.2 Surface Controls

Surface controls refine the mesh on a specific surface of the model. This can be especially useful for complicated interfaces between regions of differing materials or phases. Surface controls were used to refine the mesh on the inlet and outlet surfaces, the interface between the insulation and outlets, and the regions of discontinuity on the inner insulation surfaces.

The target surface size for the interface and the discontinuous regions was 0.15m, or 50% of the base size for solid features, while the target surface size on the inlets was 0.002 m, only 1% of base, due to the very small inlet surface area, relative to the other features of the cryostat. The inlet surfaces were only five centimeters in diameter, so a much smaller mesh size was required to ensure a sufficient number of cells on the inlet surfaces. The outlet surfaces utilized used a 0.01 m base size, 5% of the base size of the liquid region. The inlets and outlets also customized the number of prism layers and total prism layer thickness to resolve the fluid flow. Figure 3.12 highlights the mesh areas customized by a surface control.
3.6 Remeshing Discontinuous Regions

Some areas of the mesh produced discontinuous or illogical values for the temperature in the initial solutions. This indicated an error in the mesh calculations. Since the computational mesh already consisted of over 50 million cells, further refining the base size would result in a large reduction of computational efficiency. Therefore, a custom control was required to refine the areas causing the discontinuities without refining the entire model. These areas were found using the threshold values discussed in the next section.

3.6.1 Threshold Values

The threshold function in Star-CCM+ can be used to highlight groups of cells inside or outside a specified range of values. This function was used to search and separate regions of cells that reached an illogical solution. Since the liquid argon is
entering the cryostat at 87 K, varying less than 1 K throughout the cryostat, and the ambient temperature surrounding the insulation is 294 K, a threshold function was created to find cells that returned temperature values greater than 300 K or less than 85 K.

These cells were grouped into a cell set and tagged for remeshing. Then a custom surface control was applied to this cell set and the mesh for these cells was refined. The surface control refined the cells within the set to 50% of the base cell size for the solid regions. Subsequent simulations showed that these refinements resulted in solutions without discontinuities. Figure 3.13 shows the cell set of these threshold cells highlighted in Star-CCM+.

![Figure 3.13 Cell set highlighting areas containing discontinuous solution of initial mesh.](image-url)
3.7 Physics Models

3.7.1 Turbulence Models

The selection of the proper turbulence models was based on previous work conducted at South Dakota State University. Simulations for previous models yielded results similar to those seen in the experimental prototypes conducted at CERN. Since the Far Detector is expected to run similarly, though on a larger scale, than previous prototypes, similar turbulence techniques will be applied for the application of the Far Detector.

The $k-\omega$ turbulence and SST (Menter) models were found to be preferable to the $k-\varepsilon$ turbulence model for the conditions under consideration. The $k-\omega$ model delivers superior performance near walls, and though the $k-\varepsilon$ model often produces better results for open flows, the SST modification to the $k-\omega$ model yields improved freestream performance. This provides more versatile modelling of natural convection, ideal for the complex geometry seen in the Far Detector.

3.7.2 Heat Transfer Properties

The heat transfer from the ambient air surrounding the Far Detector to the insulation was modelled with a convective boundary condition. The heat transfer coefficient was approximated as 10 W/m$^2$-K. An approximation was deemed sufficient for the heat transfer coefficient after the thermal resistance due to convection was shown to be negligible relative to that for conduction through the insulation. As the calculations below show, the thermal resistance due conduction is more than 300 times the resistance due to convection, therefore even a change of 10-50\% the convection coefficient would
have a negligible effect on the temperature within the cryostat. The calculations for the ratio of resistance from convection to conduction, are shown here:

Conduction Area (Inner walls):

\[ A_{\text{cond}} = 2 \times (62 \text{ m} \times 13.37\text{m}) + 2 \times (15.1\text{m} \times 13.37\text{m}) = 2061.65 \text{ m}^2 \quad \text{Eq. 3.3} \]

Convection Area (Outer walls):

\[ A_{\text{conv}} = 2 \times (63.6\text{m} \times 14.17\text{m}) + 2 \times (16.7\text{m} \times 14.17\text{m}) = 2275.70 \text{ m}^2 \quad \text{Eq. 3.4} \]

\[ k = 0.00012222 \times \text{T} + 0.0048706 \quad \text{Eq. 3.5} \]

\[ k_{\text{Outer surface}} = 0.00012222 \times (294.15) + 0.0048706 = 0.0157115 \text{ W/m-K} \]

\[ k_{\text{Inner Surface}} = 0.00012222 \times (88.7) + 0.0048706 = 0.0408216 \text{ W/m-K} \]

\[ k_{\text{Median}} = 0.028267 \text{ w/m-K} \]

\[ R_{\text{cond}} = \frac{L}{K \times A_{\text{cond}}} = \frac{0.8}{0.028267 \times 2061.65} = 0.0137 \text{ K/W} \quad \text{Eq. 3.6} \]

\[ R_{\text{conv}} = \frac{1}{K \times A_{\text{conv}}} = \frac{1}{10 \times 2275.70} = 0.0000439 \text{ K/W} \quad \text{Eq. 3.7} \]

\[ \frac{R_{\text{conv}}}{R_{\text{cond}}} = \frac{0.0000439}{0.0137} = 0.0032 \quad \text{Eq. 3.8} \]

The heat transfer conditions for most solid features within the cryostat was set to adiabatic. In Star-CCM+ this indicates that the boundary surface is set to the temperature of the adjacent fluid. The electronics, however, were set to a heat source boundary condition. Prior experimental work and studies on the Proto-DUNE model have shown that the electronics within the cryostat give off heat into the liquid argon. Each of the six sections of electronics, one section location above and below each of the three APA planes, were estimated to provide 3,950 W to the cryostat [8].
3.7.3  Physics Settings

The physics settings used in this simulation are the same as used and validated in previous work completed at South Dakota State University [7]. These settings have been validated by comparison to experimental results. Table 3.2 shows the physics settings for the liquid argon and for the solid continua.
Table 3.3 Physics settings used in Star-CCM+ model.

<table>
<thead>
<tr>
<th>Continua</th>
<th>Physics Model</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid &amp; Solids</td>
<td>Constant Density</td>
<td>Density changes neglected except in liquid buoyancy term calculated by Boussinesq approximation</td>
</tr>
<tr>
<td>Liquid</td>
<td>Boussinesq Model</td>
<td>Models buoyancy due to density differences</td>
</tr>
<tr>
<td>Liquid</td>
<td>Segregated Flow</td>
<td>Solves flow and energy equations independently</td>
</tr>
<tr>
<td>Liquid &amp; Solids</td>
<td>Steady State</td>
<td>Assumes solution does not vary with time</td>
</tr>
<tr>
<td>Solid</td>
<td>Segregated Energy</td>
<td>Energy equation for thermal profile</td>
</tr>
</tbody>
</table>

The properties of liquid argon used in the simulation are shown in Table 3.3.

Table 3.4 Properties of liquid argon for Star-CCM+ model.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>1387.0 kg/m³</td>
</tr>
<tr>
<td>Dynamic Viscosity</td>
<td>2.4982 × 10⁻⁴ Pa-s</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>1118.9 J/kg-K</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>0.12647 W/m-K</td>
</tr>
<tr>
<td>Thermal Expansion Coefficient</td>
<td>0.0045075 / K</td>
</tr>
<tr>
<td>Turbulent Prandtl Number</td>
<td>0.9</td>
</tr>
</tbody>
</table>

The solid continua modelled within the simulation include the polyurethane insulation and stainless steel. Stainless steel is used for several features inside the cryostat including the CPA planes and ground planes. The properties used for solid features in the Star-CCM+ simulation are listed in Table 3.4.
Table 3.5 Properties of solid features used in Star-CCM+ model.

<table>
<thead>
<tr>
<th>Property</th>
<th>Stainless Steel Value</th>
<th>Insulation Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>8055.0 kg/m$^3$</td>
<td>1050.0 kg/m$^3$</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>480.0 J/kg-K</td>
<td>1450.0 J/kg-K</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>15.1 W/m-K</td>
<td>*Field Function</td>
</tr>
</tbody>
</table>

The thermal conductivity of the polyurethane insulation is dependent on the temperature. Therefore, the thermal conductivity varies through the insulation layer of the Far Detector. The value ranges from 0.0157 W/m-K at the inner surface of the insulation to 0.0408 W/m-K at the outside surface. The insulation thermal conductivity is approximated by Equation 3.9:

$$ k = 0.00012222 * T + 0.0048706 $$  
Eq. 3.9

3.8 Liquid-Ullage Interface Conditions

The conditions at the liquid-ullage interface are critical to the accuracy of the solution. The conditions at this interface were studied in previous work at South Dakota State University and validated by experimental results produced by CERN [9]. The optimal shear stress specification at this interface was the slip condition for most of the ProtoDUNE simulations, but this analysis further examined the effect of shear stress specification on the Far Detector simulations. Simulations were completed for both the slip and no-slip conditions, and the results are compared in Chapter Four of this analysis. The temperature of this interface was set to the saturation temperature of liquid argon under the assumed conditions, 87.593 K.
Studies at Fermilab have shown most of impurities enter the liquid region through the ullage region, so the impurities were set to enter the liquid region through this interface by means of a passive scalar flux. The important feature of the impurities to be determined by this analysis was the relative distribution of impurities, rather than the absolute quantity, therefore a unit flux of impurities was sufficient to model the impurities, and the actual quantity of impurities was not important.

3.9 Using Passive Scalars to Model Impurities

3.9.1 Passive Scalar Definition

A passive scalar is an inert variable that can be used in CFD simulations to track fluid flow characteristics similar to the injection of a dye into a fluid [18]. The passive scalar is a user-defined variable that does not affect the flow of the fluid in the simulation. Since the predicted impurities in the Far Detector are on the scale of parts per trillion (ppt), they will have negligible impact on the physical flow of liquid argon. Modelling the simulation to a resolution where the distribution of impurities on a scale of parts per trillion is resolved is not feasible with the current capabilities of processing power, however, so using passive scalars to model a relatively higher concentration of impurities with impacting fluid flow or characteristics is ideal.

3.9.2 Turbulent Schmidt Number Study

The turbulent Schmidt number characterizes the ratio of the rate of turbulent transport of momentum and mass for numerical simulations, as discussed in the literature review section of this report. The turbulent Schmidt number is difficult to characterize for the case of the DUNE Far Detector because the experimental model of the Far Detector
has not been completed at the time of this analysis to measure properties that would indicate a proper value for the turbulent Schmidt number. In order to determine the value for the turbulent Schmidt number, a study on the effect of varying the turbulent Schmidt number has been completed as part of this analysis. The simulation was run at the using turbulent Schmidt numbers of 0.5, 0.9, and 2.0 to compare the impact on the relative distribution of impurities.

3.9.3 Electron Lifetime

The electron lifetime is an important characteristic to determine that the cryostat impurity level is low enough to allow proper neutrino detection. The electron lifetime must be long enough to allow electrons to drift to APA planes for detection before they attach to the impurities in the form of water and oxygen. Studies by Fermilab have determine the equation for estimating the electron lifetime, with all impurities converted to impurity equivalent water molecules for simplification [7], given in Equation 3.10:

$$
\tau_{\text{electron}} \,[\mu s] = \frac{30 \times MW_{H_2O}}{10^9 \times MW_{Ar}} \frac{kg_{H_2O}}{kmol} \frac{kg_{H_2O}}{kg_{Ar}} \frac{kg_{Ar}}{kmol} \frac{kmol}{IMPURITY DENSITY} \frac{IMPURITY DENSITY}{kg_{Ar}} \frac{IMPURITY DENSITY}{kg_{Ar}}
$$

Eq. 3.10

3.9.4 Normalizing Impurity

The impurity values were scaled so that the average impurity within the cryostat was equal to one. The absolute impurities values are divided by the volume average of impurities to determine the value of impurities at each location, relative to the average. Then the standard deviation, and maximum and minimum values of impurity were determined. This provides insights into where impurities gather within the cryostat and can be used to determine possible design modifications.
4. RESULTS AND DISCUSSION

A discussion of the results of the simulations of the LBNF Far Detector will be presented in this section. The first part of this chapter will analyze the results of the mesh refinement study, comparing the results of three levels of mesh refinement for the temperature, impurity distribution, and fluid velocities. Next, the effect of the diffusivity setting on the passive scalar approximation will be examined. Then, the results for the slip and no-slip condition at the liquid-ullage interface will be compared. Finally, a comparison between the results predicted by the prototype detectors and the simulation results for the Far Detector will be discussed, as well as an evaluation of the updated Far Detector results compared to previous, simpler simulations of the Far Detector performed at SDSU.

It should be noted that the solutions presented in this chapter show a snapshot of the solution at 100,000 iterations. Though, the solution has converged at this point, the solutions still fluctuate slightly about the convergence point. This fluctuation is demonstrated by Figure 4.1, which shows the residuals of the simulation, which is the relative error at the current iteration compared to the initial error [18]. Therefore, slight variations may be expected with time. This analysis will look for trends and patterns to compare significant differences, rather than getting bogged down in the minutiae. These trends will be discussed further in the respective sections.
Figure 4.1 Plot of the residuals on Mesh 4 (60.7 million cells) from 95,000 to 100,000 iterations.

In reference to the coordinates displayed for the results, the outlets at one end of the detector are located at $Z = -29.35$ m, while the front end of the APA planes (opposite of the outlets) are located at $Z = +30.735$ m. The location for the $X = 1$m plane is a slice between the center APA plane and the CPA plane, while $X = -1$m is the same on the opposite side, and the $X = 4$m plane falls between the CPA plane and the outer APA plane. Figures 4.2 and 4.3 show a visual representation of these slices within the detector.
Figure 4.2 Geometry scene of surface slices in the Z direction, with field cage front and back planes shown in yellow.

Figure 4.3 Geometry scene of surface slices in the X direction.
4.1 Mesh Refinement Study

A mesh refinement study was completed to determine whether the solution was mesh independent. Mesh independence indicates that a small increase in the mesh density does not result in a significant change in the solution. To determine whether the model was independent of the mesh, the simulation was run for several different levels of mesh refinement. The custom control settings were kept constant but, as a percentage of the base size, they also changed to reflect changes in the base size of the mesh. The mesh refinement statistics are discussed in the methodology section and shown in Table 3.2.

4.1.1 Temperature Comparison

Below is a comparison of the temperature results for the differing mesh refinement levels. In each figure the results are shown from the coarsest mesh (Mesh 1) on the top left, to the most refined (Mesh 6) on the bottom right. The arrows show the velocity vectors of fluid flow tangential to the plane shown within the cryostat. These results are shown in Figures 4.4-4.10.
Figure 4.4 Temperature comparison at cross-section $Z = 20$ m.
Mesh 1

Mesh 2

Mesh 3

Mesh 4

Mesh 5

Mesh 6

Figure 4.5 Temperature comparison at cross-section Z = 0 m.
Figure 4.6 Temperature comparison at cross-section $Z = -20$ m.
Figure 4.7 Temperature comparison at cross-section Z = -28 m.
Figure 4.8 Temperature comparison at cross-section X = -1 m.
Figure 4.9 Temperature comparison at cross-section $X = 1$ m.
Figure 4.10 Temperature comparison at cross-section X = 4m.
Table 4.2 shows a comparison of the temperature results for the differing levels of mesh refinement. The table displays the average temperature within the liquid region, the surface temperature of slices throughout the cryostat, and the ranges of the values for the separate meshes. Figure 4.11 shows a plot of the volume average temperature compared to the mesh size. Figures 4.2 and 4.3 show the locations of these slices within the detector.

Table 4.1 Temperatures within the detector for differing levels of mesh refinement.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>cells (millions)</th>
<th>Volume Avg Temp (K)</th>
<th>Surface Avg Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Z = 20</td>
<td>Z = 0</td>
</tr>
<tr>
<td>1</td>
<td>40.8</td>
<td>87.6066</td>
<td>87.6062</td>
</tr>
<tr>
<td>2</td>
<td>56</td>
<td>87.6056</td>
<td>87.6053</td>
</tr>
<tr>
<td>3</td>
<td>58.9</td>
<td>87.6073</td>
<td>87.6069</td>
</tr>
<tr>
<td>4</td>
<td>60.7</td>
<td>87.6075</td>
<td>87.6075</td>
</tr>
<tr>
<td>5</td>
<td>65.5</td>
<td>87.6057</td>
<td>87.6055</td>
</tr>
<tr>
<td>6</td>
<td>151.6</td>
<td>87.6052</td>
<td>87.6050</td>
</tr>
<tr>
<td>Max</td>
<td></td>
<td>87.6075</td>
<td>87.6075</td>
</tr>
<tr>
<td>Min</td>
<td></td>
<td>87.6052</td>
<td>87.605</td>
</tr>
<tr>
<td>Range</td>
<td></td>
<td>0.0023</td>
<td>0.0025</td>
</tr>
</tbody>
</table>

Figure 4.11 Plot of volume average temperature within the detector by mesh size.
4.1.2 Impurity Comparison

The following results will compare the impurity results for the differing mesh refinement levels. In each figure the results are shown from the coarsest mesh (Mesh 1) on the top left, to the most refined (Mesh 6) on the bottom right. The arrows show the velocity vectors of fluid flow tangential to the plane shown within the cryostat. Figures 4.12-4.18 show the scaled impurity distribution plots for the surfaces throughout the detector.
Figure 4.12 Scaled impurity comparison at cross-section $Z = 20$ m.
Figure 4.13 Scaled impurity comparison at cross-section Z = 0 m.
Figure 4.14 Scaled impurity comparison at cross-section $Z = -20$ m.
Mesh 1

Mesh 2

Mesh 3

Mesh 4

Mesh 5

Mesh 6

Figure 4.15 Scaled impurity comparison at cross-section $Z = -28$ m.
Figure 4.16 Scaled impurity comparison at cross-section X = -1 m.
Figure 4.17 Scaled impurity comparison at cross-section X = 1 m.
Figure 4.18 Scaled impurity at cross-section X = 4 m.
Table 4.2 shows a comparison of the impurity results for the differing levels of mesh refinement. The table displays the average impurities within the liquid region, the surface average impurities of slices throughout the cryostat, and the ranges of the values for the separate meshes. Figures 4.1 and 4.2 show the locations of these slices within the detector.

Table 4.2 Comparison of impurities at differing levels of mesh refinement.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>cells (millions)</th>
<th>Volume Unscaled Imp.</th>
<th>Surface Avg Scaled Impurities</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Z = 20</td>
</tr>
<tr>
<td>1</td>
<td>40.8</td>
<td>0.9386</td>
<td>1.0009</td>
</tr>
<tr>
<td>2</td>
<td>56</td>
<td>0.9368</td>
<td>1.0016</td>
</tr>
<tr>
<td>3</td>
<td>58.9</td>
<td>0.9398</td>
<td>1.0023</td>
</tr>
<tr>
<td>4</td>
<td>60.7</td>
<td>0.9418</td>
<td>1.0006</td>
</tr>
<tr>
<td>5</td>
<td>65.5</td>
<td>0.9415</td>
<td>1.0017</td>
</tr>
<tr>
<td>6</td>
<td>151.6</td>
<td>0.9389</td>
<td>1.0009</td>
</tr>
<tr>
<td>Max</td>
<td></td>
<td>0.9418</td>
<td>1.0023</td>
</tr>
<tr>
<td>Min</td>
<td></td>
<td>0.9368</td>
<td>1.0006</td>
</tr>
<tr>
<td>Range</td>
<td></td>
<td>0.0050</td>
<td>0.0017</td>
</tr>
</tbody>
</table>

Figure 4.19 shows a plot of the average unscaled concentration of impurities within the detector compared to the mesh density. It should be noted that a unit flux of impurities was applied to the detector rather than the actual amount of impurities that are expected to enter the detector, so the values in this plot are significant only for comparison, and not for predicting actual impurity concentration within the detector. The figure shows relatively small changes of the impurity concentration, likely due to fluctuations in the solution as shown by the previous residuals plot. The relatively consistent values despite the large variance in the number of cells, indicates that all meshes adequately capture the physics of the solution. If the coarsest mesh was
inadequate, the results would be expected to show gradual change until the first adequate mesh was achieved, before the solution approached convergence.

![Graph](image)

**Figure 4.19** Comparison of impurity concentration to number of cells in the mesh.

### 4.1.3 Summary of Mesh Refinement Study

The results of the mesh refinement study show very similar results across differing levels of mesh refinement. Though some levels of refinement show maximum and minimums in slightly differing locations, it should be noted that these simulations did not account for solution variations with time. As discussed previously, the solutions oscillate about the convergence point, rather than staying constant.

The maximum temperature range at any of the planes examined in this study for differing levels of mesh refinement is approximately 0.004 K, within the range of variance over time seen in the prototype detectors [40]. Additionally, the maximum range of scaled impurities for the planes was 0.004, or 0.4%. This data supports that the
simulations are relatively robust to changes in the mesh size, and the mesh refinement at critical locations was able to accurately capture the important features of the detector.

The plots of temperature and impurity concentrations show slight differences in the distributions, but the range of these plots should be considered. These plots require extremely narrow ranges to show the relative differences between meshes, and the slight differences in trends can likely be attributed to solution fluctuation. With this in mind, the mesh levels were considered for use in following turbulent Schmidt and slip vs no-slip studies. The tabular values show that Mesh 4 did not contain the extreme (maximum or minimum) values for the surface averages at the slices considered, so this mesh was determined as most representative of the median values for the differing levels of mesh refinement.

Despite the findings that even the coarsest mesh considered in this study resulted in relatively accurate simulation of the Far Detector, Mesh 1 was nearing the coarsest limits that were possible to achieve results. Coarser meshes were attempted but these meshes resulted in simulation errors and overflow errors, due to the oversized mesh being unable to fit multiple cells in narrow geometric spaces between features. This resulted in computation errors that propagated throughout the mesh and caused the simulation to crash when a solution spiraled out of control, reaching temperatures outside the bounds of the software capability. By concentrating the mesh refinement in crucial areas, however, the model was able to achieve relatively high accuracy even for meshes near the coarsest possible allowed by the geometry.
4.2 Passive Scalar Turbulent Schmidt Number

An investigation was completed to determine the optimum turbulent Schmidt number, which would model the transport of the impurities most closely to the experimental detector. As discussed previously, the turbulent Schmidt number characterizes the ratio of the rate of turbulent transport of momentum compared to mass. Historically, there has been debate about the ideal value for CFD use, with 0.9 the most widely used value, but certain studies claiming that lower values yield better results, especially for simpler geometries, as discussed in the literature review chapter of this thesis. This thesis examines results for CFD simulations using turbulent Schmidt values of 0.5, 0.9, and 2.0.

4.2.1 Temperature Comparison

By definition, a passive scalar should not affect the temperature of the fluid in CFD simulations. The temperature differences in the following comparisons for differing values of turbulent Schmidt numbers is most likely due to solution oscillation about the convergence point, rather than significant differences caused by the turbulent Schmidt number. Figure 4.20 shows a plot of temperature relative to the turbulent Schmidt number, demonstrating that the turbulent Schmidt number does not significantly impact the temperature.
Figure 4.20 Plot of volume average temperature relative to the turbulent Schmidt number.

Table 4.4 shows a comparison of the temperature results for the differing levels of the turbulent Schmidt number. The table shows the volume average temperature in the liquid regions, the surface average temperature at planes within the detector, and the maximum, minimum, and range values for differing turbulent Schmidt numbers.

Table 4.3 Temperatures within the detector for varying turbulent Schmidt numbers.

<table>
<thead>
<tr>
<th>Turbulent Schmidt #</th>
<th>Volume Avg</th>
<th>Surface Avg Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Z = 20</td>
<td>Z = 0</td>
</tr>
<tr>
<td>0.5</td>
<td>87.6071</td>
<td>87.6083</td>
</tr>
<tr>
<td>0.9</td>
<td>87.6075</td>
<td>87.6075</td>
</tr>
<tr>
<td>2</td>
<td>87.6071</td>
<td>87.6069</td>
</tr>
<tr>
<td>Max</td>
<td>87.6075</td>
<td>87.6083</td>
</tr>
<tr>
<td>Min</td>
<td>87.6071</td>
<td>87.6069</td>
</tr>
<tr>
<td>Range</td>
<td>0.0004</td>
<td>0.0014</td>
</tr>
</tbody>
</table>
4.2.2 Scaled Impurity Comparison

Figure 4.21 Scaled Impurity comparison at $z = 20$ m (0.5- left, 0.9- center, 2-right).

Figure 4.22 Scaled Impurity comparison at $z = 0$ m (0.5- left, 0.9- center, 2-right).

Figure 4.23 Scaled Impurity comparison at $z = -20$ m (0.5- left, 0.9- center, 2-right).

Figure 4.24 Scaled Impurity comparison at $z = -28$ m (0.5- left, 0.9- center, 2-right).
Figure 4.25 Scaled Impurity comparison at x = -1 m (0.5- top, 0.9-center, 2-bottom).
Figure 4.26 Scaled Impurity comparison at x = 1 m (0.5- top, 0.9-center, 2-bottom).
Figure 4.27 Scaled Impurity comparison at x = 4 m (0.5- top, 0.9-center, 2-bottom).
4.2.3 Summary of Results for Varying the Turbulent Schmidt Number

The temperature differences seen in the simulations with different values for the turbulent Schmidt number are very small, with the greatest temperature range between simulations at any plane of 0.0014 K, and all others within the range of 0.0006 K. This shows that the surface average temperature for any plane examined here is nearly identical for almost all values of the turbulent Schmidt number considered. This meets the expectation that the turbulent Schmidt number does not affect the temperature of the solution, and differences are due to solution oscillation.

The scaled impurity distribution also yielded highly similar results for the planes considered, with the greatest difference found at the plane X = 4m where the difference between the 0.5 and 0.9 turbulent Schmidt number was 0.0081, but the range for most slices (5 of 7) was less than 0.0012. The unscaled impurities, accounting for the total concentration of impurities within the cryostat rather than scaled to an average, also ranged less than 0.17%.

Interestingly, in both these cases the impurities for 2.0 value of the turbulent Schmidt number was between the values of the 0.5 and 0.9 values, rather continuing the pattern seen from adjusting the value from 0.5 to 0.9. This was not true for most of the
planes, however. Based on the results seen in the tables and plots of sections 4.4.1-4.4.2, it does not appear that varying the turbulent Schmidt number from 0.5-2.0 had a significant impact on the temperature or impurity distributions within the Far Detector.

4.3 **Slip vs No-Slip Boundary Condition**

4.3.1 **Temperature Comparison**

An investigation was pursued to compare the no-slip boundary condition at the liquid-ullage interface with the slip boundary condition. Note that the temperature scales are slightly different for the no-slip plots to clearly show gradients, but the range is the same for all plots, 0.038 K.

![Figure 4.28](image1.png) **Figure 4.28** Comparison of No-Slip and Slip Boundary condition at liquid-ullage interface at z = 20 m (slip, left and no-slip, right).

![Figure 4.29](image2.png) **Figure 4.29** Comparison of No-Slip and Slip Boundary condition at liquid-ullage interface at z = 0 m (slip, left and no-slip, right).
Figure 4.30 Comparison of No-Slip and Slip Boundary condition at liquid-ullage interface at z = -20 m (slip, left and no-slip, right).

Figure 4.31 Comparison of No-Slip and Slip Boundary condition at liquid-ullage interface at z = -28 m (slip, left and no-slip, right).
Figure 4.32 Temperature comparison at x = -1 m (slip, top and no-slip, bottom).

Figure 4.33 Temperature comparison at x = 1 m (slip, top and no-slip, bottom).
Figure 4.34 Temperature comparison at x = 4 m (slip, top and no-slip, bottom).

Table 4.5 Shows the temperature results for the slip and no-slip conditions.

<table>
<thead>
<tr>
<th></th>
<th>Surface Avg Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh</td>
<td>Volume Avg</td>
</tr>
<tr>
<td>Slip</td>
<td>87.6075</td>
</tr>
<tr>
<td>No-Slip</td>
<td>87.8005</td>
</tr>
<tr>
<td>Range</td>
<td>0.193</td>
</tr>
<tr>
<td>Average Range of Surfaces</td>
<td>0.192671</td>
</tr>
</tbody>
</table>
4.3.2 Scaled Impurity Comparison

Figure 4.35 Scaled Impurity comparison at z = 20 m (slip, left and no-slip, right).

Figure 4.36 Scaled Impurity comparison at z = 0 m (slip, left and no-slip, right).

Figure 4.37 Scaled Impurity comparison at z = -20 m (slip, left and no-slip, right).
Figure 4.38 Scaled Impurity comparison at $z = -28$ m (slip, left and no-slip, right).

Figure 4.39 Scaled Impurity comparison at $x = -1$ m (slip, top and no-slip, bottom).
Figure 4.40 Scaled Impurity comparison at x = 1 m (slip, top and no-slip, bottom).

Figure 4.41 Scaled Impurity comparison at x = 4 m (slip, top and no-slip, bottom).

Table 4.6 Summary of results for the impurity for the slip and no-slip conditions.

<table>
<thead>
<tr>
<th></th>
<th>Surface Avg Scaled Impurities</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh</td>
<td>Volume Unscaled</td>
</tr>
<tr>
<td>Slip</td>
<td>0.9418</td>
</tr>
<tr>
<td>No-Slip</td>
<td>0.9444</td>
</tr>
<tr>
<td>Range</td>
<td>-0.0026</td>
</tr>
<tr>
<td>Average Range of Surfaces</td>
<td>0.0014</td>
</tr>
</tbody>
</table>
4.3.3 Slip vs. No-Slip Summary

The slip and no-slip boundary conditions on the liquid-ullage interface yielded significantly different results in the simulations. Some similar temperature trends were observed, though often with a slight translation of placement, but the results showed a temperature shift upwards of very near 0.193 K for all surfaces of the no-slip boundary condition. For conditions where significant temperature gradients are measured in millikelvin, 0.193 K is a noteworthy change.

As will be discussed further in the comparison to the ProtoDUNE results, it has been hypothesized that this jump in cryostat temperature for the no-slip condition is due to the no-slip condition underpredicting the heat transfer coefficient. With zero fluid velocity at the boundary, the no-slip condition predicts less mixing at the interface, and this lack of exposure results in lower predicted heat transfer between the liquid and ullage regions.

The results also indicate a higher level of impurities for the no-slip boundary condition, especially near the top of the liquid region in the detector. The impurities enter the liquid region via a constant flux at the liquid-ullage interface, so the lower level of impurities at the surface in the slip results is likely due to the fluid velocity at the boundary “sweeping away” the impurities more quickly at the point of entry to mix into the rest of the ullage region.

The distribution of impurities was also different for the slip and no-slip conditions. The slip boundary condition showed relatively higher concentrations of impurities farthest from the outlets, compared to the average, while the no-slip condition
showed relatively higher impurities concentrated at the outlet end of the detector. Further investigation would be required to determine the cause of this discrepancy.

4.3.4 Comparison to ProtoDUNE Slip vs. No-Slip

The slip and no-slip boundary conditions were also compared in the for the ProtoDUNE simulations. One advantage in testing the slip and no-slip conditions is that there is experimental data for the ProtoDUNE detectors that can be used to verify which condition produces results more comparable to the experimental results. Previous work at SDSU concluded that the slip boundary condition at the liquid-ullage interface produced results more similar to the experimental results than the no-slip condition [9]. The following graphs and tables will be discussed to corroborate these conclusions.

Figures 4.42 and 4.43 show a comparison of the CFD simulations and the experimental results for the ProtoDUNE simulations [9]. The first figure shows the results for the slip condition at the liquid-ullage interface, while the second shows the results for the no-slip condition.
The values for the comparison were corrected by applying a correction factor calculated so that the average temperature within the detector was equal for the CFD simulations and for the experimental results. The correction was applied to allow easier comparison on the temperature profiles between the simulation and experimental results. Table 4.8 shows the correction adjustment applied to the CFD results for two different
temperature probes. These results show that the slip condition required much less adjustment than the no-slip condition to match the average temperature within the detector.

The table also shows that the no-slip boundary conditions predicts significantly higher temperatures than those seen in the experimental results. This is likely due to an under prediction of the heat transfer coefficient at the liquid-ullage interface due to the assumption of no fluid movement at the interface boundary. Without the correct heat transfer coefficient, the temperature within the liquid is overpredicted.

Table 4.7 Temperature correction adjustment for ProtoDUNE simulations.

<table>
<thead>
<tr>
<th></th>
<th>Static Probe Correction (K)</th>
<th>Dynamic Probe Correction (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slip</td>
<td>+0.061</td>
<td>+0.062</td>
</tr>
<tr>
<td>No-Slip</td>
<td>-0.454</td>
<td>-0.454</td>
</tr>
</tbody>
</table>

Table 4.9 shows the mean squared error for the ProtoDUNE simulations under different conditions, including the slip and no-slip conditions for circulation pumps on or off as well as constant surface temperature or heat flux at the liquid-ullage surface. These results also show that the slip condition more closely matched the experimental results for a vast majority of the scenarios studied.
Table 4.8 Mean squared error *10⁶ based on probe type and boundary conditions after correcting.

<table>
<thead>
<tr>
<th></th>
<th>Static Temperature Probe</th>
<th>Dynamic Temperature Probe</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Surface Temperature</td>
<td>Heat Flux</td>
</tr>
<tr>
<td></td>
<td>Slip</td>
<td>No-Slip</td>
</tr>
<tr>
<td>Pump On</td>
<td>4.09</td>
<td>5.14</td>
</tr>
<tr>
<td>Pump Off</td>
<td>1.18</td>
<td>7.21</td>
</tr>
</tbody>
</table>

4.3.5 Slip vs. No-Slip Conclusions

The results in this study and previous work at SDSU have indicated that the slip boundary condition better simulates the expected conditions within the detectors. The no-slip condition appears to under predict the heat transfer between the liquid and ullage regions. Additionally, the slip condition appears to provide more realistic mixing of the impurities within the detector. The no-slip condition shows significantly higher impurity concentrations near the top of the liquid region and the outlet end within the detector compared to the no-slip condition. The relatively uniform mixing of impurities desired and seen in the prototype (35 ton and ProtoDUNE) detectors’ experimental results [7] & [9], more closely matches the results seen using the slip boundary condition at the liquid-ullage interface.

4.4 Comparison to ProtoDUNE Detectors

Before comparing the results of the Far Detector simulations completed in this work with the ProtoDUNE simulations and experimental results, it is important to note important design differences that will affect the results. First, the Far Detector is much larger than the ProtoDUNE detector, with a volume more than 28 times that of the ProtoDUNE detector. Additionally, the Far Detector simulations contain more detailed
consideration of geometric elements such as the ground planes and service floor. Table 4.10 highlights further differences between the detectors.

**Table 4.9 Design differences between the ProtoDUNE and Far Detectors.**

<table>
<thead>
<tr>
<th></th>
<th>ProtoDUNE</th>
<th>Far Detector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Argon flow rate (kg/s)</td>
<td>1.668</td>
<td>10</td>
</tr>
<tr>
<td>Inlet Temperature (K)</td>
<td>88.1634</td>
<td>Outlet + 0.4418</td>
</tr>
<tr>
<td>Number of Inlets</td>
<td>4</td>
<td>128 total, 64 active at a time</td>
</tr>
<tr>
<td>Inlet Location</td>
<td>Bottom along one side of detector</td>
<td>Bottom along both sides of detector</td>
</tr>
<tr>
<td>Number of Outlets</td>
<td>1</td>
<td>4</td>
</tr>
</tbody>
</table>

Despite these differences the simulations show a remarkable level of similarities. As shown in Figure 4.44 the temperature distribution taken at a slice near the center of the cryostat is remarkably similar for the ProtoDUNE and Far Detector simulations. Both plots have a temperature scale from 87.0 K to 87.7 K.

![Figure 4.44 Comparison of ProtoDUNE (left) and Far Detector (right) temperatures near center.](image)
Figure 4.45 shows a comparison of the impurity ranges on a slice through the cryostat. Both plots range from 95.35-105 % of the average impurity concentration within the liquid argon. This figure shows highly similar levels of scaled impurities within the detectors, despite the design differences. This supports the design hypothesis that the Far Detector will provide similar conditions to those seen in the ProtoDUNE detector.

4.5 Comparison to Previous Far Detector Simulations

Exact comparison to previous simulations is complicated by the updated boundary conditions in the detector. Previous simulations at South Dakota State University used an argon saturation temperature of 88.348 K, and varying inlet and outlet locations [7]. These conditions have been updated after further work on the ProtoDUNE experimental detectors and Far Detector design updates, and the argon saturation temperature is now expected to be 87.593 K, at the pressure of 104.5 kPa [9], and new inlet and outlet locations have been selected. The new saturation temperature has resulted in significantly lower temperatures throughout the detector, as seen in Figure 4.46.

Despite the decrease in overall temperature, however, the temperature range within the TPC region is very similar. Figure 4.46 shows a comparison, with both plots
having an overall temperature range of 0.07 K, despite a 1.41 K shift down in the temperature. Figure 4.46 also highlights the differences caused by placing the inlets below the service floor and including the service floor and ground plane geometries. It is clear that these features separate the warmer incoming argon from the rest of the liquid region, creating a warmer area near the floor of the detector.

Figure 4.46 Shows a comparison of the temperature distribution for previous simulations at SDSU [7] and the most recent simulations for the plane at Z = 0m.

These results show a significantly greater range in the impurity concentration for the newer simulations. This is likely due to the additionally modeling details included in the updated version of the geometry. Previous simulations at SDSU neglected the ground plane and service floor geometry, as discussed in the methodology chapter of this thesis, and as shown in Figure 4.47. The updated simulations show lower impurities below the service floor than seen in previous simulations, as indicated by the dark blue region in the impurities plot. The updated inlet location is beneath the service floor, as opposed to at
the top of the detector. Thus, the pure liquid argon enters below the service floor and is partially separated from the main area of the detector by the service floor.

![Diagram showing fluid flow and impurity distribution](image)

**Figure 4.47** Shows a comparison of the impurity distribution for previous simulations at SDSU [7] and the most recent simulations for the plane at \( Z = 0 \) m.

The area of greatest concern for the impurity concentration, however, is the TPC, as discussed in previous chapter of this thesis. **Figure 4.47** Shows that the impurity concentration within the TPC is similar for both the current and previous simulations, between 0.99 and 1.01. The differing flow patterns and impurity distribution is likely due to the revised inlet and outlet conditions.
5. CONCLUSIONS AND FUTURE WORK

5.1 Conclusions

The CFD models developed and assessed in this study show high agreement, with only 0.5% range in the average impurities and less than 0.01% range for average temperature, for varying levels of mesh refinement. This supports that the model has achieved grid independence, where the solution is not significantly changed by small increases in mesh refinement. The coarsest mesh was able to provide similar design insights to the highest resolution model, while resulting in a file size less than half that of the highest resolution model and requiring much lower computational costs.

This verifies and expands on findings from previous literature. That large and geometrically complex systems can be accurately modelled while reducing computational costs has important applications in industry. This efficient modelling is achieved by concentrating the mesh in areas critical to determining important flow characteristics. Reducing the computational cost results in saving time and money for high level CFD simulations.

The effect of varying the turbulent Schmidt number from 0.5-2.0 was much less than expected, showing virtually identical temperatures and impurity variations of less than 0.17% between simulations. It was hypothesized that lower turbulent Schmidt numbers would result less uniform spreading of impurities with most impurities concentrated near the source, while higher values would result in more uniform concentrations throughout the detector. This agrees with the findings summarized in the literature review that further, and more comprehensive studies on the turbulent Schmidt
number are required to create an accurate guideline for setting the turbulent Schmidt number.

The no-slip boundary condition yielded significantly different results than the slip boundary condition, notably an approximately +0.193 K temperature shift. It has been hypothesized that this temperature shift is due to an underprediction of the heat transfer coefficient resulting from less mixing near the liquid-ullage interface due to the no-slip condition.

The no-slip boundary condition also resulted in significantly higher impurities, especially near the liquid-ullage interface. It is suspected that this higher concentration of impurities near the source is due to the lack of physical mixing resulting from setting the fluid velocity to zero relative to the interface.

As indicated by the most recent studies in the literature review, more complex boundary conditions than the simplified slip and no-slip conditions may be required to achieve the highest level of accuracy at a fluid-fluid interface. In the case of the DUNE detectors, however, the slip condition reaches reasonable agreement and better performance compared to experimental results that the no-slip condition.

The results showed similar distribution patterns to previous work at SDSU, though the introduction of more detailed geometry yielded a higher range of impurities due to geometric separation of the inlets for pure liquid argon from the main body of the detector by the impermeable service floor.

This research studied the effect of mesh refinement, varying turbulent Schmidt numbers, and the slip vs. no-slip boundary condition at a fluid-fluid interface on the solution of a geometrically complex cryogenic neutrino detection chamber using CFD. It
was determined that refining the mesh in areas of critical flow was more significant to the solution than the global mesh refinement. The turbulent Schmidt number was determined to have negligible effect over a range of 0.5-2.0. The no-slip boundary condition was found to significantly under predict the heat transfer coefficient at the fluid-fluid interface.

5.1.1 Limitations

One limitation of this work is the solution variance due to fluctuations between iterations. Calculating a mean solution over a range of iterations after the simulation has converged may result in more precise comparisons between simulations and allow more conclusive determination of boundary condition effects.

Since all levels of mesh refinement considered in this study appeared to sufficiently resolve the mesh, observing coarser mesh sizes to find the minimum acceptable level of mesh refinement would seem a desirable goal. Coarser meshes than studied in this work, however, were attempted and failed to run to completion. Coarser meshes would be difficult to achieve due to geometric limitations, the narrow clearance of some features, of the Far Detector.

5.2 Future Work

Future work should be completed to simulate the gaseous Argon flow in the ullage region of the single-phase detector. Temperature and impurity results from the ullage region should be used as the input boundary conditions on the liquid ullage interface for the simulation of the liquid region. Another goal of simulating the ullage region will be used validate the proposed design for the ullage region. The location and
number of ports through the ullage region is still under consideration by the consortium. This work is expected to be completed as soon as more information on the ullage ports is available.

In addition, a similar analysis to that contained within this report should be completed for the dual phase detector. The dual phase detector is planned for construction at SURF after the single-phase detector design has been finalized and constructed. Therefore, it is important to validate the proposed design soon for the dual phase detector before the construction process begins. The methods and results used in this analysis as well as those in previous work at SDSU may be leveraged to provide important insight into the methodology for simulating the dual phase detector.
6. BIBLIOGRAPHY


