PARAMETRIC STUDY VIA NUMERICAL SIMULATIONS OF NATURAL CONVECTION IN LATERALLY HEATED CYLINDRICAL ENCLOSURES:
INVESTIGATING CHARACTERISTIC LENGTH

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PARAMETRIC STUDY VIA NUMERICAL SIMULATIONS OF NATURAL CONVECTION IN LATERALLY HEATED CYLINDRICAL ENCLOSURES:

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Thesis

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ii
ABSTRACT

This study numerically investigates the laterally heated vertical cylinder and the length scale associated with this reactor. For natural convection the important dimensionless characteristic is the Rayleigh number, which predicts the flow regime as laminar, transitional, or turbulent. The Rayleigh number is useful as a design tool for scaling a reactor. Up to this point the associated length scale has been assumed as various definitions of length and diameter and has not yet been thoroughly investigated.

The current assumed definitions for the length scale: height, diameter, and volume to lateral surface area, are directly studied in a multi-dimensional (2D and 3D) numerical parametric study involving these length scales and aspect ratio (height/diameter). Other important characteristics such as the ratio of heating to cooling and thickness of the divider (insulator) between heating and cooling are also studied. The study begins with turbulent transient 2D axisymmetric simulations and proceeds to turbulent transient 3D simulations then compares the 3D and 2D simulations. Finally, 2D and 3D laminar simulations are investigated.

Presented are the results of the fluid flow speeds, thermal environments, flow patterns, boundary layer thickness, boundary layer velocity, and normal probability density functions which provide a unique way of studying how the Rayleigh number is influenced by variables. The numerical simulations are examined for spatial step, time
step, and relative convergence by a mesh study, time step study, and thermal analysis, respectively. The turbulence model used (k-ω SST) is based on recent published studies. All simulations were conducted with the commercially available software ANSYS FLUENT. Findings are discussed when they prove significant, and aid in developing a fundamental understanding of the physics occurring inside this reactor setup.

The results indicate that the current length scales assumed for this reactor are incorrect, and a new definition needs to be considered. A new length scale is proposed but needs continued investigation. A significant finding is that two-dimensional (axisymmetric) simulations do not properly capture the flow physics, and result in large modeling errors. These errors dramatically affect the design of a reactor and need to be addressed with three-dimensional simulations.
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# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>LIST OF TABLES</th>
<th>ix</th>
</tr>
</thead>
<tbody>
<tr>
<td>LIST OF FIGURES</td>
<td>xi</td>
</tr>
</tbody>
</table>

## 1 INTRODUCTION AND LITERATURE REVIEW ............................................. 1

1.1 Introduction ......................................................................................... 1

1.2 Literature review ................................................................................ 5

1.2.1 2D previous work ............................................................................ 6

1.2.2 3D previous work ........................................................................... 12

1.2.3 2D to 3D comparative previous work ............................................. 16

1.2.4 Overview ......................................................................................... 17

## 2 SCOPE OF WORK .................................................................................. 20

2.1 Turbulent 2D parametric study of geometric parameters affecting
characteristic length ..................................................................................... 21

2.2 Turbulent 3D parametric study of geometric parameters affecting
characteristic length ..................................................................................... 21

2.3 Turbulent and Laminar 2D-3D effects are studied. .............................. 22

## 3 THEORY ............................................................................................... 23

3.1 Governing Equations ............................................................................ 23

3.1.1 Continuity ....................................................................................... 23
5 RESULTS .............................................................................................................. 67

5.1 Turbulent 2D parametric study ........................................................................ 69

5.1.1 Changing Rayleigh number ........................................................................... 70

5.1.2 Changing aspect ratio – constant diameter .................................................. 77

5.1.3 Changing aspect ratio – constant length ....................................................... 82

5.1.4 Overview of aspect ratio ................................................................................. 87

5.1.5 Changing insulator length .............................................................................. 92

5.1.6 Changing the heating to cooling ratio \( \frac{L_h}{L_c} \) ................................................. 95

5.1.7 2D Overview .................................................................................................. 103

5.2 Turbulent 3D parametric study ......................................................................... 104

5.2.1 Changing Rayleigh ........................................................................................ 105

5.2.2 Changing aspect ratio .................................................................................... 109

5.3 2D 3D comparisons .......................................................................................... 131

5.3.1 Turbulent ........................................................................................................ 131

5.3.2 Laminar .......................................................................................................... 132

5.3.3 Inversion ......................................................................................................... 138

6 CONCLUSION .................................................................................................... 140

BIBLIOGRAPHY .................................................................................................... 144

APPENDICES ......................................................................................................... 153

APPENDIX A. NPDF CONVERGENCES ................................................................. 154

APPENDIX B. 3D EXTRA ....................................................................................... 161

APPENDIX C. NOMENCLATURE .......................................................................... 171
LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 1</td>
<td>Summary of 2D enclosures and parameters studied</td>
<td>18</td>
</tr>
<tr>
<td>Table 2</td>
<td>Summary of 3D enclosures and parameters studied</td>
<td>19</td>
</tr>
<tr>
<td>Table 3</td>
<td>Rayleigh number for all simulations based on three definitions</td>
<td>39</td>
</tr>
<tr>
<td>Table 4</td>
<td>Water properties of standard turbulent simulations</td>
<td>40</td>
</tr>
<tr>
<td>Table 5</td>
<td>2D and 3D parametric study of aspect ratio by changing length</td>
<td>44</td>
</tr>
<tr>
<td>Table 6</td>
<td>2D and 3D parametric study of aspect ratio by changing diameter</td>
<td>44</td>
</tr>
<tr>
<td>Table 7</td>
<td>2D parametric study of heated to cooled lateral surfaces</td>
<td>44</td>
</tr>
<tr>
<td>Table 8</td>
<td>2D parametric study of insulator sizes</td>
<td>45</td>
</tr>
<tr>
<td>Table 9</td>
<td>2D and 3D study of Rayleigh</td>
<td>45</td>
</tr>
<tr>
<td>Table 10</td>
<td>2D mesh sizes</td>
<td>47</td>
</tr>
<tr>
<td>Table 11</td>
<td>3D mesh sizes</td>
<td>48</td>
</tr>
<tr>
<td>Table 12</td>
<td>3D residual heat flux, start of numerical sampling</td>
<td>56</td>
</tr>
<tr>
<td>Table 13</td>
<td>2D residual heat flux, start of numerical sampling</td>
<td>57</td>
</tr>
<tr>
<td>Table 14</td>
<td>Maximum y+ for 3D simulations</td>
<td>66</td>
</tr>
<tr>
<td>Table 15</td>
<td>Maximum y+ for 2D simulations</td>
<td>66</td>
</tr>
<tr>
<td>Table 16</td>
<td>Changing Rayleigh, 2D setup</td>
<td>70</td>
</tr>
<tr>
<td>Table 17</td>
<td>Changing length, 2D, setup for Figures 27-30,35, and 36</td>
<td>77</td>
</tr>
<tr>
<td>Table 18</td>
<td>Changing diameter, 2D, setup for Figures 31-36</td>
<td>83</td>
</tr>
</tbody>
</table>
Table 19  Changing aspect ratio, 3D, setup for Figures 48-53. ........................................ 110
Table 20  2D simulation values of important characteristics............................................. 138
LIST OF FIGURES

Figure 1 Two different reactor setups, retrograde and forward ........................................... 3
Figure 2 Illustration of discretizing a scalar transport equation .................................................. 34
Figure 3 Cell centroid evaluation .................................................................................................. 35
Figure 4 Numerical Algorithm ....................................................................................................... 37
Figure 5 Temperature dependent properties of water ................................................................. 41
Figure 6 Temperature dependent characteristics of water .......................................................... 42
Figure 7 General dimensions of the reactor .................................................................................. 43
Figure 8 2D mesh setups with detailing ........................................................................................ 46
Figure 9 3D mesh setup with detailing .......................................................................................... 47
Figure 10 NPDF example showing sampling independence ......................................................... 53
Figure 11 2D spatial convergence, aspect ratio 5:1 ..................................................................... 58
Figure 12 2D spatial convergence, aspect ratio 10:1 .................................................................... 58
Figure 13 2D spatial convergence, aspect ratio 20:1 .................................................................... 59
Figure 14 2D spatial convergence of Lh/Lc 1, aspect ratio 5:1 ..................................................... 59
Figure 15 2D spatial convergence of Lh/Lc 2, aspect ratio 5:1 ..................................................... 60
Figure 16 2D spatial convergence of Lh/Lc 3, aspect ratio 5:1 ..................................................... 60
Figure 17 2D spatial convergence of Lh/Lc 6, aspect ratio 5:1 ..................................................... 61
Figure 18 3D spatial convergence, aspect ratio 5:1 ..................................................................... 62
Figure 19 2D time convergence, aspect ratio 5:1 ............................................................................... 64
Figure 20 Near-Wall regions and corresponding y+ values ................................................................. 65
Figure 21 Boundary layers occurring inside the reactor ................................................................. 68
Figure 22 Changing Rayleigh, 2D temperature and vector maps ................................................ 72
Figure 23 Changing Rayleigh, 2D velocity magnitude maps .......................................................... 73
Figure 24 Changing Rayleigh, 2D NPDF of velocity magnitude ..................................................... 74
Figure 25 Changing Ra, 2D boundary layer thickness and velocity .............................................. 74
Figure 26 Changing Rayleigh, 2D velocity vectors ........................................................................ 75
Figure 27 Changing length, reactors without scaling for Figures 28-30 ........................................ 78
Figure 28 Changing length, 2D temperature & vector maps ...................................................... 79
Figure 29 Changing length, 2D velocity magnitude maps ............................................................ 80
Figure 30 Changing length, 2D velocity vectors ........................................................................... 81
Figure 31 Changing diameter, reactors without scaling for Figures 32-34 below....................... 83
Figure 32 Changing diameter, 2D temperature and vector maps .............................................. 84
Figure 33 Changing diameter, 2D velocity magnitude maps ....................................................... 85
Figure 34 Changing diameter, 2D velocity vectors ..................................................................... 86
Figure 35 2D NPDF of velocity magnitude ....................................................................................... 89
Figure 36 2D boundary layer thickness and velocity .................................................................... 90
Figure 37 Changing insulator, 2D temperature maps .................................................................. 93
Figure 38 Changing insulator, 2D velocity magnitude maps ...................................................... 94
Figure 39 Changing insulator, 2D NPDF of velocity magnitude ................................................. 95
Figure 40 Changing \( \text{Lh}/\text{Lc} \), 2D temperature & vector maps .................................................. 96
Figure 41 Changing \( \text{Lh}/\text{Lc} \), 2D velocity magnitude maps .......................................................... 97
Figure 42  Changing Lh/Lc, 2D velocity vectors ................................................. 98
Figure 43  Changing Lh/Lc, 2D NPDF of velocity magnitude ................................. 100
Figure 44  Changing Lh/Lc, 2D boundary layer thickness and velocity .................... 101
Figure 45  Changing Ra, 3D temperature, velocity magnitude, and vector maps ...... 106
Figure 46  Changing Rayleigh, 3D NPDF of velocity magnitude ............................ 107
Figure 47  Changing Rayleigh, 3D boundary layer thickness and velocity ................. 108
Figure 48  Changing aspect ratio, 3D reactor without scaling for Figures 49-51 ...... 110
Figure 49  3D temperature & vector maps .......................................................... 111
Figure 50  Changing AR, 3D velocity magnitude maps ......................................... 112
Figure 51  Changing aspect ratio, 3D velocity vectors ......................................... 113
Figure 52  Changing aspect ratio, 3D NPDF of velocity magnitude .......................... 114
Figure 53  Changing AR, 3D boundary layer thickness and velocity ........................ 115
Figure 54  3D temperature cross-sections, AR 5:1 ................................................ 118
Figure 55  3D axial velocity cross-sections, aspect ratio 5:1 .................................... 119
Figure 56  3D temperature cross-sections, aspect ratio 2.5:1 .................................... 120
Figure 57  3D axial velocity cross-sections, aspect ratio 2.5:1 .................................... 121
Figure 58  3D temperature cross-sections, aspect ratio 10:1 ..................................... 122
Figure 59  3D axial velocity cross-sections, aspect ratio 10:1 ..................................... 123
Figure 60  3D temperature cross-sections, aspect ratio 5:0.5 ..................................... 124
Figure 61  3D axial velocity cross-sections, aspect ratio 5:0.5 ..................................... 125
Figure 62  3D temperature cross-sections, aspect ratio 5:2.15 ................................... 126
Figure 63  3D axial velocity cross-sections, aspect ratio 5:2.15 ................................... 127
Figure 64  3D temperature cross-sections Rayleigh increased an order ...................... 128
Figure 65 3D axial velocity cross-sections, Rayleigh increased an order ............... 129
Figure 66 2D and 3D laminar temperature and velocity magnitude maps .............. 133
Figure 67 3D laminar temperature cross-sections, aspect ratio 5:1...................... 135
Figure 68 3D laminar axial velocity cross-sections, aspect ratio 5:1................... 136
Figure 69 3D laminar axial velocity cross-sections, aspect ratio 5:1.................... 137
CHAPTER I

INTRODUCTION AND LITERATURE REVIEW

1.1 Introduction

Crystals play a large role in developing technologies. They are used in many applications including LED’s, sonars, and ultrasound applications. The quartz crystal is a commonly grown crystal; the most well-known application is the quartz clock. The quality of the crystal has a significant impact on its use and performance. Different growing methods produce varying crystal quality. There is a growing economic demand for larger and higher quality crystals; this demand has sparked a plethora of research. There are many ways to grow crystals; the method examined here is based on hydrothermal reactors.

Hydrothermal growth reactors have been used for a long time to grow quartz crystals, but it wasn’t until rather recently when the ammonothermal reactor was developed to grow gallium nitride (GaN) crystals. This new growth method gained interest when Fukuda and Ehrentraut published [1] which compared ammonothermal to hydride vapor-phase epitaxy (HVPE) reactors. HVPE was the leading GaN crystal growth method at the time. They determined that the ammonothermal growth method had the greatest potential to produce large high-quality crystals on an industrial scale. They also showed that the
HVPE, had inherent problems of scale, cost, and crystal quality. When they compared the current experiments of both methods, the ammonothermal method showed greater scalability and higher quality crystals.

The proof of concept for the ammonothermal reactor was shown in an early experiment [2] where gallium nitride crystals were grown in an ammonothermal reactor. The crystals grown were small, but it was experimentally shown that GaN crystals could be grown in an ammonothermal reactor operating on the same principles of a hydrothermal reactor. More recent published experimental results by Bao and others in [3] and [4] show ammonothermal reactors capable of growing larger GaN crystals at faster rates than the earlier studies.

As mentioned before, the basic operating principles of ammonothermal and hydrothermal reactors are similar; the main difference is the ‘mineralizers’, ammonia and water, respectively. The mineralizers are used for transporting the crystal component species, Gallium and Silicon, respectively. For GaN, the solubility curve can be either positive or negative dependent upon the specific mineralizer. A retrograde or negative solubility reactor, shown in Figure 1a, operates by etching the necessary nutrients from a nutrient basket in the cooler upper portion of the reactor. Driven by natural convection, the nutrients are then advected to the lower warmer portion of the reactor, where they deposit through mass transfer in crystal form onto a pre-existing seed. For a forward soluble reactor shown in Figure 1b, the internal configuration is inverted compared to the retrograde setup. The positive solubility of forward soluble reactors means etching, deposition, and mass transfer occurs in the opposite direction compared to the retrograde reactor.
Figure 1  Two different reactor setups, retrograde and forward
One for negative and another for positive solubility a) retrograde setup b) forward setup.

Nutrient transport through natural convection is key to growing high quality crystals. It occurs when a fluid is differentially heated, which induces a difference in density of the fluid. The difference in density results in the upward and respective downward moving boundary layers. The boundary layers entrain the interior fluid core, which opposes the boundary layer flow. This force is the driving force of many reactors. The strength of this force depends on many factors, including the geometry being studied, the magnitude of differential heating, the fluid properties, and not least the positions of the nutrients, seeds, and baffle.

There have been many studies of natural convection in different shaped reactors. In [5] Aydin and Yesiloz studied a two-dimensional circular quadrant. The study examined specifically the effect of cooling the vertical wall and heating the bottom horizontal wall of the circular quadrant. The paper also presented experimental data to validate the numerical simulation. According to the authors, this geometry had not been studied
Another geometry that involved mixed wall heating, vertical and horizontal was presented in [6]. The authors presented a vertical cylinder with lateral side heating and top cap cooling. The study investigated the aspect ratio of the reactor and how it affected the flow patterns and the temperature field. A more common configuration was studied by Schneider and Straub [7]. It consisted of a cylindrical enclosure with top and bottom heating. This study looked at different wall temperatures, geometries, and inclination angles of the reactor. This was an early investigation of cylindrical enclosures and neglected the usual internal components industrial reactors actually contain. Another common enclosure was studied by Li, Xing, and Braun [8], a cubic cavity bottom heated and top cooled. Contours of temperature and flow patterns of the fluid were experimentally and numerically investigated. The numerical simulations were validated by showing a strong correlation with the experimental results. This correlation was used as a justification for farther numerical investigation.

Another set of papers published by Braun et al. [9], [10], and [11] had a geometry different from those previously mentioned. The geometry studied was a rectangular parallelepipedic enclosure where the lower lateral walls were heated and the top cooled. All three articles presented both experimental and numerical results, with strong correlations between the two. Braun et al. [9] presented a look into the effect of aspect ratio of the rectangular enclosure and offered an optimal design range for such a reactor. The second publication [10] examined the formation of the wall boundary layers both numerically and experimentally and compared the effects of different aspect ratios, as well as temperature deviations along the wall. In [11] the authors studied the resultant
flow patterns of said geometry, both numerically and experimentally, and explained the flow structures that developed in the experiment and numerical simulation.

The same authors also examined top cap cooled and lateral side bottom heating compared to only lateral heating for vertical cylinder. Braun and Li [12] numerically investigated the two heating methods. They detailed fundamental flow and heat transfer differences between the two different thermal configurations, and concluded that the mixed heating condition produced a more favorable crystal growth environment. In [13] the same authors compared the laterally heated cylindrical enclosure to the laterally heated rectangular enclosure. A similar analysis was presented as in the previous paper with an additional grid convergence study to support the accuracy of the numerical simulations.

The aforementioned studies represent a stepping stone for the detailed review that follows. The geometry of concern henceforward is the laterally heated cylindrical reactor.

1.2 Literature review

Directly determining the fluid properties, flow patterns, and concentrations inside an actual reactor is rather prohibitive if not impossible both technically and financially. The working temperature and pressure is exceedingly high, 300°F and above, under pressures often exceeding 100 MPa; this environment makes building an apparatus to measure internal conditions economically unfeasible. The alternative approach is to numerically simulate the reactor using validated software and models and once validated, extrapolate the numerical model to actual conditions. This provides valuable insight into the internal conditions, and can be a useful tool for improving efficiency of a reactor and quality of
the crystals. However, numerical simulations can be computationally expensive as well, so many times simplifying assumptions are often imposed.

A review of the currently published work shows that many simplifying assumptions have been used at times, such as, neglecting the seeds, porous media, mass transfer, and baffle in order to facilitate computation; often times these assumptions are used in conjunction with a simple wall heating configuration, such as constant internal wall temperature or heat flux condition. Presented below is a summary of what is currently the state of the art knowledge for laterally heated cylinders.

1.2.1 2D previous work

One of the major assumptions made to significantly simplify the complexity of any numerical simulation is that it can be modeled two dimensionally. The third dimension depending on geometry is either infinite in scale or axisymmetric. In some cases this assumption is valid, but mainly it saves on computational difficulties arising from a full 3D analysis.

*Laminar 2D*

Hu, Chen, and Prasad [14] used a finite volume method to solve Navier Stokes equations in the fluid domain and the Darcy-Brinkman-Forcheimer extended model for the porous region. The cylindrical reactor incorporated a porous medium, a baffle, and seed crystals, with a functional wall-imposed temperature and considered the reactor radius as the characteristic length of the Grashof number. The authors studied the effect of changing the structure of the porous media, and found that depending on the porosity of the medium and thermal conditions the fluid may not have enough momentum to penetrate the medium. For a similar setup the authors in [15] studied the effect of the
baffle opening. It was shown that the opening size needs to be carefully chosen to optimize the temperature difference across the baffle and create ideal crystal growth conditions. The ideal conditions allow enough fluid to be transferred through the baffle to allow for mass transfer, yet also produce a thermal difference across the baffle to encourage deposition. The baffles effects were studied again in [16] where various designs were introduced using a similar setup as [15]. It was concluded that smaller opening baffles were not as suitable for crystal growth. Chen and Prasad [17] also modeled an ammonothermal reactor of retrograde solubility of GaN. They used a baffle directly comparable to their previous work and found a different temperature distribution and flow pattern resulting from the retrograde solubility, when compared to the forward solubility.

The dissertation of Kakhki [18] models a retrograde based ammonothermal crystal growth reactor. The numerical model solves Navier-Stokes, Darcy-Brinkman-Forcheimer, and chemical kinetic equations. The model was used to study multiple geometric setups and their effects on crystal growth. It studied the effects of the gap between the nutrient basket (porous media) and the sidewall, changing the location of the upper heater, different baffle openings including center and wall openings, and lastly, how crystal growth volumetric changes affect the flow field in the reactor. For the interested reader the full results and conclusions are presented in detail in the dissertation.

Enayati, Chandy, and Braun [19] investigate the onset of transition in a laterally heated cylindrical reactor. They used the commercial software ANSYS FLUENT and studied flows characterized by Rayleigh numbers ranging from 750-28,000. To vary the Rayleigh number the authors changed the thermal expansion coefficient of the fluid $\beta$. 
The characteristic length used by the authors was the ratio of volume to lateral surface area, which amounts to half the radius of the reactor. By studying the resulting velocity fluctuations and streamlines of fluid flow in various locations of the reactor, the authors were able to conclude that the critical Rayleigh number occurred around 2800.

Turbulent 2D

Li, Evans, and Wang [20] investigated the turbulent flow regime in a reactor with a baffle with no gap at the wall. It employed constant lateral wall temperature (bottom hot top cooled) and used a k-ω [21] model for turbulence. Their investigation claimed the resulting flow patterns of a fully 3D simulation resulted in 2D flow. There was not however, any results presented confirming this statement. The authors continued with 2D simulations and studied the resulting flow patterns and temperature contours of various aspect ratios for thermal growth environments. The same authors studied a heat flux wall boundary condition in [22]. They employed the same reactor model as before, but this time they attempted to reach desired thermal distributions. In this manner they continued to adjust the heat flux boundary condition until the desired thermal distribution was reached. The paper concluded with a way to estimate the required heat fluxes to generate user specified thermal distribution.

A more detailed model of an ammonothermal reactor is presented by Pendurti, Chen, and Prasad [23]. This study used a k-ε model for turbulence, seeds, a baffle, charge, internal wall temperatures, and mass transfer models for solubility and growth rates. It set the seed location, and studied how various baffle configurations affected crystal growth.

A reactor devoid of a baffle and seeds was studied by Papanicolaou and Belessiotis [24] using the stream function and multiple turbulence models. The sidewall used an
imposed heat flux condition, and the authors ran multiple simulations with different aspect ratios at different Rayleigh numbers. They compared the different turbulence models by investigating the vertical velocity profiles, turbulent kinetic energy, and wall Nusselt numbers. The boundary layer formation and transient development of the flow were also studied. At the time of publication there was no experimental data on high Rayleigh number flow (1E14), and thus the authors were not able to validate their numerical results with experimental data.

The first of several publications by Masuda et al. [25] studied two hydrothermal growth reactors, one containing a baffle the other a baffle and porous medium. The numerical setup included a reactor wall thickness with a temperature imposed on the outside, similar to that of an actual autoclave. Turbulence was modeled by a modified k-ε model, employed by commercial software SC/Tetra. They studied the effects of angled baffles without a porous media and examined the resulting thermal contours and velocity vectors. Then they extended their study to different baffle angles in conjunction with a porous media. This allowed the authors to study the interaction between the porous medium and the angled baffle. The numerical study lead to the conclusion that the optimal thermal environment resulted from a funnel shaped baffle of twenty degrees. The thermal environment showed enough fluid transport through the baffle for effective mass transport with a strong temperature differential above and below the baffle.

A second article by Masuda et al. [26] detailed a simplified reactor. The same turbulence model was used as above, along with similar reactor geometry including seeds. The seed width was varied and the resulting flow patterns were analyzed. They found that two main patterns would occur depending on the width of the seeds: a) the first
pattern resulted in a single large elongated circulation alongside the seed, and b) the second resulted in multiple recirculation zones occurring near the seeds. The authors were able to show that the different flow patterns greatly affected the thermal distribution within the reactor and caused the temperature on the seeds to drop when recirculation developed.

Masuda et al. [27] studied the same reactor setup and also examined fluid transport property effects. The three fluid properties investigated were, specific heat capacity, thermal conductivity, and viscosity. The variation of the properties was estimated by using the property tables of water. Then each fluid property was studied by varying individual properties while holding all others constant. From this systematic approach it was determined that the effect of thermal conductivity had the least impact on flow patterns and heat transfer, while heat capacity and viscosity greatly affected the flow structure.

Masuda et al. [28] numerically and experimentally investigated GaN crystal growth. The paper details the experimental setup, and reviews the quality and growth of the GaN crystals. In their experiment two different setups were considered. The main difference between them was the inclusion of an insulator on top, bottom, and in between the lower and upper heaters which created a larger gap between the lower and upper heaters. The numerical simulations showed that the flow patterns in the reactor can be changed by moving the position of the heater or baffle. The thermal contours were found to establish a more favorable crystal growth environment when the lower heater was positioned farther below the baffle, which they concluded greatly increased crystal growth rate in the experimental setup.
The same authors [29] numerically investigated the effects of changing the distance between the top and bottom heaters and the effects of baffle openings in. Similar conditions were used to simulate the reactor, which now included seeds. Three different distances between the two heaters, and four different baffle openings were simulated yielding twelve different numerical simulations. The results of the temperature contours were given, along with the temperatures of the surface on the seeds. The authors concluded that the baffle needed to have an opening of at least thirty percent for a favorable crystal growing environment.

Enayati, Chandy, and Braun [30] aimed to determine numerically where the transitional flow regime sets in for the laterally heated cylindrical reactor. The model involved an imposed wall temperature boundary condition and the Boussinesq approximation. The Rayleigh number was used as a parameter with a characteristic length defined as volume to lateral surface area i.e., half the radius. Simulations of various Rayleigh numbers from 750-8.8E10 were conducted, and studied. The Rayleigh number was varied in the same manner as in their previous work [19]. From examining flow patterns, temperature contours, boundary layers, and turbulent intensity values it was determined that the transitional regime began around 2800 and ended around 8.8E5 Rayleigh number.

The same authors in [31] numerically studied the effects of the porous media. This investigation varied the permeability and positioning of the porous media. Additionally, the ratio of heating to cooling was examined.
1.2.2 3D previous work

There are a limited number of simulations of three dimensional reactors. Such simulations are computationally expensive, many requiring days of CPU run time for a single simulation. In order to avoid performing such studies, an error concept threshold is established between two and three-dimensional simulations. If the error is small enough the study can be simulated with the two-dimensional model. This often times is useful for a quick study of specific parameters, but accuracy can then be very limited. In an ammonothermal reactor, the kinetics governing the solubility of gallium are so sensitive to temperature, that a small error in temperature can result in poor crystal growth, or wide off-the-mark predictions.

In order to simplify both setup and limit computational expense, laminar flow regimes can be studied to enhance understanding of the physics. However, all too often, a laminar flow is not what really governs the actual flow environment, and a turbulent simulation must be conducted instead. This farther complicates the numerical difficulties as direct numerical simulations (DNS) or large eddy simulations (LES) are expensive to implement and conduct. Thus, many times a turbulence model is employed, but again an error is incurred by using a turbulence model. Unfortunately, different turbulence models too often give different results; therefore, validation with experiments is always necessary to determine which turbulence model is most applicable.

Laminar 3D

Popov et al. [32] studied a hydrothermal autoclave. Specifically, they simulated numerically the autoclave using Navier-Stokes equations for the fluid, Darcy-Brinkman-Forchheimer equations for the porous medium, and the convection diffusion equations to
model the concentration. They included a baffle, with a specified opening and studied the effects of changing the vertical position of the porous medium. The results showed the different temperature and concentration contours along with the different flow patterns that resulted from changing the vertical position of the porous medium.

In [33] Chen et al. used a similar geometry in the context of an ammonothermal reactor. The study included modeling of crystal growth, and was able to determine the growth rates of GaN crystals. They examined the effects of a larger diameter reactor and the effects of a different baffle opening. They presented the flow patterns and temperature contours of the reactor and specifically studied the flow through the baffle. The goal was to learn about fluid transport through the baffle and how its opening and the reactor diameter affected the flow.

Li and Braun [13] as presented before, compared the cylindrical and rectangular reactors. The cylindrical reactor had imposed wall temperature boundary conditions and a baffle. The flow patterns were studied along with temperature distributions inside the reactor. It was clearly noted that the baffle shape needed to be carefully chosen to generate a favorable crystal growing environment. Li and Braun [12] as previously mentioned, studied the cylindrical reactor with two different thermal boundary conditions. The first heating configuration was the lateral heating and cooling configuration compared to laterally heated bottom and top cooled upper surface. As in [13], temperature distributions and velocities were compared.

Li et al. [34] also studied a cylindrical hydrothermal reactor. Their numerical simulation was compared directly to an in-house experiment. The reactor used water as the working fluid, had laterally heated walls, and contained a baffle. The time averaged
temperatures of the experiment and simulation were compared and proved to correspond closely. The same study also presented the difference in flow behavior and temperatures when constant temperature and constant heat flux boundary conditions for the lower heated wall are used. It was determined that the heating condition had little effect on the thermal environment provided the heat flux remained comparable.

The same authors [35] studied a similar geometry, but added a porous medium. The numerical simulation was compared directly to an in-house experiment which showed similar flow patterns. The authors investigated the effects of porosity of a porous block formed out of spheres and lower wall heat flux. They were able to determine that all of these parameters had various effects, but the impact of the upper portion on the chamber was negligible compared to the effects on the lower chamber. They also considered the effect of a tilted reactor, when the angle of tilt was relatively small. They found that the overall flow was minimally impacted, and that the main effect resides with changing the wall boundary layer thickness in the direction of tilt.

_Turbulent 3D_

In 2004 Li et al. [36] published the effects of non-axisymmetric heating conditions of a hydrothermal autoclave. The authors employed a k-ω turbulence model and presented the difference in behavior between a reactor with and without a baffle. The reactor with a baffle had a thermal distribution that was less asymmetric and provided a better growing environment for crystals. It did not eliminate asymmetric thermal conditions in the upper portion of the reactor where crystal growth would occur. The authors concluded that keeping the upper growing chamber thermally axisymmetric was of utmost importance for uniform crystal growth.
The same authors [37] also studied the effects of single versus multi-hole baffle designs. Multiple opening designs were simulated and their effects compared. The baffles had a set total opening area, to keep the total opening a constant when comparing the different designs. The authors described the flow patterns and the resulting thermal distributions. They conclude that an eight-hole axisymmetric patterned baffle provided the best thermal environment for crystal growth.

Another baffle geometry study is presented by Li and Braun [38]. A similar geometry was used as the previously mentioned article [37]. However, the baffles in this study had a single opening, a sixteen-hole symmetric opening, and a homogeneously perforated baffle respectively. They modeled the perforated baffle as a porous plate. Again, the total area of the openings was kept constant for a direct comparison. The flow patterns and thermal environments were compared, and the authors concluded that the perforated baffle allowed the greatest fluid and heat transfer exchange, and that any multi-hole baffle designs should only have holes away from the wall, at least half the distance of the radius of the reactor from the wall.

The same authors investigated the effects of single opening baffle areas in another paper [39]. Geometry and boundary conditions were the same as [37] and [38]; the difference was that single baffle opening baffles of 5, 10, 15, and 20 percent along with different aspect ratio reactors were simulated. The authors investigated thermal distributions and flow patterns along with heat transfer rate across the baffle opening. The effects of the aspect ratio and baffle opening were shown. The authors also discuss the characteristic length scale, and acknowledged that it is dependent upon the autoclave diameter, chamber height, and baffle hole diameter.
Another study by Enayati, Chandy, and Braun [40] studied a very similar reactor as [39] with larger baffle openings. Their results showed a large thermal change occurring inside the reactor dependent upon on the baffles opening. In [41] and [42] the same authors also investigated the effects of a rack and seeds. They compared an empty reactor to one with a rack and another with rack and seeds to determine how the different internal configurations affected the fluid flow.

1.2.3 2D to 3D comparative previous work

There is a limited number of 2D-3D comparative works in the literature. The works that exist show the great importance of actually modeling the reactor three dimensionally. Most of the time studies that employ a three-dimensional model, compare it to a two-dimensional model, and show the assumption to be within some acceptable error. They use this error to justify continued use of the two-dimensional model. In this section, it will be shown how this 2D assumption and the errors that result from it may play an important role. However, the total literature studying direct effects is limited generally to very specific cases.

Erlekampf et al. [43] employed two and three-dimensional simulations to study the effect of different baffle shapes. The work specifically focuses only on three-dimensional simulations and does not directly compare with the two-dimensional results. It focused on showing non-axisymmetric flow patterns and thermal distributions and the importance of using three dimensional simulations. The authors also showed how each baffle shape affected the thermal distribution and showed where the fluid flow fluctuations occurred.

The dissertation of Moldovan [44] presented direct comparisons between two and three-dimensional simulations. It also directly compared turbulence models to determine
the most appropriate model. This was very important, as it presented evidence supporting the use of the \( k-\omega \) model for turbulence. The dissertation compares thermal distributions and flow patterns and presents temperature location data to determine effects in a methodical way. For more details and studies the reader is referred to [44].

A simplified reactor geometry is studied in great depth by Enayati et al. [45]. The authors employed a LES to model fluid flow in the reactor, and were able to directly compare to an in-house experiment. Numerical and experimental flow patterns were compared and showed a strong correlation. Reynolds Averaged Navier Stokes (RANS) and LES simulations in three dimensions were directly compared, along with two dimensional simulations. The authors demonstrated that it is most recommended to simulate the reactor fully three dimensionally using a LES simulations to accurately determine the correct thermal distribution. The 2D RANS simulations produced incorrect thermal distributions; while the three-dimensional RANS simulation was much closer to the LES simulation.

1.2.4 Overview

This chapter summarized the many experimental and numerical studies that have been conducted on the laterally heated vertical cylinder. The studies referenced above were broken down into 2D and 3D groupings, with sub groups divided farther into laminar and turbulent categories. Not every paper fit neatly into these categories, some studied both laminar and turbulent regimes. And often times comparing works is impossible because of the different assumptions, geometry, and/or models for numerical simulations.
A large number of two-dimensional parametric studies involving various geometries, internal and external have been conducted. The majority of these studies have investigated the effects of the internal reactor geometries, such as seed placement, baffle shapes, and porous medium site and its location. The most commonly studied internal feature of the reactor is the baffle. Many different configurations have been studied, and vary from the size of the opening, to types of openings, and different baffle shapes altogether. The least studied feature of this cylindrical reactor is the external geometry. I.e. the length, diameter, or a ratio of these lengths and how they affect the overall fluid flow. The tables shown below, briefly categorize the studies and break down what parameters were studied.

Table 1  Summary of 2D enclosures and parameters studied

<table>
<thead>
<tr>
<th>Reference</th>
<th>2D</th>
<th>Simulation Employed</th>
<th>Internal Geom</th>
<th>Studied Parameters</th>
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<tr>
<td>2D</td>
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<td>Fluid Props f(T)</td>
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Table 2  Summary of 3D enclosures and parameters studied

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<th>Simulation Employed</th>
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<th>Studied Parameters</th>
<th>Reference 3D</th>
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</table>

The characteristic length has not been studied exclusively for the laterally heated vertical cylinder. Without knowledge of this critical length scale, scalability for industry would be difficult. Every reactor would need to have its own independent study. The most commonly assumed scales for this configuration are: the length or height of the reactor, the diameter or radius of the reactor, or a volume to surface area ratio of the reactor. At this time, none of these lengths scales have been investigated in systematic detail to determine the correct scaling factor(s).
CHAPTER II

SCOPE OF WORK

The literature presented in Chapter I reviewed aspects of the laterally heated cylindrical reactor. However, there has not been a comprehensive length scale study. The current work proposes to investigate the characteristic length and determine what other geometric parameters may affect the length scale. A laterally heated vertical cylindrical enclosure will be studied for simplicity. The cylinder does not contain seeds, baffles, or porous media. The study will involve a multi parameter study, through numerical simulations involving: a) the geometric aspect ratio, b) length, c) diameter, d) the ratio of laterally heated to laterally cooled sections of the reactor, e) changing the insulator thickness, and finally f) two compared to three-dimensional simulations in a turbulent and laminar regime. The study focuses on mostly turbulent simulations, as most reactors operate in a turbulent regime. Not every parameter was studied in a three-dimensional environment due to computational constraints, nor did every study have its own convergence study. Sections 2.1-2.3 present an itemized list of the studies that will be undertaken.
2.1 Turbulent 2D parametric study of geometric parameters affecting characteristic length.

i. Numerical simulations were conducted to study specific parametric influences while holding all other parameters constant including fluid properties.
   a. Effect of aspect ratio – constant diameter.
   b. Effect of aspect ratio – constant length.
   c. Effect of changing the size of the insulator.
   d. Effect of changing the sidewall heating to cooling ratio.

ii. The simulations were evaluated for numerical accuracy and error.
   a. Quantifying a basis of change in Rayleigh number.
   b. The relative convergence of each case is determined.
   c. Spatial convergence of the grid is evaluated.
   d. Temporal convergence and stability is examined.
   e. The wall y+ condition for turbulence is examined.

iii. Comparisons of the effects of each parameter are examined.
   a. Normal probability density functions of velocity magnitude.
   b. Examination of how the boundary layer is affected.
   c. Contour maps of important fluid properties and dependent variables.

2.2 Turbulent 3D parametric study of geometric parameters affecting characteristic length.

i. Numerical simulations were conducted to study specific parametric influences while holding all other parameters constant including fluid properties.
   a. Effect of aspect ratio - changing length.
b. Effect of aspect ratio - changing diameter.

ii. The simulations were evaluated for numerical accuracy and error.
   a. Quantifying a basis of change in Rayleigh number.
   b. The relative convergence of each case is determined.
   c. Spatial convergence of the grid is evaluated.
   d. The wall y+ condition for turbulence is examined.

iii. Comparisons of the effects of each parameter were evaluated.
   a. Normal probability density functions of velocity magnitude.
   b. Examination of how the boundary layer is affected.
   c. Contours of important fluid properties and dependent variables.

2.3 Turbulent and Laminar 2D-3D effects are studied.

i. The simulated turbulent cases are then compared.
   a. Individual cases - 2D to 3D.
   b. Aspect ratio trends - 2D to 3D.

ii. Laminar 2D and 3D comparisons.
   a. Normal probability density functions of velocity magnitude.
   b. Examination of how the boundary layer is affected.
   c. Contours of important fluid properties and dependent variables.
CHAPTER III

THEORY

All numerical simulations were performed using ANSYS FLUENT. A commercially available program that solves sets of complex fluid flow governing equations utilizing the finite volume method in Cartesian coordinates. The simulations are governed either for laminar or turbulent flow by three main equations: continuity, momentum, and energy. The working fluid used was water, and a discussion of its properties is given. Dimensionless numbers are used to categorize specific flow characteristics. Generally, the simulations employed three-dimensional Cartesian coordinate systems of the equations, whereas for two dimensional simulations the equations were reduced to the two-dimensional axis-symmetric equations.

3.1 Governing Equations

3.1.1 Continuity

The following conservation equations will be explained in context of [46]: continuity, momentum, and energy. Mass conservation is given by:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m
\]
the equation applies to both compressible and incompressible fluids and $S_m$ represents a mass source term.

3.1.2 Momentum

*The Laminar Regime*

The three conservation of momentum equations in vector form for an inertial reference frame are given by:

$$\frac{\partial}{\partial t}(\rho \hat{v}) + \nabla \cdot (\rho \hat{v} \hat{v}) = -\nabla p + \nabla \cdot (\vec{r}) + \rho \hat{g} + \vec{F}$$

where $p$ is static pressure, $\rho \hat{g}$ is the gravitational body force, $\vec{F}$ are external body sources that are model dependent, and $\vec{r}$ is the stress tensor. The stress tensor is defined:

$$\vec{r} = \mu \left[ (\nabla \hat{v} + \nabla \hat{v}^T) - \frac{2}{3} \nabla \cdot \hat{v}I \right]$$

where $\mu$ is dynamic viscosity, $I$ is the unit tensor, and $\nabla \hat{v}^T$ is the effect of volume dilation.

*The Turbulent Regime*

To solve the instantaneous Navier-Stokes equations in turbulence on very fine grids is very difficult and extremely computationally expensive. This is the definition of a Direct Numerical Simulation (DNS). Computational difficulties arise when the governing momentum equations are no longer dominated by viscous forces, but by momentum forces; this change means the equations have transformed from a parabolic system of equations into a system of hyperbolic equations. To simplify the problem, the equations are time averaged, yielding the Reynolds Averaged Navier Stokes (RANS). These equations have additional unknowns that involve the instantaneous velocities $\hat{u}_i$ and form the Reynolds Stresses. There are no extra equations to account for the Reynolds Stresses,
and therefore need to be modeled. The RANS equations will be developed in a brief manner as presented in [46].

\[ u_i = \bar{u}_i + u'_i \]
\[ \phi = \bar{\phi} + \phi' \]

Where \( \bar{u}_i \) and \( \bar{\phi} \) are for the time averaged velocity components and scalar properties respectively. The instantaneous velocities are given by \( u'_i \) and instantaneous scalar properties given by \( \phi' \). When the above expressions are substituted into the instantaneous continuity and momentum equations and integrated with respect to time the time averaged continuity and momentum equations are generated.

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \]
\[ \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_i} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right] + \frac{\partial}{\partial x_j} \left( -\rho u'_i u'_j \right) \]

The above are the RANS equations. The last term on the right-hand side (rhs) represent the Reynolds stresses.

The Reynolds stresses are typically modeled using the Boussinesq hypothesis. This hypothesis relates the mean velocity gradients to the Reynolds stresses.

\[ -\rho \bar{u}_i \bar{u}_j = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left( \rho k + \mu_t \frac{\partial u_k}{\partial x_k} \right) \delta_{ij} \]

This hypothesis will be used in all turbulence models of concern in this work. The difficulty now lay in modeling the transport of turbulent kinetic energy and turbulent viscosity, represented by \( k \) and \( \mu_t \) respectively. Additionally, in two equation models \( \epsilon \) or \( \omega \) is included as turbulent dissipation or specific dissipation.
The \( k-\epsilon \) model

The first two equation turbulence model reviewed is the standard \( k-\epsilon \) model. It was the first to be developed, and many other models follow a similar concept. The model is presented following [46] as shown below.

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho ku_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \epsilon - Y_m + S_k
\]

\[
\frac{\partial}{\partial t} (\rho \epsilon) + \frac{\partial}{\partial x_i} (\rho \epsilon u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + C_{1\epsilon} \frac{\epsilon}{k} (G_k + C_{3\epsilon} G_b) - C_{2\epsilon} \rho \frac{\epsilon^2}{k} + S_\epsilon
\]

It should be noted here that these sets of equations ultimate purpose is to compute the turbulent viscosity which is related to the Reynolds Stresses. The empirically determined constants are: \( C_{1\epsilon}, C_{2\epsilon}, C_{3\epsilon}, \sigma_\epsilon, \sigma_k \), and \( C_\mu \) shown below for defining turbulent viscosity.

\[
\mu_t = \rho C_\mu \frac{k^2}{\epsilon}
\]

The generation of turbulence is \( G_k \), the generation of turbulent kinetic energy due to buoyancy is \( G_b \), and the contribution of compressible turbulence in \( Y_m \). The generation of turbulence and generation of turbulent kinetic energy due to buoyancy is shown below.

\[
G_k = -\rho \bar{\dot{u}_i \dot{u}_j} \frac{\partial \bar{u}_j}{\partial x_i}
\]

\[
G_k = \mu_t S^2
\]

Where \( S \) is the modulus of the mean rate-of-strain tensor

\[
S \equiv \sqrt{2 S_{ij} S_{ij}}
\]

Buoyancy generates turbulence defined as

\[
G_b = \beta g_i \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i}
\]
where $Pr_t$ is the turbulent Prandtl number, which is a constant in the standard model. The coefficient of thermal expansion, $\beta$, is defined as

$$\beta = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p$$

and will be discussed later and in Section 3.4.

The $k$-$\omega$ model

The second two equation turbulence model presented here is the standard $k$-$\omega$ model. Again, the model will be presented following [46], starting with the transport equations for $k$ and $\omega$ representing kinetic energy and vorticity respectively.

$$\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left[ \Gamma_k \frac{\partial k}{\partial x_j} \right] + G_k - Y_k + S_k$$

$$\frac{\partial}{\partial t} (\rho \omega) + \frac{\partial}{\partial x_i} (\rho \omega u_i) = \frac{\partial}{\partial x_j} \left[ \Gamma_\omega \frac{\partial \omega}{\partial x_j} \right] + G_\omega - Y_\omega + S_\omega$$

$\Gamma_k$ and $\Gamma_\omega$ represent the effective diffusivity of $k$ and $\omega$ respectively; $G_k$ $G_\omega$ represents the generation of turbulent kinetic energy due to velocity gradients and generation of $\omega$, respectively. $Y_k$ and $Y_\omega$ represent the dissipation of $k$ and $\omega$, respectively; and $S_k$ and $S_\omega$ are user defined source terms. The effective diffusivity is given by

$$\Gamma_k = \mu + \frac{\mu_t}{\sigma_k}$$

$$\Gamma_\omega = \mu + \frac{\mu_t}{\sigma_\omega}$$

where $\sigma_k$ and $\sigma_\omega$ are the turbulent Prandtl numbers for $k$ and $\omega$ respectively. Turbulent viscosity is computed slightly differently than the $k$-$\epsilon$ model as shown below.

$$\mu_t = a^* \frac{\rho k}{\omega}$$
The $a^*$ coefficient damps the turbulent viscosity, which causes a low-Reynolds number correction given by

$$ a^* = a_\infty^* \left( \frac{a^*_0 + Re_t/R_k}{1 + Re_t/R_k} \right) $$

$$ Re_t = \frac{\rho k}{\mu \omega} $$

where $R_k$, and $a^*_0$ are empirically derived constants.

Modeling the production of kinetic energy ($G_k$) is the same as the k-$\epsilon$ model. Modeling the production of $\omega$ is given by

$$ G_\omega = \alpha \frac{\omega}{k} G_k $$

$$ \alpha = \frac{a_\infty}{a^*} \left( \frac{a_0 + Re_t/R_\omega}{1 + Re_t/R_\omega} \right) $$

$$ R_\omega = 2.95 \ a^* $$

Modeling the turbulent dissipation of $k$ is given by

$$ Y_k = \rho \beta^* f_{\beta^*} k \omega $$

$$ f_{\beta^*} = \begin{cases} 
1 & \chi_k \leq 0 \\
1 + 680 \chi_k^2 & \chi_k > 0 
\end{cases} $$

$$ \chi_k \equiv \frac{1}{\omega^3} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} $$

$$ \beta^* = \beta_i^* \left[ 1 + \zeta^* F(M_t) \right] $$

$$ \beta_i^* = \beta_\infty^* \left( \frac{4/15 + (Re_t/R_\beta)^{4*}}{1 + (Re_t/R_\beta)^{4*}} \right) $$

where $\zeta^*$, $R_\beta$, and $\beta_i^*$ are constants and $F(M_t)$ is a compressibility correction.
The dissipation of $\omega$ is given by

$$Y_\omega = \rho \beta f_\beta \omega^2$$

$$f_\beta = \frac{1 + 70 \chi_\omega}{1 + 80 \chi_\omega}$$

$$\chi_\omega = \frac{|\Omega_{ij}\Omega_{jk}S_{kl}|}{(\beta_\infty \omega)^3}$$

$$\Omega_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right)$$

$$\beta = \beta_i \left[ 1 - \frac{\beta^*_i}{\beta_i} \xi^* F(M_t) \right]$$

where $\beta_i$, $\alpha_{\infty}$, $\alpha_0$, $\sigma_k$, and $\sigma_\omega$ are all model constants.

**The k-\omega Shear-Stress Transport model**

The last two equation turbulence model reviewed is the k-\omega Shear-Stress Transport (SST) model. This is the model used in all turbulent simulations and is a combination of the standard k-\epsilon and k-\omega models. This combination model uses the accurate k-\omega model near the wall region and the k-\epsilon in the far field. This requires that the k-\epsilon model be transformed into a k-\omega model and a function defining the dependence between the two. This model was chosen because it has often been used in the literature and has been directly compared to a LES model with reasonable accuracy in [45]. Again using [46] and starting with the transport equations below.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[ \Gamma_k \frac{\partial k}{\partial x_j} \right] + G_k - Y_k + S_k$$

$$\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_j}(\rho \omega u_j) = \frac{\partial}{\partial x_j}\left[ \Gamma_\omega \frac{\partial \omega}{\partial x_j} \right] + G_\omega - Y_\omega + D_\omega + S_\omega$$

$G_k, Y_k, Y_\omega, S_k, and S_\omega$ were all previously described and are defined the same way as the
k-ω model. $I_k$ and $I_ω$ are calculated the same way, with a change in how $μ_t$, $σ_k$, and $σ_ω$ are defined. $D_ω$ represents the cross-diffusion term; the changes are given below

$$μ_t = \frac{ρk}{ω} \frac{1}{\max\left[\frac{1}{α^*}, \frac{SF_2}{a_1ω}\right]}$$

where $S$ is the strain rate magnitude. The new turbulent Prandtl numbers defined by

$$σ_k = \frac{1}{F_1/σ_{k,1} + (1 - F_1)/σ_{k,2}}$$

$$σ_ω = \frac{1}{F_1/σ_{ω,1} + (1 - F_1)/σ_{ω,2}}$$

The blending functions $F_1$ and $F_2$ are defined by

$$F_1 = tanh(ϕ_1^*)$$

$$ϕ_1 = min\left[max\left(\frac{\sqrt{k}}{0.09ωy}, \frac{500μ}{ρy^2ω}\right), \frac{4ρk}{σ_{ω,2}D_ω^+y^2}\right]$$

$$D_ω^+ = max\left[2ρ \frac{1}{σ_{ω,2}} \frac{1}{ω} \frac{∂k}{∂x_j} \frac{∂ω}{∂x_j}, 10^{-10}\right]$$

$$F_2 = tanh(ϕ_2^2)$$

$$ϕ_2 = max\left[2 \frac{\sqrt{k}}{0.09ωy}, \frac{500μ}{ρy^2ω}\right]$$

where $y$ is the distance to the next wall and $D_ω^+$ is the positive portion of the cross-diffusion term. The cross-diffusion term results from transforming the k-$c$ model into a k-ω model, given by

$$D_ω = 2(1 - F_1)ρ \frac{1}{ωσ_{ω,2}} \frac{∂k}{∂x_j} \frac{∂ω}{∂x_j}$$

Production of $ω$ in the term $G_ω$ is redefined by
\[ G_\omega = \frac{\alpha}{\nu_t} G_k \]

also differing by

\[ \alpha_{\infty} = F_1 \alpha_{\infty,1} + (1 - F_1) \alpha_{\infty,2} \]

\[ \alpha_{\infty,1} = \frac{\beta_{i,1}}{\beta_{\infty}^*} - \frac{\kappa^2}{\sigma_{\omega,1} \beta_{\infty}^*} \]

\[ \alpha_{\infty,2} = \frac{\beta_{i,2}}{\beta_{\infty}^*} - \frac{\kappa^2}{\sigma_{\omega,2} \beta_{\infty}^*} \]

where \( \kappa \) is a constant.

Both dissipation terms are defined similarly to the k-\( \omega \) model. \( Y_k \) is modeled with \( f_{\beta^*} \)
equal to 1 and \( Y_\omega \) is changed by evaluating \( \beta_i \) differently expressed by

\[ \beta_i = F_1 \beta_{i,1} + (1 - F_1) \beta_{i,2} \]

The new model constants are: \( \sigma_{k,1}, \sigma_{k,2}, \sigma_{\omega,1}, \sigma_{\omega,2}, \alpha_1, \beta_{i,1}, \) and \( \beta_{i,2} \). The other constants are the same as the k-\( \omega \) model.

The wall boundary conditions are treated with a wall function approach. Where the \( \omega \) equation switches automatically between the viscous sublayer formulation to the wall function depending on the grid. The wall function was optimized using Couette flow. The value of \( \omega \) at the wall is defined by

\[ \omega_w = \frac{\rho (u^*)^2}{\mu} \omega^+ \]

The laminar sublayer

\[ \omega^+ = \frac{6}{\beta_i (y^+)^2} \]

And logarithmic region
\[ \omega^* = \frac{1}{\sqrt{\beta^*_\infty}} \frac{du^*_{turb}}{dy^*} \]

**Boussinesq approximation**

As very briefly mentioned, the coefficient of thermal expansion \( \beta \) defined again as

\[ \beta = \frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p \]

shows the relationship between density and temperature in a constant pressure environment. Typically, as the temperature of a fluid is increased, the density decreases. If the fluid were not to exhibit this property, then natural convection could not occur. \( \beta \) is constant if the change of density and temperature is linear. If this change is not linear, then \( \beta \) becomes a function of temperature. The assumption used for this study is that the fluid density changes linearly with respect to temperature, as such a constant density fluid can be assumed for the fluid with an additional force resulting from \( \beta \). This assumption simplifies the model, as the fluid is modeled as constant density which in turn decreases computational effort. This assumption is valid for fluids when either: (1) the fluid has a very linear density temperature relationship or (2) the temperature difference is small, such that \( \beta(T) \) is essentially the same as a constant \( \beta \).

### 3.1.3 Energy

The process in the reactor is driven purely by thermal gradients, produced by some form of differential heating. Therefore, energy conservation needs to be introduced. The conservation of energy is given by

\[
\frac{\partial}{\partial t}(\rho E) + \nabla \cdot \left( \hat{\rho} (\rho E + p) \right) = \nabla \cdot \left( k_{eff} \nabla T - \sum_j h_j \hat{f}_j + \left( \hat{\tau}_{eff} \cdot \hat{\nu} \right) \right) + S_h
\]
where \( k_{\text{eff}} \) is the effective conductivity (\( k+k_t \) where \( k_t \) is the turbulent thermal conductivity, defined in accordance with the turbulence model). \( \mathcal{J} \) is the diffusion flux of the specific species \( j \) and \( S_h \) are any other volumetric heat sources. Other terms are defined such as

\[
E = h - \frac{p}{\rho} + \frac{v^2}{2}
\]

and the sensible enthalpy for incompressible flows is defined by

\[
h = \sum_j Y_j h_j + \frac{p}{\rho}
\]

\[
h_j = \int_{T_{\text{ref}}}^{T} c_{p,j} dT
\]

where the reference temperature is defined by the solver and models used.

3.2 Discretization and Solvers

ANSYS uses the control volume method for solving the governing equations. The transport equation in integral form is used for discretizing the governing equations about each control volume. This is shown below by considering an unsteady conservation equation for a scalar quantity \( \phi \) in control volume \( \mathcal{V} \).

\[
\int_{\mathcal{V}} \frac{\partial \rho \phi}{\partial t} dV + \oint_{\partial \mathcal{V}} \rho \phi \mathbf{\hat{v}} \cdot d\mathbf{A} = \oint_{\partial \mathcal{V}} \mathcal{I}_\phi \nabla \phi \cdot d\mathbf{A} + \int_{\mathcal{V}} S_\phi dV
\]

Where

\[
\rho = \text{density}
\]

\[
\mathbf{\hat{v}} = \text{velocity vector}
\]

\[
\mathbf{\hat{A}} = \text{surface area vector}
\]
\[ \Gamma_\phi = \text{diffusion coefficient for } \phi \]
\[ \nabla \phi = \text{gradient of } \phi \]
\[ S_\phi = \text{source of } \phi \text{ per unit volume} \]

the above formulation is applied to every control volume in the domain. Discretizing on every cell, an example of two cells is shown in Figure 2, yields

\[
\frac{\partial \rho \phi}{\partial t} V + \sum_{f} \rho_f \bar{v}_f \phi_f \cdot \hat{A}_f = \sum_{f} \Gamma_\phi \nabla \phi_f \cdot \hat{A}_f + S_\phi V
\]

where

\[ N_{faces} = \text{number of faces enclosing cell} \]
\[ \phi_f = \text{value of } \phi \text{ convected through face } f \]
\[ \rho_f \bar{v}_f \phi_f \cdot \hat{A}_f = \text{mass flux through the face} \]
\[ \hat{A}_f = \text{area of face } f \]
\[ \nabla \phi_f = \text{gradient of } \phi \text{ at face } f \]
\[ V = \text{cell volume} \]

Figure 2 Illustration of discretizing a scalar transport equation
and $\frac{\partial \rho \phi}{\partial t} V$ is the Temporal Discretization. The temporal discretization is necessary for transient simulations, the time evolution of a variable $\phi$ is given by

$$\frac{\partial \phi}{\partial t} = F(\phi)$$

where $F$ is any spatial discretization, i.e. first, second, etc. forward or backward differences can be used. This will in turn develop either an implicit or explicit scheme for time integration. For more information on the different discretization’s refer to [46]. The study presented here used a second order implicit formulation (QUICK Scheme).

The gradients of the scalar variable $\phi$ must be evaluated. There are multiple ways FLUENT defines the gradients: Green-Gauss Cell-Based, Green-Gauss Node-Based, and Least Squares Cell-Based. Only the Least Squares Cell-Based method will be reviewed, as this was the method used in all simulations. Coming from [46] the solution is assumed to vary linearly. In Figure 3 below, the change in cell values between cell $c_0$ and $c_i$ along the vector $\delta r_i$ from the centroid of cell $c_0$ to cell $c_i$, can be expressed as

$$(\nabla \phi)_{c_0} \cdot \Delta r_i = (\phi_{c_i} - \phi_{c_0})$$
Since similar equations characterize each surrounding cell c0, the following system is obtained, and can be written in compact form as:

\[ [J](\nabla \phi)_{c0} = \Delta \phi \]

where \([J]\) is the coefficient matrix that is purely a function of geometry. The objective is to determine the gradient of the cell boundaries by solving the minimization problem for the system of the non-square coefficient matrix in a least-squares sense. Using a Gram-Schmidt process a matrix of weights are produced for each of the faces of cell c0.

\[ (W_{i0}^x, W_{i0}^y, W_{i0}^z) \]

The gradient at the cell center can be computed by multiplying the weight factors by the difference vector resulting in

\[ \Delta \phi = (\phi_{c1} - \phi_{c0}) \]

\[ (\phi_x)_{c0} = \sum_{i=1}^{n} W_{i0}^x \cdot (\phi_{ci} - \phi_{c0}) \]

\[ (\phi_y)_{c0} = \sum_{i=1}^{n} W_{i0}^y \cdot (\phi_{ci} - \phi_{c0}) \]

\[ (\phi_z)_{c0} = \sum_{i=1}^{n} W_{i0}^z \cdot (\phi_{ci} - \phi_{c0}) \]

It is important to note that FLUENT incorporates limiters. By default, the standard limiter, the minmod function, was used in the simulations.

The solver used in the simulations was a pressure-based solver. The SIMPLE and PISO algorithms were both used, dependent on the speed of the simulation. They are both segregated algorithms where pressure corrections are used to enforce continuity. The algorithm for the numerical solution is shown in Figure 4.
The discretization used was second order. For the full detailing of these algorithms refer to [46].

3.3 Dimensionless Parameters

There are three main dimensionless numbers that characterize the reactor: Prandtl, Grashof, and Rayleigh numbers. Each describes a different physical phenomenon that occurs inside the reactor. The first is the Prandtl number defined by

$$Pr = \frac{\mu c_p}{k}$$

where $k$, $\mu$, and $c_p$ are the thermal conductivity, dynamic viscosity and specific heat of the fluid, respectively. The Prandtl number is the ratio of the momentum diffusion rate to the thermal diffusion rate. Its value gives an indication of the relationship between the momentum boundary layer, $\delta$, to the thermal boundary layer, $\delta_t$, when Prandtl is one and $\delta$ is equal to $\delta_t$. Prandtl greater than one implies $\delta$ greater than $\delta_t$; and less than one implies the opposite relationship.
The second important dimensionless number represents the ratio buoyancy forces to viscous forces. The Grashof number is defined by

\[ Gr = \frac{g \beta \Delta T \rho^2 X^3}{\mu^2} \]

where \( g \), \( \beta \) and \( \rho \) are the gravitational acceleration, thermal expansion coefficient, and density of the fluid respectively. \( \Delta T \) was defined as the difference between the hot and cold wall temperatures. The characteristic length, \( X \), is not universally agreed upon for this specific geometry and consequently will have various definitions.

The last dimensionless number, the Rayleigh number is defined by

\[ Ra = Gr Pr = \frac{c_p g \beta \Delta T \rho^2 X^3}{\mu k} \]

which describes the primary mode of heat transfer. In this respect Rayleigh is dependent upon both Grashof and Prandtl. Higher Rayleigh numbers indicate heat transfer dominated by convection, while lower Rayleigh indicates a conduction dominated process. The value of this number is also an indicator for laminar, transitional, or turbulent flows. For the reactor geometry studied, the flow regimes were identified in [19] and [30].

Depending on the researcher, the literature offers multiple definitions for the characteristic length, \( X \). The three main definitions are: volume to lateral surface area, height, and the diameter or radius of the reactor. The effect of using each will be investigated and studied. Table 3 references all the cases simulated in the present work, and their respective Rayleigh numbers based on three different length scales. The specific
details of each case are given in Section 4.1.1. The table is referenced when comparing different simulations.

### Table 3  Rayleigh number for all simulations based on three definitions

<table>
<thead>
<tr>
<th>Aspect Ratio L:D</th>
<th>( Ra \frac{L}{A} )</th>
<th>( Ra ) L</th>
<th>( Ra ) D</th>
</tr>
</thead>
<tbody>
<tr>
<td>5:1</td>
<td>8.8004e+06</td>
<td>7.8220e+10</td>
<td>5.6323e+08</td>
</tr>
<tr>
<td>2.5:1</td>
<td>8.8004e+06</td>
<td>9.7775e+09</td>
<td>5.6323e+08</td>
</tr>
<tr>
<td>10:1</td>
<td>8.8004e+06</td>
<td>6.2575e+11</td>
<td>5.6323e+08</td>
</tr>
<tr>
<td>20:1</td>
<td>8.8004e+06</td>
<td>5.0060e+12</td>
<td>5.6323e+08</td>
</tr>
<tr>
<td>5:0.5</td>
<td>1.1001e+06</td>
<td>7.8220e+10</td>
<td>7.0403e+07</td>
</tr>
<tr>
<td>5:2.15</td>
<td>8.8007e+07</td>
<td>7.8220e+10</td>
<td>5.6324e+09</td>
</tr>
<tr>
<td>5:5</td>
<td>1.1001e+09</td>
<td>7.8220e+10</td>
<td>7.0403e+10</td>
</tr>
</tbody>
</table>

To study the effects of changing the magnitude of the Rayleigh number a parameter had to be studied. Subramanian [47] presents a relationship between Reynolds number and Grashof number. The Reynolds number is defined below and how it correlates to Gr.

\[
Re = \frac{\rho v X}{\mu}
\]

Where, by an order of magnitude analysis.

\[
v = \sqrt{g\beta \Delta T X}
\]

\[
Re^2 = \frac{v^2 \rho^2 X^2}{\mu^2} = \frac{g\beta \Delta T \rho^2 X^3}{\mu^2} = Gr
\]

This implies that the velocity occurring inside the domain is related to the Grashof number and because the Prandtl number was kept constant, velocity becomes the most important parameter to investigate when determining if the magnitude of the Rayleigh number changed. Not only can the overall flow velocity be investigated but as well as the velocity of the boundary layers. Significant changes in flow speeds inside the reactor or inside the boundary layer indicates large changes in the magnitude of the Rayleigh number.
3.4 Fluid Properties

The objective of this work is to study how different geometric parameters affect the flow process in the reactor, independent of the fluid properties. The general working fluid considered is water with the simplifying assumption of constant fluid properties. This simplified the model and eliminated the non-linear effects introduced by property variation. To approximate the buoyancy forces, the Boussinesq approximation was used, that is, the properties of the fluid throughout the equations are kept constant with the exception of the source term. The properties were chosen based on a temperature between the heated and cooled walls. The properties of the standard fluid case are shown in Table 4.

Table 4 Water properties of standard turbulent simulations

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>ρ</td>
<td>997.1</td>
<td>kg/m³</td>
</tr>
<tr>
<td>β</td>
<td>2.57e-4</td>
<td>1/K</td>
</tr>
<tr>
<td>μ</td>
<td>8.5384e-4</td>
<td>kg/ms</td>
</tr>
<tr>
<td>c_p</td>
<td>4180.9</td>
<td>J/kgK</td>
</tr>
<tr>
<td>k</td>
<td>0.61028</td>
<td>W/mK</td>
</tr>
</tbody>
</table>

To evaluate the approximations the temperature dependent properties according to NIST [48] are shown below in blue in the Figure 5. They were fitted with second order polynomial functions to make the data continuous, shown as the green line. The fits were found using MATLAB [49] and its nonlinear minimization solver (fminsolve); the unknown second order polynomial coefficients were determined by minimizing the sum of the squared errors. The fits exhibited R values very close to one, and cover up the data in blue. The temperature range examined was the lowest and highest temperature boundary condition.
Figure 5  Temperature dependent properties of water

The temperature dependent properties imply that the dimensionless numbers and thermal expansion coefficient are functions of temperature. Figure 6 shows these relationships, with an assumed length scale of volume to lateral surface area of the standard reactor (AR = 5:1). It is important to note, that for the current study, constant properties were used (the values in Table 4) to avoid the ranges of dimensionless numbers shown in Figure 6. Figures 5 and 6 are given for completeness on the study of water, showing the potential error by assuming constant water properties compared to the real properties of water as an experiment will exhibit.
The current study needed to be able to quantify a change in $Ra$. The only way to affect the $Ra$ number is to change the fluid properties or wall condition. The easiest parameters to change were $g$, $\beta$, or $\Delta T$. In this study the thermal expansion coefficient $\beta$ was changed, to avoid changing the boundary condition and to abide by the necessary conditions to use the Boussinesq approximation. This fluid is not based on a real fluid but the Rayleigh numbers would assume, theoretically, dynamic similitude for a generic case that runs at that value of the Rayleigh. An experimental approach would be to put the reactor into a centrifuge to artificially increase gravity. Another would be to increase the temperature differential; however, this will increase the non-linear property variations which will affect the internal conditions.
CHAPTER IV

NUMERICAL IMPLEMENTATION

The geometry, fluid properties, boundary conditions, convergence criterion, and post processing are detailed below. It is important to mention that the original geometry is based off of an actual reactor, thus scaling factors and ratios were not round. The aspect ratio, \( AR \), is an improper ratio defined each time for the reader to easily identify reactor scale changes. The proper aspect ratio, \( \bar{h} \), defined by \( L/D \) is given in the tables.

4.1 Geometries and Setup

![Figure 7 General dimensions of the reactor](image_url)
The general geometry is given in Figure 7. It has been used for all 2D and 3D simulations presented herein. The centerline represents the axis of symmetry in a 2D simulation. The red, blue, and yellow lines indicate heated \((L_h)\), cooled \((L_c)\), and insulated \((L_i)\) walls, respectively. The top and bottom of the reactor were considered adiabatic.

4.1.1 Dimensions

Tables 5-9 details in bold the parameters that were changed. The standard case is italicized for significance, as this is the baseline case to compare changes to. An asterisk indicates only a two-dimensional study was performed of the specific case in Tables 5, 6, and 9.

Table 5 2D and 3D parametric study of aspect ratio by changing length

<table>
<thead>
<tr>
<th>(AR)</th>
<th>(\bar{h})</th>
<th>(L) (mm)</th>
<th>(D) (mm)</th>
<th>(L_h) (mm)</th>
<th>(L_c) (mm)</th>
<th>(L_i) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5:1</td>
<td>2.59</td>
<td>411.05</td>
<td>158.75</td>
<td>243.84</td>
<td>160.86</td>
<td>6.35</td>
</tr>
<tr>
<td>5:1</td>
<td>5.18</td>
<td>822.10</td>
<td>158.75</td>
<td>487.68</td>
<td>321.72</td>
<td>12.7</td>
</tr>
<tr>
<td>10:1</td>
<td>10.36</td>
<td>1644.19</td>
<td>158.75</td>
<td>975.36</td>
<td>643.43</td>
<td>25.4</td>
</tr>
<tr>
<td>20:1*</td>
<td>20.71</td>
<td>3288.39</td>
<td>158.75</td>
<td>1950.72</td>
<td>1286.87</td>
<td>50.8</td>
</tr>
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</table>

Table 6 2D and 3D parametric study of aspect ratio by changing diameter

<table>
<thead>
<tr>
<th>(AR)</th>
<th>(\bar{h})</th>
<th>(L) (mm)</th>
<th>(D) (mm)</th>
<th>(L_h) (mm)</th>
<th>(L_c) (mm)</th>
<th>(L_i) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5:0.5</td>
<td>10.36</td>
<td>822.10</td>
<td>79.375</td>
<td>487.68</td>
<td>321.72</td>
<td>12.7</td>
</tr>
<tr>
<td>5:1</td>
<td>5.18</td>
<td>822.10</td>
<td>342.02</td>
<td>487.68</td>
<td>321.72</td>
<td>12.7</td>
</tr>
<tr>
<td>5:2.15</td>
<td>2.40</td>
<td>822.10</td>
<td>793.75</td>
<td>487.68</td>
<td>321.72</td>
<td>12.7</td>
</tr>
<tr>
<td>5:5*</td>
<td>1.04</td>
<td>822.10</td>
<td>793.75</td>
<td>487.68</td>
<td>321.72</td>
<td>12.7</td>
</tr>
</tbody>
</table>

Table 7 2D parametric study of heated to cooled lateral surfaces

<table>
<thead>
<tr>
<th>(AR)</th>
<th>(L_h/L_c)</th>
<th>(L) (mm)</th>
<th>(D) (mm)</th>
<th>(L_h) (mm)</th>
<th>(L_c) (mm)</th>
<th>(L_i) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5:1</td>
<td>1</td>
<td>822.10</td>
<td>158.75</td>
<td>404.70</td>
<td>404.70</td>
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</tr>
<tr>
<td>5:1</td>
<td>2</td>
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<td>158.75</td>
<td>539.60</td>
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<td>158.75</td>
<td>607.05</td>
<td>202.35</td>
<td>12.7</td>
</tr>
<tr>
<td>5:1</td>
<td>6</td>
<td>822.10</td>
<td>158.75</td>
<td>693.77</td>
<td>115.63</td>
<td>12.7</td>
</tr>
</tbody>
</table>
Table 8  2D parametric study of insulator sizes

<table>
<thead>
<tr>
<th>$AR$</th>
<th>$Li/L$</th>
<th>$L$ (mm)</th>
<th>$D$ (mm)</th>
<th>$Lh$ (mm)</th>
<th>$Lc$ (mm)</th>
<th>$Li$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5:1</td>
<td>.015</td>
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<td>158.75</td>
<td>404.70</td>
<td>404.70</td>
<td>12.7</td>
</tr>
<tr>
<td>5:1</td>
<td>.031</td>
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<td>158.75</td>
<td>398.35</td>
<td>398.35</td>
<td>25.4</td>
</tr>
<tr>
<td>5:1</td>
<td>.077</td>
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<td>158.75</td>
<td>379.30</td>
<td>379.30</td>
<td>63.5</td>
</tr>
<tr>
<td>5:1</td>
<td>.155</td>
<td>822.10</td>
<td>158.75</td>
<td>347.55</td>
<td>347.55</td>
<td>127</td>
</tr>
</tbody>
</table>

Table 9  2D and 3D study of Rayleigh

<table>
<thead>
<tr>
<th>$AR$</th>
<th>$\beta$ (1/K)</th>
<th>$\Delta T$ (K)</th>
<th>$L$ (mm)</th>
<th>$D$ (mm)</th>
<th>$Lh$ (mm)</th>
<th>$Lc$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5:1</td>
<td>2.57E-4</td>
<td>7</td>
<td>822.10</td>
<td>158.75</td>
<td>487.68</td>
<td>321.72</td>
</tr>
<tr>
<td>5:1</td>
<td>2.57E-3</td>
<td>7</td>
<td>822.10</td>
<td>158.75</td>
<td>487.68</td>
<td>321.72</td>
</tr>
<tr>
<td>5:1*</td>
<td>2.57E-4</td>
<td>70</td>
<td>822.10</td>
<td>158.75</td>
<td>487.68</td>
<td>321.72</td>
</tr>
<tr>
<td>5:1*</td>
<td>2.57E-5</td>
<td>7</td>
<td>822.10</td>
<td>158.75</td>
<td>487.68</td>
<td>321.72</td>
</tr>
</tbody>
</table>

4.1.2 Initializing the Fluid Domain

The interior of the domain, shown later in Figures 8a and 9a, was initialized with zero velocity and uniform temperature of 300K at atmospheric pressure.

4.1.3 Boundary Conditions

For the 2D and 3D simulations all walls were no slip walls. From Figure 7, the cooled top lateral wall labeled $Lc$, had a constant temperature of 296.15K ($Tc$) while the bottom lateral wall labeled $Lh$, had a temperature of 303.15K ($Th$). The top and bottom of the reactor were considered adiabatic, as well as the insulator region of the lateral wall ($Li$).

These conditions were applied for both the 2D and 3D simulations, with two exceptions, one occurring in Table 9. The table has listed a $\Delta T$ case of 70, this specific simulation used $Th$ of 350K and $Tc$ of 280K. The other case, the laminar case, had a different thermal boundary condition of $Th$ 310K and $Tc$ 290K. The laminar case was different because 2D data was provided by Hooman Enayati.
4.1.4 Grids

The 2D numerical grids were all setup with a structured orthogonal mesh. Areas where boundary layers formed had extra layers for catching small scale flow details. The basic mesh is shown in Figure 8 with the details highlighted.

On all simulations the refined region of the mesh was of the same thickness, 15mm. This helped capture the structure of the turbulent boundary layer. Presented below in Table 10 are the details of each mesh. Note, that when a parameter doubles or halves the number of elements did not scale perfectly, as the boundary layers near the wall affected the scaling. The final size of each mesh is meant to hold the same refined boundary area and provide similar interior mesh sizes. In some cases, the entire mesh was inadequate, and thus a new more refined mesh was used. When multiple mesh sizes are listed, the bolded size is the final size used in the study.

![Figure 8](image)

**Figure 8** 2D mesh setups with detailing
a) entire domain b) detail of corner refinement c) detail of sidewall refinement with corresponding scale shown.
Table 10  2D mesh sizes

<table>
<thead>
<tr>
<th>$AR$</th>
<th>Parameter Studied</th>
<th>Grid Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5:1</td>
<td>$AR, \Delta L$</td>
<td>20k</td>
</tr>
<tr>
<td>5:1</td>
<td>Base case for comparison</td>
<td>40k,80k</td>
</tr>
<tr>
<td>10:1</td>
<td>$AR, \Delta L$</td>
<td>80k,120k</td>
</tr>
<tr>
<td>20:1</td>
<td>$AR, \Delta L$</td>
<td>160k,240k</td>
</tr>
<tr>
<td>5:0.5</td>
<td>$AR, \Delta D$</td>
<td>20k</td>
</tr>
<tr>
<td>5:2.15</td>
<td>$AR, \Delta D$</td>
<td>100k</td>
</tr>
<tr>
<td>5:5</td>
<td>$AR, \Delta D$</td>
<td>200k</td>
</tr>
<tr>
<td>5:1</td>
<td>$L_i = 25.4, 63.5, 127mm$</td>
<td>40k</td>
</tr>
<tr>
<td>5:1</td>
<td>$Lh/L_c = 1, 2, 3$</td>
<td>40k,80k</td>
</tr>
<tr>
<td>5:1</td>
<td>$Lh/L_c = 6$</td>
<td>80k,120k</td>
</tr>
<tr>
<td>5:1</td>
<td>$\beta = 2.57e-5, 2.57e-3, \Delta T = 70$</td>
<td>40k</td>
</tr>
</tbody>
</table>

FLUENT only uses Cartesian coordinates for numerical simulations; therefore, the 3D mesh was not a cylindrical mesh. To improve accuracy a layer of refined cells near the walls were created to capture boundary layers. The interior consisted of mostly hexahedrons. The top and bottom caps had a refinement to capture boundary layers. The basic mesh is shown in Figure 9.

Figure 9  3D mesh setup with detailing
a) entire domain b) top view of mesh c) top view detail of wall refinement.
Table 11 specifies the size of each 3D mesh used in this study. All meshes kept roughly uniform cell sizes, no larger than 7mm in any direction. The one 3D mesh convergence test was 5:1. It was important to verify that the standard case was sufficiently meshed, as the rest of the simulations are based around mesh scaling similar in size. Bold indicates the size used in the study.

<table>
<thead>
<tr>
<th>AR</th>
<th>Parameter Studied</th>
<th>Grid Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5:1</td>
<td>$AR$, $\Delta L$</td>
<td>434k, 853k</td>
</tr>
<tr>
<td>5:1</td>
<td>Base case for comparison</td>
<td>255k, 578k</td>
</tr>
<tr>
<td>10:1</td>
<td>$AR$, $\Delta L$</td>
<td>1066k</td>
</tr>
<tr>
<td>5:0.5</td>
<td>$AR$, $\Delta D$</td>
<td>213k</td>
</tr>
<tr>
<td>5:2.15</td>
<td>$AR$, $\Delta D$</td>
<td>1568k</td>
</tr>
</tbody>
</table>

Aspect ratio 2.5:1 in Table 11 had two meshes conducted because of a strange flow pattern that developed inside the insulator region. Only the flow pattern was confirmed with the refined mesh, not an entire study of this mesh was conducted. The spatial convergence test is in Section 4.3.2.

4.2 Data processing

The Fluent data was farther processed by using Tecplot and MATLAB. This allowed for manipulation of the data in order to make comparisons more meaningful. This also allows for the results to be time averaged and/or circumferentially averaged. There is an intrinsic difficulty when different sized domains are compared, because without the appropriate scaling factors direct comparisons are difficult. The typical approach of geometrically scaling the domains and comparing similarly scaled positions was avoided. Thus, another way to compare different domains was necessary, and subsequently introduced.
4.2.1 Time and circumferential averaging

Instantaneous results are difficult to present and understand and sometimes are actually not meaningful. In many cases it is easier to present time averaged results. The results from time averaging the 2D and 3D transient flow simulations are presented. The 3D simulations were circumferentially averaged, to represent the flow in a single plane for comparisons to 2D simulations. Time averaging or circumferential averaging are represented by a single bar over the scalar variable being averaged, and if the averaging is done in both time and space the variable will have a double bar. Results were averaged by extracting the data from fluent files into Tecplot where the cell centered data was exported into arrays of data containing the position and flow solution. The arrays contained the positioning of all points in chronological order, meaning that the entire domain was specified with the results then it was repeated every time the data was sampled. The 3D simulations had rather large meshes and due to the extensive number of instantaneous samples taken, resulting Matlab matrices were large.

*Time averaging*

These transient data files were then further processed into time averaged and circumferentially averaged files. The 2D and 3D simulations were first time averaged. According to the formula

\[ \sum_{1}^{n} \frac{\phi_{xyz}}{n} \]

where,

\[ n = \text{number of samples} \]
\[ \phi_{xyz} = \text{scalar property or } u,v,w \text{ component of velocity at similar } x,y,z \text{ locations} \]

which greatly decreased the size of the data.

**Circumferential averaging**

The 3D simulations then were also circumferentially averaged. This was done by built in MATLAB functions “meshgrid” and “griddata”. This allowed the non-uniform slices of the 3D mesh to be interpolate into a set of polar data. All the variables were transformed from Cartesian coordinates \((x,y,z)\) into cylindrical polar coordinates \((r,\theta,z)\).

It was important to make this transformation into cylindrical coordinates before averaging, otherwise few points would coincide for averaging. The circumferential averaging was done by

\[
\sum_{1}^{m} \frac{\phi_{rz}}{m}
\]

where,

\[ m = \text{number of points} \]

\[ \phi_{rz} = \text{scalar property or } v_r, v_{\theta}, w \text{ component of velocity at the same } r,z \text{ locations} \]

and the remaining data now represented data corresponding to \(r,z\) coordinates, and was directly compared to the 2D simulations.

**Double averaging**

When the 3D results were double averaged (first time averaged then spatially averaged) the averaging is a communitive property. A short proof is explained below.

Matrix \(\Phi\) of size n,m represents the scalar property of a set 3D transient data. This set of data is at a constant radius constant height, at various times \(t\), and various angles \(\theta\).
\[ \Phi_{n,m} = \]

<table>
<thead>
<tr>
<th>Time</th>
<th>( \theta_1 )</th>
<th>( \theta_2 )</th>
<th>( \theta_3 )</th>
<th>...</th>
<th>( \theta_m )</th>
<th>Spatial avg.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t_1 )</td>
<td>( \Phi_{1,1} )</td>
<td>( \Phi_{1,2} )</td>
<td>( \Phi_{1,3} )</td>
<td>...</td>
<td>( \Phi_{1,m} )</td>
<td>( \frac{\sum_{j=1}^{m} \Phi_{1,j}}{m} )</td>
</tr>
<tr>
<td>( t_2 )</td>
<td>( \Phi_{2,1} )</td>
<td>( \Phi_{2,2} )</td>
<td>( \Phi_{2,3} )</td>
<td>...</td>
<td>( \Phi_{2,m} )</td>
<td>( \frac{\sum_{j=1}^{m} \Phi_{2,j}}{m} )</td>
</tr>
<tr>
<td>( t_3 )</td>
<td>( \Phi_{3,1} )</td>
<td>( \Phi_{3,2} )</td>
<td>( \Phi_{3,3} )</td>
<td>...</td>
<td>( \Phi_{3,m} )</td>
<td>( \frac{\sum_{j=1}^{m} \Phi_{3,j}}{m} )</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>( t_n )</td>
<td>( \Phi_{n,1} )</td>
<td>( \Phi_{n,2} )</td>
<td>( \Phi_{n,3} )</td>
<td>...</td>
<td>( \Phi_{n,m} )</td>
<td>( \frac{\sum_{j=1}^{m} \Phi_{n,j}}{m} )</td>
</tr>
</tbody>
</table>

Time avg. \( \frac{\sum_{i=1}^{n} \Phi_{i,1}}{n} \), \( \frac{\sum_{i=1}^{n} \Phi_{i,2}}{n} \), \( \frac{\sum_{i=1}^{n} \Phi_{i,3}}{n} \), ... \( \frac{\sum_{i=1}^{n} \Phi_{i,m}}{n} \)

Double averaging was computed by time averaging then spatially averaging, shown as,

\[
\overline{\Phi} = \frac{\sum_{i=1}^{n} \Phi_{i,1}}{n} + \frac{\sum_{i=1}^{n} \Phi_{i,2}}{n} + \frac{\sum_{i=1}^{n} \Phi_{i,3}}{n} + \ldots + \frac{\sum_{i=1}^{n} \Phi_{i,m}}{n}
\]

but double averaging can also be computed by spatially averaging then time averaging, shown as,

\[
\overline{\Phi} = \frac{\sum_{j=1}^{m} \Phi_{1,j}}{m} + \frac{\sum_{j=1}^{m} \Phi_{2,j}}{m} + \frac{\sum_{j=1}^{m} \Phi_{3,j}}{m} + \ldots + \frac{\sum_{j=1}^{m} \Phi_{n,j}}{m}
\]

but both are mathematically equivalent to,

\[
\overline{\Phi} = \frac{\sum_{j=1}^{m} \sum_{i=1}^{n} \Phi_{i,j}}{nm}
\]

which means that the order of double averaging is commutative.

Great care was taken while post-processing the results. Rounding errors, such as machine error had to be dealt with; otherwise similar coordinate positions could not be determined. This problem arose when cartesian coordinate meshes were transformed into cylindrical polar meshes. Matlab is not able to re-grid and re-mesh data directly from cartesian coordinates into cylindrical coordinates, the mesh has to be transformed.
manually. This induces machine errors in the radius of each position, thus identifying similar radii becomes problematic. This was overcome by rounding all data to ten significant figures. The grid transformations were carefully chosen to avoid interpolation errors while simultaneously precise enough to resolve the boundary layers as determined from the original data. Furthermore, the 2D time averaged data was gridded onto the same set of coordinates for direct comparison to the 3D double averaged data.

4.2.2 Normal probability density function

The normal probability density function (NPDF) allows the results of different domains to be compared. It shows the overall flow intensity of a simulation when velocity magnitude is used as the input. This function allows dissimilar reactors to be normalized and directly compared. A scalar from multiple domains can be plotted as sets of curves. The NPDF was computed using MATLAB’s built in functions. It is defined in [49] by:

\[ y = f(x|\mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \]

and for the evaluation used in this study,

\[ \mu = \text{mean of the sample} \]
\[ \sigma = \text{standard deviation of the sample} \]
\[ x = \text{the data, the scalar quantity describing the fluid} \]
\[ y = \text{the likelihood, appearance, or probability per units of } 1/x \]

There are a few necessary conditions for comparing different domains. The first is that the sampled domain must be uniform. This is to ensure that the entire domain is represented evenly, without bias. The data has to be re-gridded and meshed before input
into a NPDF because the original grid is not uniform. Secondly, a finer re-gridding of the domain cannot result in a change of the NPDF curve. Refinement can be both in x or y directions, and independence to both directions needs to be determined. Hence, careful choices of the resolution of the grid were made. To confirm independence finer resolutions were compared. An example is provided in Figure 10.

The example provided shows the importance of choosing a well refined sampling grid for NPDFs otherwise results will not be independent of sampling. It also shows that the domain converges to a single curve, which will prove useful when comparing different sized domains. As the sampling reaches the resolution or passes the resolution of the original numerical domain the linear interpolation used in the griddata function converges the sample to a unique curve representative of the domain. The griddata function can use spline and cubic interpolation methods as well. These methods were tested and produced the same results on an NPDF, hence the linear method was used. The convergence of each domain and its sampling size is presented in Appendix A.

![Figure 10](image)

**Figure 10** NPDF example showing sampling independence
4.2.3 Contour details

Similar to the NPDF grid independence of the new gridded data for contours had to be determined. In each case, when contours are presented a grid study was conducted to determine independence of the contours and grid. This was especially important for the circumferential averaging, as poor gridding generated poor averages, resulting in contours that were not smooth.

4.2.4 Boundary layers

Boundary layer thickness, $\delta$, was defined as the distance from the wall where the absolute axial velocity stopped increasing. This was found by calculating the gradient of the absolute axial velocity from the wall and determining where it became negative. In order to determine a smoother boundary layer, the absolute axial velocity was circumferentially and or time averaged first. A second value was also determined from finding the boundary layer, that was the velocity of the boundary layer, $\delta_v$. This velocity is the absolute axial velocity where the boundary layer ends. This velocity shows how the velocity of the boundary layer changes with respect to height in the reactor. This method does not capture a boundary layer inside or near the insulator region. This location is where the boundary layers impinge and disintegrate. The results show clear evidence of where the boundary layers break down in chapter 5.

4.2.5 Normalization of results

When results are presented in chapter 5 the length and radius of the reactors are shown as normalized lengths, $L^*$ and $R^*$, respectively. These are defined by:

$$L^* = \frac{L_{max}}{L}$$
\[ R^* = \frac{R_{\text{max}}}{R} \]

where max is actual dimension of the reactor. This means that \( L^* \) and \( R^* \) will be defined from zero to one. Velocity magnitude, \( |V| \), and temperature, \( T \), are also normalized for contour maps and are defined from zero to one. Their normalization is defined by:

\[ |V|^* = \frac{|V|_{\text{max}}}{|V|} \]

\[ T^* = \frac{T - T_c}{T_h - T_c} \]

4.3 Convergence and numerical considerations

There are multiple convergences that had to be evaluated to determine the accuracy of the simulations. These are: relative, spatial, and time step convergence. The first is the relative convergence of the simulation. This evaluates, how long, in numerical time, it takes to reach a steady or quasi-steady state solution. The second, spatial convergence is based upon the accuracy of the mesh. Another important factor considered was the quality of the mesh near the wall. Every numerical simulation needed to capture the boundary layer sufficiently, and was evaluated by examining the \( y^+ \) value. Lastly, the Courant-Friedrichs-Lewy (CFL) condition was considered.

4.3.1 Relative convergence

The relative convergence was evaluated for every case, and for a case to be considered converged it had to meet a set of conditions. The sets of conditions varied slightly from 2D to 3D simulations. These conditions were met before numerical sampling occurred. The conditions were:
1. The case needed to reach 400 seconds for a 2D simulation 600 seconds for a 3D simulation.

2. The net heat flux had to be around 10% or less of the total heat flux for all simulations.

3. The flow had to be relatively repetitive. 3D simulations were allowed more variance.

4. 2D numerical sampling was for 100 seconds every second and 3D numerical sampling was for 200 seconds every second.

If condition 2 or 3 had not been met when condition 1 was satisfied, the case was simulated longer before numerical sampling began. This ensured that, the case had reached a quasi-steady state and that the sampled data was converged. The imposed minimum numerical time, given in condition 1, is to ensure relative convergence and for 3D cases, a minimum 600 was chosen based on research in [45] where 3D simulations were studied from 780-900 seconds. These 3D simulations were directly comparable in fluid properties, and boundary conditions, hence a similar convergence criterion was imposed. Tables 12 and 13, shows the heat flux convergence at the beginning of sampling for the 3D and 2D simulations.

<table>
<thead>
<tr>
<th>AR (3D cases)</th>
<th>Parameter Studied</th>
<th>Heat Flux + (Watts)</th>
<th>Heat Flux – (Watts)</th>
<th>Net Heat Flux (Watts)</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5:1</td>
<td>AR, ΔL</td>
<td>104.13</td>
<td>-104.72</td>
<td>-0.60</td>
<td>.57</td>
</tr>
<tr>
<td>5:1</td>
<td>Base for comparison</td>
<td>170.76</td>
<td>-169.10</td>
<td>1.68</td>
<td>.99</td>
</tr>
<tr>
<td>10:1</td>
<td>AR, ΔL</td>
<td>302.23</td>
<td>-276.58</td>
<td>25.65</td>
<td>9.27</td>
</tr>
<tr>
<td>5:0.5</td>
<td>AR, ΔD</td>
<td>75.38</td>
<td>-75.29</td>
<td>0.09</td>
<td>.12</td>
</tr>
<tr>
<td>5:2.15</td>
<td>AR, ΔD</td>
<td>383.99</td>
<td>-370.68</td>
<td>13.31</td>
<td>3.59</td>
</tr>
<tr>
<td>5:1</td>
<td>Ra increased</td>
<td>326.46</td>
<td>-320.92</td>
<td>5.54</td>
<td>1.73</td>
</tr>
</tbody>
</table>
Table 13  2D residual heat flux, start of numerical sampling

<table>
<thead>
<tr>
<th>AR (2D cases)</th>
<th>Parameter Studied</th>
<th>Heat Flux + (Watts)</th>
<th>Heat Flux - (Watts)</th>
<th>Net Heat Flux (Watts)</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5:1</td>
<td>AR, ΔL</td>
<td>88.94</td>
<td>-91.73</td>
<td>-2.80</td>
<td>3.15</td>
</tr>
<tr>
<td>5:1</td>
<td>Base for comparison</td>
<td>159.41</td>
<td>-152.03</td>
<td>7.38</td>
<td>4.85</td>
</tr>
<tr>
<td>10:1</td>
<td>AR, ΔL</td>
<td>256.09</td>
<td>-241.88</td>
<td>14.21</td>
<td>5.87</td>
</tr>
<tr>
<td>20:1</td>
<td>AR, ΔL</td>
<td>350.84</td>
<td>-326.00</td>
<td>24.84</td>
<td>7.62</td>
</tr>
<tr>
<td>5:0.5</td>
<td>AR, ΔD</td>
<td>69.22</td>
<td>-68.38</td>
<td>0.84</td>
<td>1.23</td>
</tr>
<tr>
<td>5:2.15</td>
<td>AR, ΔD</td>
<td>375.57</td>
<td>-358.86</td>
<td>16.71</td>
<td>4.66</td>
</tr>
<tr>
<td>5:1*</td>
<td>β = 2.57e-5</td>
<td>77.29</td>
<td>-90.96</td>
<td>-13.66</td>
<td>17.67</td>
</tr>
<tr>
<td>5:1*</td>
<td>β = 2.57e-3</td>
<td>310.27</td>
<td>-312.42</td>
<td>-2.15</td>
<td>.69</td>
</tr>
<tr>
<td>5:1*</td>
<td>ΔT = 70</td>
<td>3193.29</td>
<td>-3086.17</td>
<td>107.12</td>
<td>3.47</td>
</tr>
<tr>
<td>5:1</td>
<td>Lh/Lc = 1</td>
<td>161.23</td>
<td>-163.98</td>
<td>-2.75</td>
<td>1.71</td>
</tr>
<tr>
<td>5:1</td>
<td>Lh/Lc = 2</td>
<td>146.83</td>
<td>-140.90</td>
<td>5.93</td>
<td>4.21</td>
</tr>
<tr>
<td>5:1</td>
<td>Lh/Lc = 3</td>
<td>128.94</td>
<td>-115.60</td>
<td>13.34</td>
<td>11.54</td>
</tr>
<tr>
<td>5:1</td>
<td>Lh/Lc = 6</td>
<td>99.77</td>
<td>-90.00</td>
<td>9.77</td>
<td>10.86</td>
</tr>
<tr>
<td>5:1</td>
<td>I = 12.7mm</td>
<td>161.23</td>
<td>-163.98</td>
<td>-2.75</td>
<td>1.71</td>
</tr>
<tr>
<td>5:1</td>
<td>I = 25.4mm</td>
<td>159.82</td>
<td>-162.37</td>
<td>-2.55</td>
<td>1.60</td>
</tr>
<tr>
<td>5:1</td>
<td>I = 63.5mm</td>
<td>150.87</td>
<td>-161.07</td>
<td>-10.20</td>
<td>6.76</td>
</tr>
<tr>
<td>5:1</td>
<td>I = 127mm</td>
<td>144.64</td>
<td>-150.11</td>
<td>-5.47</td>
<td>3.78</td>
</tr>
</tbody>
</table>

4.3.2 Spatial convergence

Spatial convergence was tested for multiple 2D simulations and one 3D simulation. The test meshes are outlined in Section 4.1.4, Tables 10 and 11. Comparisons are not made on a point by point location data, because the flow is oscillatory; also, no contour comparisons are given because it is impossible to visually discern a difference in many cases. The spatial convergences are given below in Figures 11-18. The normal probability density function is explained and defined in Section 4.2.2. The NPDF sampling independence is shown in Appendix A.
2D Aspect Ratio

![Graph](image)

**Mesh size**
- 80k mesh
- 40k mesh

Figure 11  2D spatial convergence, aspect ratio 5:1
The time averaged velocity magnitude studied in a normal probability density function.

![Graph](image)

**Mesh size**
- 80k mesh
- 120k mesh

Figure 12  2D spatial convergence, aspect ratio 10:1
The time averaged velocity magnitude studied in a normal probability density function.
Figure 13 2D spatial convergence, aspect ratio 20:1
The time averaged velocity magnitude studied in a normal probability density function.

2D Ratio of heating to cooling

Figure 14 2D spatial convergence of $L_h/L_c$ 1, aspect ratio 5:1
The time averaged velocity magnitude studied in a normal probability density function.
Figure 15  2D spatial convergence of $L_h/L_c$ 2, aspect ratio 5:1
The time averaged velocity magnitude studied in a normal probability density function.

Figure 16  2D spatial convergence of $L_h/L_c$ 3, aspect ratio 5:1
The time averaged velocity magnitude studied in a normal probability density function.
Figure 17  2D spatial convergence of \( \frac{L_h}{L_c}  \), aspect ratio 5:1
The time averaged velocity magnitude studied in a normal probability density function.

The spatial convergences shown in an NPDF provide strong evidence that the current mesh density provided sufficient accuracy for further analysis. Figures 11-16, 18 show very similar overall flow intensity and thus demonstrate mesh convergence. Figure 17 shows a small deviation between mesh sizes 80k and 120k. This simulation showed a large amount of sporadic oscillations and demonstrated a flow more similar to a transitional regime. The simulations studying the ratio of heating to cooling, Figures 15-17, in general had the greatest amount of variance, as these flows were the most oscillatory in time of the 2D simulations.

Only one 3D spatial convergence test was conducted. The test was conducted on the standard aspect ratio (5:1), with the standard, fine mesh of 578k (a) checked against the coarse 255k (b) mesh. Figure 18 shows the spatial convergence and clearly shows similar overall flow speeds inside the reactor.
Figure 18 3D spatial convergence, aspect ratio 5:1
The double averaged velocity magnitude studied in a normal probability density function.

The 3D double averaged velocity magnitude and temperature contours comparing the two meshes are not shown here because of their similarity. These contours are shown in Appendix B for completeness.

4.3.3 Temporal convergence and stability

The Courant-Friedrichs-Lewy condition is a necessary condition for convergence governing the system of partial differential equations described earlier in Section 3.1.2. This condition limits the spatial to time step ratio, otherwise the governing system will be numerically unstable. The worst-case scenario was taken from all cases to estimate the CFL condition. How the CFL number is calculated is shown below.

\[ C_{\text{max}} > \frac{u_x \Delta t}{\Delta x} + \frac{u_y \Delta t}{\Delta y} + \frac{u_z \Delta t}{\Delta z} \]

The assumptions used are given below.
• $C_{max} = 1$, was estimated as worst case. An implicit time stepping method was employed which makes this a conservative estimate.

• The velocity is estimated as the maximum instantaneous velocity magnitude occurring in any of the simulations ($\|V_{max}\| = 77 \text{ mm/s}$) and applied for $u_x$, $u_y$, and $u_z$.

• The minimum grid dimension is estimated by the boundary layer thickness ($\delta = 3\text{ mm}$). This was another very conservative estimate, as the majority of the grid spacing located away from the boundary layer was coarser.

• The timestep was kept constant for all simulations, $\Delta t$ was equal to 0.01.

\[
\frac{0.77(0.01)}{0.03} + \frac{0.77(0.01)}{0.03} + \frac{0.77(0.01)}{0.03} = 0.77
\]

Noting that the above assumptions are for the strictest definitions of each variable and that the maximum velocities and minimum spacing does not correspond to the same locations in the simulations it is reasonable to assume that the CFL is satisfied.

Additionally, there was a numerical time step convergence performed. The convergence was found by comparing a 2D simulation with another of a smaller time step, by holding everything but the time step constant, in this case .005 second was checked.

Figure 19 shows that .01 seconds is a sufficiently small time step for time convergence. The smaller time step is overlapped completely by the larger time step; this shows the independence of time step to the solution, and hence 0.01 was used as the time step for all cases.
4.3.4 Wall condition y+

Following [46], the y+ value is used to identify the regions near the wall. There are three general regions near the wall, from nearest to farthest: the viscous sublayer, the blending region, and the fully turbulent region. Each region describes different flow characteristics based upon the y+ value. Figure 20 is given to show these regions.

The effects of turbulence near-wall regions result in two approaches. The first is to model the effects of the wall and modify the equations, in Section 3.1.2 according to [46], to account for these effects. The second approach is to resolve the near wall regions by creating a very refined computational grid on boundary layers. A sufficiently resolved boundary layer contains roughly ten grid points and has a y+ value around 1. The value of y+ was also used as a guideline for capturing the boundary layer sufficiently. The definition of y+ is shown below
where $y$ is the distance from the wall. For reference $\mu_t$ is the turbulent viscosity discussed in Section 3.1.2. Tables 14 and 15 show the maximum $y+$ values occurring anywhere in the domain for 3D and 2D simulations. The 2D and 3D simulations have almost ten layers in the boundary layers and should resolve the viscous sublayer sufficiently without wall functions. All simulations with standard fluid properties had a $y+$ value below 1. Because the simulations have roughly ten grid points in the boundary layer and have a sufficiently low value of $y+$ the viscous sublayer should be captured without wall models. These are not the maximum values through time, only the maximum values occurring at the beginning of the sampling. An asterisk denotes a non-standard fluid property, standard fluid properties given in Table 4.

Figure 20  Near-Wall regions and corresponding $y+$ values
Table 14  Maximum $y^+$ for 3D simulations

<table>
<thead>
<tr>
<th>$AR$ (3D cases)</th>
<th>Parameter Studied</th>
<th>$y^+_{max}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5:1</td>
<td>$AR, \Delta L$</td>
<td>0.36</td>
</tr>
<tr>
<td>5:1</td>
<td>Base for comparison</td>
<td>0.38</td>
</tr>
<tr>
<td>10:1</td>
<td>$AR, \Delta L$</td>
<td>0.49</td>
</tr>
<tr>
<td>5:0.5</td>
<td>$AR, \Delta D$</td>
<td>0.41</td>
</tr>
<tr>
<td>5:2.15</td>
<td>$AR, \Delta D$</td>
<td>0.38</td>
</tr>
<tr>
<td>5:1*</td>
<td>$Ra$ increased</td>
<td>0.95</td>
</tr>
</tbody>
</table>

Table 15  Maximum $y^+$ for 2D simulations

<table>
<thead>
<tr>
<th>$AR$ (2D cases)</th>
<th>Parameter Studied</th>
<th>$y^+_{max}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5:1</td>
<td>$AR, \Delta L$</td>
<td>.62</td>
</tr>
<tr>
<td>5:1</td>
<td>Base for comparison</td>
<td>.64</td>
</tr>
<tr>
<td>10:1</td>
<td>$AR, \Delta L$</td>
<td>.51</td>
</tr>
<tr>
<td>20:1</td>
<td>$AR, \Delta L$</td>
<td>.50</td>
</tr>
<tr>
<td>5:0.5</td>
<td>$AR, \Delta D$</td>
<td>.63</td>
</tr>
<tr>
<td>5:2.15</td>
<td>$AR, \Delta D$</td>
<td>.66</td>
</tr>
<tr>
<td>5:5</td>
<td>$AR, \Delta D$</td>
<td>.68</td>
</tr>
<tr>
<td>5:1*</td>
<td>$\beta = 2.57E-5$</td>
<td>.30</td>
</tr>
<tr>
<td>5:1*</td>
<td>$\beta = 2.57E-3$</td>
<td>1.47</td>
</tr>
<tr>
<td>5:1*</td>
<td>$\Delta T = 70$</td>
<td>1.47</td>
</tr>
<tr>
<td>5:1</td>
<td>$Lh/Lc = 1,2,3,6$</td>
<td>.46 max</td>
</tr>
<tr>
<td>5:1</td>
<td>$I = 12.7,25.4,63.5,127mm$</td>
<td>.66 max</td>
</tr>
</tbody>
</table>

Specific details about the simulations presented in Tables 14 and 15 can be found in Section 4.1.1. Tables 5-9 give the conditions of all the simulations shown in the above two tables.
CHAPTER V

RESULTS

It is necessary to provide a quick overview of how the fluid moves through the reactor. Refer to Figure 21 for the general geometry of the reactor and the boundary layers that develop due to natural convection. The fluid is driven by the boundary layers, with each respective section driving fluid towards the insulator; in Figure 21 the heated wall shown by Lh forms a natural convective boundary layer of upward moving fluid, while wall Lc forms a downward moving natural convective boundary layer of fluid. When the fluid of the natural convective boundary layers reaches the insulator, shown by the wall Li, there are three flow patterns that can occur.

The first is that the fluid could pass through each boundary layer with a portion of fluid moving towards the core. This would imply boundary layer breakdown and is an impossible flow, as the boundary layers drive the entire flow inside the reactor. Secondly the fluid could leave the boundary layer and turn towards the center and head towards its respective cap without passing through the insulator. This means that the boundary layer separates from the wall, turns perpendicular to the wall and moves towards the centerline, then turns again towards its respective cap, and recirculates by traveling towards the cap near the centerline eventually re-entering the boundary layer by impinging on the bottom.
Boundary layers occurring inside the reactor or top cap and turning towards the sidewall. This would create four main vortices inside the reactor, two in the heated lower section and two in the cooled upper portion. Thirdly, the fluid could turn towards the center and pass through the insulator and head towards the opposite cap. The difference between the second and third flow options differentiates how much fluid manages to pass through the insulator. If no fluid travels through the insulator region then little to no advective heat transfer occurs from top to bottom and vice versa through the insulator, and thus a greater difference in thermal distribution will occur. If some of the fluid travels through the insulator the temperature differential in the core region of the reactor will be reduced due to advective heat transfer. In most instances the fluid does some combination of the second and third patterns with a small amount of boundary layer disruption occurring in certain simulations. This describes the basic fluid flow through the reactor.
The results are presented first detailing the 2D simulation results. The parameters of length, diameter, aspect ratio, heating to cooling lengths, and insulator thickness are discussed. Secondly the 3D simulations are presented, and discussed in a similar manner. Lastly a comparison is made between 2D and 3D simulations. This includes the detailing of differences and trends that are owed to the third dimension along with a comparison between 2D and 3D laminar simulations.

The results presented may be instantaneous, time averaged, circumferentially averaged, and or both types of averaging to properly depict the fluid flow characteristics. Again, variables with a single bar overtop indicate an averaging, either time or circumferential averaging, for 3D simulations the type of averaging used is understood based on the presented view. When variables have a double bar, only applicable for 3D simulations, this indicates that both circumferential and time averaging was performed.

The objective is to study how these parameters affect the magnitude of the Rayleigh number for the laterally heated cylindrical reactor. In Section 3.3 the Rayleigh number was defined and from the literature review earlier three length scales are commonly used. Table 3 presents all the Rayleigh numbers for each definition for all simulations conducted. Presented below is the 2D investigation of the parameters that affect the characteristic length.

5.1 Turbulent 2D parametric study

The following is a breakdown of the two-dimensional turbulent studies. They are categorized by parameters of length, diameter, aspect ratio, insulator thickness, and the ratio of heating. In order to evaluate how any of these parameters may affect the Rayleigh number a baseline of change must be established. For review, the Rayleigh is defined
again below, where $X$ is the characteristic length defined by the commonly used definitions given in the literature review.

$$Ra = \frac{c_p g \beta \Delta T \rho^2 X^3}{\mu k}$$

5.1.1 Changing Rayleigh number

To quantify how much the Rayleigh number varied, the standard 5:1 aspect ratio (baseline) case was compared to three different cases. The three cases are described in Table 16 below by b, c, and d, where a is the baseline case. This table also presents the relevant geometry, boundary conditions, and fluid properties of each simulation conducted. Fluid properties that are not given in Table 16 are given as the standard fluid properties, Table 4. It should be noted that the thermal difference was incorporated to confirm that the correct definition of $\Delta T$ is being used for the reactor. Bolded values in Table 16 represent a change from the standard setup.

**Table 16 Changing Rayleigh, 2D setup**
The specific fluid properties, geometry, boundary conditions, and non-dimensional values for the simulations studied in Figures 22-26.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Fig letter</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta$</td>
<td></td>
<td>2.57E-4</td>
<td>2.57E-4</td>
<td>2.57E-3</td>
<td>2.57E-5</td>
</tr>
<tr>
<td>$\Delta T$ (K)</td>
<td>7</td>
<td>70</td>
<td>7</td>
<td>7</td>
<td></td>
</tr>
<tr>
<td>Th (K)</td>
<td></td>
<td>303.15</td>
<td>350</td>
<td>303.15</td>
<td>303.15</td>
</tr>
<tr>
<td>Tc (K)</td>
<td></td>
<td>296.15</td>
<td>280</td>
<td>296.15</td>
<td>296.15</td>
</tr>
<tr>
<td>L (mm)</td>
<td></td>
<td>822.1</td>
<td>822.1</td>
<td>822.1</td>
<td>822.1</td>
</tr>
<tr>
<td>D (mm)</td>
<td></td>
<td>158.75</td>
<td>158.75</td>
<td>158.75</td>
<td>158.75</td>
</tr>
<tr>
<td>AR</td>
<td></td>
<td>5:1</td>
<td>5:1</td>
<td>5:1</td>
<td>5:1</td>
</tr>
<tr>
<td>$\bar{h}$</td>
<td></td>
<td>5.18</td>
<td>5.18</td>
<td>5.18</td>
<td>5.18</td>
</tr>
<tr>
<td>$\frac{Ra}{A}$</td>
<td>8.80E6</td>
<td><strong>8.80E7</strong></td>
<td>8.80E7</td>
<td>8.80E5</td>
<td></td>
</tr>
<tr>
<td>$Ra L$</td>
<td></td>
<td>7.82E10</td>
<td><strong>7.82E11</strong></td>
<td>7.82E11</td>
<td>7.82E9</td>
</tr>
<tr>
<td>$Ra D$</td>
<td></td>
<td>5.63E8</td>
<td><strong>5.63E9</strong></td>
<td>5.63E9</td>
<td>5.63E7</td>
</tr>
<tr>
<td>Figures</td>
<td></td>
<td>22-26</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

70
Conducting these simulations provided insight as to how the Rayleigh number magnitude associates with the temperature and velocity maps occurring in the reactor. Without these simulations there was no way to determine how much other parameters affect the reactor with respect to a changed Rayleigh number.

Table 16 shows that cases b and c have identical Rayleigh numbers, independent of the characteristic length definition. These cases provide the relationship between β and ΔT. Examining Figures 22-23 cases b and c show that the time averaged contour maps of normalized temperature and normalized velocity magnitude are nearly identical. It is also shown that the overall flow intensity (time averaged velocity magnitude) occurring inside the reactor, shown by the NPDF, is nearly identical in Figure 24 cases b and c. Lastly the boundary layers and flow patterns of both simulations are nearly identical in Figures 25 and 26 cases b and c. The results provide evidence that the definition of ΔT is equivalent to Tc from Th. These results also provide evidence that changing β or ΔT will yield identical normalized simulation results provided the Boussinesq assumption is still valid.

For every case, changing the magnitude of the Rayleigh number had a direct effect on the speed of the flow. In Figures 23, 24, and 25bb cases b and c the magnitude was increased an order and in case d the magnitude decreased an order, compared to a, regardless to the definition of X. There is a clear trend that when the magnitude of the Rayleigh increases the overall flow speed and boundary layer speed increases inside the reactor, similarly when the magnitude is decreased the overall flow speed (Figures 23-24) and boundary layer speed (Figure 25bb) decreases. It is important to note and keep in mind how the NPDF (Figure 24) showed a significant change when the Rayleigh had
Figure 22  Changing Rayleigh, 2D temperature and vector maps  
All are 5:1 aspect ratio shown with normalized lengths and normalized temperature. Standard water properties unless specified otherwise. a) baseline case b) $\Delta T$ increased to 70 c) $\beta$ increased an order d) $\beta$ decreased an order.
Figure 23  Changing Rayleigh, 2D velocity magnitude maps
All are 5:1 aspect ratio shown with normalized lengths. Time averaged normalized velocity magnitude with standard water properties unless specified otherwise. a) baseline case b) ΔT increased to 70 c) β increased an order d) β decreased an order.
Figure 24  Changing Rayleigh, 2D NPDF of velocity magnitude
All are 5:1 aspect ratio shown and standard water properties unless specified otherwise. Time averaged velocity magnitude as the input. a) baseline case b) \( \Delta T \) increased to 70 c) \( \beta \) increased an order d) \( \beta \) decreased an order.

Figure 25  Changing Ra, 2D boundary layer thickness and velocity
Boundary layers were time averaged. aa) and bb) respectively. a) baseline case b) \( \Delta T \) increased to 70 c) \( \beta \) increased an order d) \( \beta \) decreased an order.
Figure 26  Changing Rayleigh, 2D velocity vectors

Note: the vectors are not scaled against each simulation and are time averaged. All are 5:1 aspect ratio shown with normalized lengths, radii, and standard water properties unless specified otherwise. a) baseline case b) ΔT increased to 70 c) β increased an order d) β decreased an order.
been changed by an order of magnitude. Figure 24 will be used as a comparison when comparing the effects of other parameters on the magnitude of the Rayleigh number.

The boundary layer thickness, $\delta$, shown in Figure 25a, changed significantly due to the differences in boundary layer velocity, 25bb. The faster the boundary layer velocity, the more the boundary layer was sheared, which resulted in a smaller boundary layer thickness; this effect is shown in cases b and c. The opposite is also shown true, the slower the boundary layer velocity, the larger the boundary layer grew; shown by case d. The differences in the momentum boundary layer explain the thermal boundary layer differences found near the wall in Figure 22. In Section 3.3 the Prandtl number is presented and discussed, and is noted to relate the momentum boundary layer thickness to the thermal boundary layer thickness. In these simulations the Prandtl number was never varied. This implies that as $\delta$ changes the thermal boundary layer should change in a similar corresponding manner; if $\delta$ increases so does thermal boundary layer and vice versa. In Figure 22, cases b and c have significantly smaller thermal boundary layers compared to case a. This is due to the decreased size of the momentum boundary layer thickness $\delta$. Case d shows a significantly larger thermal boundary layer compared to a, which also corresponds directly to the changes shown by $\delta$ (increased boundary layer thickness). The thermal boundary layer follows the same pattern as predicted by holding Prandtl constant, thus only the momentum boundary layer will be presented in detail.

All of the cases showed that the boundary layer is destroyed in Figure 25 near and inside the insulator because this is where the lower and upper boundary layers impinge.

Examining Figure 26 shows that the time averaged flow pattern changes minimally by changing the magnitude of the Rayleigh number, at least by the currently studied
parameter changes ($\beta$ and $\Delta T$). It is important to note here that while the time averaged flow pattern remained similar, the transient nature of the flow changed. This transient flow has been covered by Enayati in previous works and the detailed results will not be given here.

5.1.2 Changing aspect ratio – constant diameter

In order to study the aspect ratios effect on the magnitude of the Rayleigh number, a two-parameter study of $L$ and $D$ was conducted. In this section the diameter was held constant while the length was varied. The results of the NPDF and boundary layers are presented in Section 5.1.4, Figures 35 and 36, as it incorporates the results of all AR cases studied.

Table 17 below presents the details of the simulation conditions for the parameter, length. The fluid properties are the standard water conditions given in Table 4, as well as the standard thermal boundary conditions given in Section 4.1.3. For the specific details of the geometry refer to Table 5. Bolded values signify differences from the standard italicized case.

<table>
<thead>
<tr>
<th>Fig letter Parameter</th>
<th>L (mm)</th>
<th>D (mm)</th>
<th>AR</th>
<th>$\bar{h}$</th>
<th>$\frac{V}{A}$</th>
<th>$Ra \frac{L}{a}$</th>
<th>$Ra D$</th>
<th>Figures</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>822.1</td>
<td>158.75</td>
<td>5:1</td>
<td>5.18</td>
<td>8.80E6</td>
<td>7.82E10</td>
<td>5.63E8</td>
<td>27-30,35,36</td>
</tr>
<tr>
<td></td>
<td>411.05</td>
<td>158.75</td>
<td>2.5:1</td>
<td>2.59</td>
<td>8.80E6</td>
<td>9.78E9</td>
<td>5.63E8</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1644.19</td>
<td>158.75</td>
<td>10:1</td>
<td>10.36</td>
<td>8.80E6</td>
<td>6.26E11</td>
<td>5.63E8</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3288.39</td>
<td>158.75</td>
<td>20:1</td>
<td>20.71</td>
<td>8.80E6</td>
<td>5.01E12</td>
<td>5.63E8</td>
<td></td>
</tr>
</tbody>
</table>
From the time averaged normalized temperature contours, Figure 28, it is clear that higher aspect ratio cases, c and d, resulted in greater temperature differentials between the lower and upper section of the reactor when compared to a, the standard reactor. In these longer reactors the fluid traveled in the boundary layer longer which allowed for more heating or cooling in the respective section. The shorter length reactor (smaller aspect ratio), case b, showed a slightly smaller temperature differential between the upper and lower sections of the reactor compared to a, the standard reactor.

It appears that the amount of fluid that penetrated the opposite section, fluid that traveled from the lower boundary layer into the upper section of the reactor or vice versa, changed minimally when increasing or decreasing the length. This is supported by the trend that increasing the length increased the temperature differentials between the upper and lower section, and decreasing the length decreased the temperature differentials between the upper and lower section.

In Figure 28 case c and d, some of the cooler upper section fluid penetrated through the insulator and traveled all the way to the bottom cap. This stagnant fluid will not move until it is heated or cooled enough for buoyancy forces to begin to take effect. The reason the fluid stagnates in the cap is because the caps are adiabatic.
Figure 28  Changing length, 2D temperature & vector maps
All use the standard water properties, boundary conditions, and diameter. Time averaged and normalized. a) standard case b) the length was halved c) the length doubled d) the length quadrupled.
Figure 29  Changing length, 2D velocity magnitude maps
All use the standard water properties, boundary conditions, and diameter. Time averaged and normalized. a) aspect ratio 5:1 b) aspect ratio 2.5:1 c) aspect ratio 10:1 d) aspect ratio 20:1.
Figure 30 Changing length, 2D velocity vectors

Note: not scaled to each other. All use the standard water properties, boundary conditions, and diameter. Time averaged. a) standard case b) the length was halved c) the length doubled compared to the standard reactor d) the length quadrupled compared to the standard reactor.
Figure 29 shows that the fastest flow occurs near the center of the reactor. This is the fluid that has moved from the boundary layer and is traveling towards a cap. The fluid in the boundary layer does not appear to move as fast as the fluid near the centerline by the insulator, which is an interesting flow result. The only way this can occur is if the flow near the center is re-entering the boundary layer well before reaching the top or bottom cap. In Figure 29 cases b-d all show signs that fluid is re-entering the boundary layer before reaching the cap.

The flow pattern for each simulation remained nearly the same, with the exception of the shorter reactor, case b. In Figure 30 case b showed that the fluid recirculated closer to the insulator, rather than nearer to the cap, which resulted in a shorter circulation.

5.1.3 Changing aspect ratio – constant length

The second parameter of the aspect ratio was the diameter. This section highlights changing the diameter, in the 2D sense changing the radius. Likewise, the boundary layers and NPDF was held until Section 5.1.4 which overviews all the aspect ratio simulations.

Table 18 below presents the details of the simulation conditions for the parameter diameter. The fluid properties are the standard water conditions given in Table 4, as well as the standard thermal boundary conditions given in Section 4.1.3. For the specific details of the geometry refer to Table 6. Again, bolded values signify differences from the standard italicized case.
Table 18  Changing diameter, 2D, setup for Figures 31-36

<table>
<thead>
<tr>
<th>Fig letter</th>
<th>Parameter</th>
<th>a</th>
<th>f</th>
<th>g</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>L (mm)</td>
<td>822.1</td>
<td>822.1</td>
<td>822.1</td>
<td>822.1</td>
<td></td>
</tr>
<tr>
<td>D (mm)</td>
<td>158.75</td>
<td>79.375</td>
<td>342.02</td>
<td>793.75</td>
<td></td>
</tr>
<tr>
<td>AR</td>
<td>5:1</td>
<td>5:0.5</td>
<td>5:2.15</td>
<td>5:5</td>
<td></td>
</tr>
<tr>
<td>( \bar{h} )</td>
<td>5.18</td>
<td>10.36</td>
<td>2.40</td>
<td>1.04</td>
<td></td>
</tr>
<tr>
<td>( Ra \frac{V}{A} )</td>
<td>8.80E6</td>
<td>1.10E6</td>
<td>8.80E7</td>
<td>1.10E9</td>
<td></td>
</tr>
<tr>
<td>Ra L</td>
<td>7.82E10</td>
<td>7.82E10</td>
<td>7.82E10</td>
<td>7.82E10</td>
<td></td>
</tr>
<tr>
<td>Ra D</td>
<td>5.63E8</td>
<td>7.04E7</td>
<td>5.63E9</td>
<td>7.04E10</td>
<td></td>
</tr>
</tbody>
</table>

Figures 31-36

Figure 31  Changing diameter, reactors without scaling for Figures 32-34 below
The green, red, yellow, and blue represent the axis of symmetry, sidewall heating of Th, insulator, and sidewall cooling of Tc, respectively. a) standard case f) aspect ratio 5:0.5 g) aspect ratio 5:2.15 h) aspect ratio 5:5.

Figure 32 shows how changing the diameter effected the thermal environment inside the reactor. Increasing the reactor diameter, decreasing the aspect ratio, caused a decrease in the temperature differential between the upper and lower section of the reactor. This is shown clearly by cases g and h when compared to a, the standard case. As the diameter increased the fluid had more area to pass through the insulator region to the opposite section. This allowed for more mixing which decreasing the temperature differential. Decreasing the diameter, or increasing the aspect ratio, increased the temperature.
Figure 32  Changing diameter, 2D temperature and vector maps
All use the standard water properties, boundary conditions, and radius. Time averaged and normalized. a) standard case f) the diameter was halved g) the diameter times 2.15 h) the diameter times five.
Figure 33  Changing diameter, 2D velocity magnitude maps
All use the standard water properties, boundary conditions, and radius. Time averaged and normalized. a) aspect ratio 5:1 f) aspect ratio 5:0.5 g) aspect ratio 5:2.15 h) aspect ratio 5:5.
Figure 34  Changing diameter, 2D velocity vectors
All use the standard water properties, boundary conditions, and radius. Time averaged. a) standard case f) the diameter was halved g) the diameter times 2.15 h) the diameter times five.
differential between the upper and lower section of the reactor show by case f compared to a in Figure 32. Case f essentially constricts the area where the fluid can pass through the insulator region, which means less fluid can penetrate through and thus a greater temperature differential.

The time averaged velocity magnitude contours, Figure 33, show very little difference in maximum flow speeds occurring inside the reactors; however, it did affect where high speed flow was located. In smaller aspect ratio cases, where the diameter was increased, there was more flow in the caps of the reactor, shown by case g and h. This can be accounted for the distance that the core has to travel to reach the boundary layer. Fluid that is near the center of the reactor has to move a greater distance to reach the wall as the diameter is increased.

The diameter did not appear to affect the flow patterns inside the reactor. Figure 34 shows nearly the same flow pattern occurring in case f, g, and h.

5.1.4 Overview of aspect ratio

Reviewing Sections 5.1.2 and 5.1.3 gives a complete view of how the aspect ratio effects the fluid flow and thermal environment inside the reactor. Reviewing Figures 28 and 32 shows the time averaged normalized thermal environments of all two-dimensional aspect ratio cases simulated. These figures confirm the trends: firstly, increasing the aspect ratio increases the thermal difference between the upper and lower section of the reactor, and secondly, decreasing the aspect ratio decreases this thermal difference inside the reactor.

The flow pattern and strength of the flow pattern does not seem to correlate with any general trend of changing the aspect ratio. Figures 29, 33, 30, and 34 show the time
averaged normalized velocity magnitude maps and time averaged velocity vectors of changing aspect ratio simulations. Comparing Figures 29 and 33 shows that the location of high speed flow is not directly correlated with aspect ratio. The only common locations of fast moving fluid occur near the insulator in the center of the reactor. Reviewing Figures 30 and 34 does not indicate any general flow field trends from changing the aspect ratio. It appears that aspect ratio and the flow patterns are unrelated to general trends.

The normal probability density function of all the simulations from each section along with the boundary layer thickness and velocity is presented below. Tables 17 and 18 should be referenced for the specifics of each case presented in Figures 35 and 36.

In Figure 35 the changing length cases (b-d) provide evidence that length directly affected the flow speed inside the reactor. In cases where the length was increased, case c and d, more fast-moving fluid and less slow-moving fluid occurs inside the reactor compared to a. In case b, where length decreased, is shown to be the slowest moving fluid inside the reactor. There seems to be an upper bound where increasing the length will not increase the overall fluid flow speed inside the reactor. Comparing case c and d shows this phenomenon as case d has slightly less fast-moving fluid and slightly more slow-moving fluid compared to case c.

The changing diameter cases (f-h) were less clear from Figure 35. Increasing the diameter too much as evidenced by case h shows a large decrease in the overall flow speed inside the reactor. Decreasing the diameter, case f also shows a decrease in overall flow speed inside the reactor. Increasing the diameter, or reaching some optimal diameter seems to generate the highest flow speeds inside the reactor, as shown by case g.
All have standard water properties. Time averaged velocity magnitude as input. a) aspect ratio 5:1 b) aspect ratio 2.5:1 c) aspect ratio 10:1 d) aspect ratio 20:1 f) aspect ratio 5:0.5 g) aspect ratio 5:2.15 h) aspect ratio 5:5.

Examining all cases in Figure 35 reveals that there appears to be optimal aspect ratios. This implies that the optimal aspect ratio to maximize the overall fluid flow speed inside the reactor is going to be specific to some scale of the reactor. Meaning that for a specific length, a specific diameter will maximize the overall flow speed inside the
reactor; however, this aspect ratio is only optimal for a single specific length, it is not the optimal aspect ratio for a different length. For example, in Figure 35 the optimal aspect ratio for the standard length of 822mm appears to be aspect ratio 5:2.15, case g. If one holds diameter as the scale length of 159mm, then the optimal aspect ratio appears to be 10:1, case c.

Figure 36  2D boundary layer thickness and velocity aa) and bb) respectively. All have standard water properties. Time averaged. a) aspect ratio 5:1 b) aspect ratio 2.5:1 c) aspect ratio 10:1 d) aspect ratio 20:1 f) aspect ratio 5:0.5 g) aspect ratio 5:2.15 h) aspect ratio 5:5.
Figures 24 and 35 alongside Tables 16-18 show how the magnitude of the Rayleigh number is affected by changing the aspect ratio. Comparing these figures shows that the flow intensity of all the cases studied are near the standard reactor. The tables note how the magnitude of the Rayleigh number changes. By noting the supposed changes in the tables based on a length scale and comparing the changes in Figure 24 with Figure 35 it is apparent that none of the current definitions of length scale are reasonable. Another way to evaluate the change in Rayleigh is to compare the velocities of the boundary layers. By comparing Figures 25bb and 36bb with the Tables 16-18 it is clear that the velocities of the boundary layers do not correspond with the current length scales as well.

The boundary layer thickness in Figure 36 aa show the effects of changing the length and diameter. Case g shows a spike of the boundary layer thickness near the top and bottom of the reactor because this reactor has more fluid moving near the caps. There are also oscillations in boundary layer thickness near the insulator, this is because of boundary layer breakdown where the two boundary layers impinge and the boundary layer no longer exists. The spike shown in case g and the oscillations near the insulator should be ignored. When the length was increased greatly, the boundary layer had longer to grow, as such it became thicker. This explains why case d had a thick boundary layer. Case h had a thick boundary layer because the core region that moves in the opposite direction of the boundary layer was far away, thus it did not shear the boundary layer as much as smaller diameter cases.

The speed of the boundary layers shown in Figure 36bb are dependent on multiple factors. Firstly, the longer the reactor the more time the boundary layer can increase in speed, shown by case b and c. Secondly, as the diameter increases the boundary layer
experiences less fluid shear with the opposite moving core. This is shown most clearly by comparing case f and g.

5.1.5 Changing insulator length

The changing insulator length simulations were setup with an even ratio of heating to cooling. This was to avoid possible interaction between heating ratios and insulator lengths. The velocity vectors were not presented because no discernable flow pattern difference resulted from changing the insulator length. The specific geometry is given in Table 8. Standard water properties and the standard boundary conditions were implemented. The current length scales used in the Rayleigh number do not incorporate an insulator length, hence the Ra number is assumed independent of the insulator length.

The below studied cases had a maximum insulator of about 15 percent of the length of the reactor, case d. From reviewing Figures 37 and 38 there are no discernable differences in the time averaged temperature maps or the time averaged normalized velocity magnitude maps. Figure 39 shows a trend suggesting that as the insulator length increases, the overall fluid flow intensity inside the reactor decreases, albeit very slightly. Physically increasing the insulator is decreasing the areas of heating and cooling on the sidewalls of the reactor, which in turn decreases the fluid flow speeds inside the reactor. It appears that as long as the insulator remains smaller than a certain threshold, it does not severely affect the magnitude of the Rayleigh number.
Figure 37 Changing insulator, 2D temperature maps
All use the standard water properties, length, and radius. Time averaged and normalized.
a) insulator length that of the standard reactor b) the insulator length doubled c) the insulator length multiplied by five d) the insulator length was multiplied by ten.
Figure 38  Changing insulator, 2D velocity magnitude maps
All use the standard water properties, length, and radius. Time averaged and normalized.
a) insulator length that of the standard reactor b) the insulator length doubled c) the insulator length multiplied by five d) the insulator length was multiplied by ten.
5.1.6 Changing the heating to cooling ratio $L_h/L_c$

The following section examines the ratio of heated area/length to cooled area/length.

To study this effect, the length of the heated section was increased and the length of the cooled section was decreased. Simulating the opposite scenario, by increasing the length of the cooled wall and decreasing the length of the heated wall will produce similar results. Standard fluid properties and the standard boundary conditions are used. The dimensions of each case are given in Table 7. The current length scales used in the
Figure 40  Changing Lh/Lc, 2D temperature & vector maps
All use the standard water properties, length, and radius. Time averaged and normalized.
a) even heating ratio b) heating ratio doubled c) heating ratio times three d) heating ratio times six.
Figure 41  Changing Lh/Lc, 2D velocity magnitude maps

All use the standard water properties, length, and radius. Time averaged and normalized.

a) even heating ratio
b) heating ratio doubled
c) heating ratio times three
d) heating ratio times six.
Figure 42  Changing Lh/Lc, 2D velocity vectors
All use the standard water properties, boundary conditions, and radius. Time averaged. a) even heating ratio b) heating ratio doubled c) heating ratio times three d) heating ratio times six.
Rayleigh number do not incorporate a heating length to cooling length ratio, hence the Rayleigh number is assumed independent of the heating to cooling length ratio.

Figure 40 shows how changing the ratio of heating to cooling effects the time averaged normalized temperature distribution inside the reactor. It is clearly presented that as the ratio of heated to cooled areas increase the temperature inside the reactor increases overall. It is also shown that in the cooled upper section of the reactor, the area above the insulator, begins to increase in temperature as well. This also implies that the temperature differential occurring inside the reactor begins to decrease as the heating to cooling ratio increases. Case b-d shows that some of the cooled fluid from the upper section manages to reach the lower cap of the reactor and stagnate at the bottom.

The time averaged velocity magnitude contours, Figure 41 show that the locations of high speed flow changes as the ratio increases. Case a shows a very symmetrical fluid speed across the insulator. This occurs because the ratios of heating to cooling are even, thus the boundary layers that develop are nearly the same, and the resulting fluid flow near the center of the reactor becomes uniform across the insulator. As this ratio grows the boundary layers become more dissimilar, and hence the fluid in the center of the reactor is affected. Figure 41 also shows that the flow begins to slow down inside the cooler section of higher ratio cases, b-d. This was the result of the decreased temperature differential between the upper and lower sections (Figure 40).

The flow patterns begin to change as the ratio is increased as well. The velocity vectors, Figure 42, show that the heated section begins to develop a very elongated flow vortex, case d. As the upper cooled section shrinks, the fluid is forced to re-circulate from
center into the boundary layer very quickly, thus developing very small vortices. These help to explain the thermal maps shown in Figure 40.

Figure 43 Changing $L_h/L_c$, 2D NPDF of velocity magnitude
All have standard water properties. Time averaged velocity magnitude as input. a) even heating ratio b) heating ratio doubled c) heating ratio times three d) heating ratio times six.
Figure 44  Changing $Lh/Lc$, 2D boundary layer thickness and velocity $aa)$ and $bb)$ respectively. All have standard water properties. Time averaged. a) even heating ratio b) heating ratio doubled c) heating ratio times three d) heating ratio times six.
The normal probability density function of time averaged velocity magnitude, Figure 43, showed a strong correlation between higher heating ratios and slower moving fluid inside the reactor. As the ratio of heating to cooling increased (cases b-d), the fluid inside the reactor began to slow down, as evidenced in Figure 43. An expected result, as uneven heating resulted in less overall heat transfer in and out of the reactor. The overall fastest moving fluid occurred in the even heating ratio simulation. Reviewing Figures 24 and 43, it does not appear that the heating ratio affected the magnitude of the Rayleigh number significantly, at least up to a heating to cooling ratio of 6.

The boundary layer thicknesses are shown in Figure 44aa. Note the oscillations in the boundary layer thickness; these occur where the heated and cooled boundary layers impinge and should be ignored. The heated boundary layer thickness increases as the ratio $L_h/L_c$ increases. This occurs because the fluid travels a greater distance thus allowing the boundary layer to grow; the opposite occurs with the cooled boundary layer. The cooled boundary layer thickness decreases as the $L_h/L_c$ ratio increases.

There was a large difference in the velocity of the boundary layers, Figure 44bb. When fluid re-enters the boundary layer from the center of the reactor, the temperature of the fluid is going to affect the velocity of the boundary layer that develops. The greater the thermal difference between the fluid entering the boundary layer and the wall temperature, the faster the velocity will increase in the boundary layer. In case a the fluid in the center upper section of the reactor is a cooler temperature than in case b. This implies that the fluid in case b is going to develop a higher velocity boundary layer faster than in case a, as shown by Figure 44bb. In the center of the lower section in case b the temperature is warmer than case a; this implies that the boundary layer velocity will
increase more slowly in b than in a. This trend increases as the ratio of heating to cooling increases, but note that it is slightly affected by the length in which the boundary layer can develop.

5.1.7 2D Overview

The turbulent 2D simulations showed that changing the length of the reactor, studied in Section 5.1.2, affected the overall speed of the flow inside the reactor more than changing the diameter. When the length was increased the overall flow speed was increased, as indicated by Figure 35; however, at higher aspect ratios eventually showed a slowing of flow near the caps. It also appeared that the length of the reactor is more correlated to the length scale, in that increasing the length appeared to increase fluid speed and decreasing the length decreased fluid speed.

Changing the diameter, studied in Section 5.1.3, had a different effect, mostly on the thermal distribution in the reactor. Where increasing the diameter of the reactor increased mixing between the lower and upper sections and decreasing the diameter restricted mixing and led to a greater temperature differential. However, the specific aspect ratio case 5:2.15 showed the highest overall flow speeds and signified that there may be optimal diameters for specific lengths that maximizes the mixing and fluid velocities. Hence length is not the only factor that effects the magnitude of the Rayleigh number.

The insulator length, studied in Section 5.1.5, appeared to have little effect on the fluid flow or temperatures inside the reactor. It did show a slight decrease in flow speed as the insulator reached a larger ratio of the total length.

The ratio of heating to cooling, studied in Section 5.1.6, appeared to have a significant effect on velocity and overall temperature distribution inside the reactor.
Equal areas provide the fastest overall flow with moderate mixing. While higher ratios eventually slowed fluid flow and caused the larger area to dominate the temperature of the reactor.

The 2D simulations all showed a basic flow pattern. The fluid traveled along the boundary layer and impinged near the insulator which forced fluid towards the centerline. In this region some fluid passed by and escaped towards the opposite cap; this occurred in a repetitive pattern where the fluid near the insulator oscillated between passing through the insulator and recirculating. However, most of the fluid was recirculated without passing through the insulator region. There was still an exchange of energy and momentum through the insulator region, even when fluid did not directly penetrate through the insulator. This flow pattern occurred because of the limitation of 2D simulations. Fluid cannot constantly pass through the insulator region, it can only pass through the insulator region in an oscillatory manner where the lower hot fluid passes to the upper cooled section and then the upper cooled fluid passes through to the lower heated section. This restriction of fluid passing through the insulator is because of continuity, one cannot have fluid from both the lower and upper sections passing through the insulator region simultaneously.

5.2 Turbulent 3D parametric study

The 3D simulations examining the length scale are presented below. The 3D simulations had significantly longer CPU run times, some exceeding two months, thus not all parameters were studied. Only the change in length and diameter effects were studied, specifically through the aspect ratio. The five 3D cases, given in Tables 5 and 6, corresponded directly to five 2D simulations, sharing the same fluid properties, given in
Table 4, and wall boundary conditions, given in Section 4.1.3. There was also a separate study examining the effect of changing the Rayleigh number, as the 3D change of the Rayleigh number may not result in a similar change as the 2D study. No comparisons between the 3D and 2D simulation are made in this section, that is held until Section 5.3.

5.2.1 Changing Rayleigh

A similar presentation of results as Section 5.1.1 follows now for 3D transient simulations. It was important to understand how directly changing the Rayleigh effected the full 3D simulation, as 2D simulations may not correspond well. Rayleigh of an order of magnitude greater was studied, the lower order of magnitude was ignored because of the long simulation run time required. Increasing the magnitude of the Rayleigh was accomplished by increasing β by an order of magnitude, refer to Section 3.3 for the Rayleigh number definition. Some of the following results are double averaged meaning the variables studied were time averaged and circumferentially averaged. For an explanation and definition of time averaging, space/circumferential averaging, and double averaging (time and space averaging) refer to Section 4.2.1. Standard fluid properties are used, given in Table 4, unless otherwise specified. The boundary conditions were the standard boundary conditions defined in Section 4.1.3. The specific geometry of the standard case can be found in Tables 5 or 6 under aspect ratio 5:1.

Figure 45 shows the double averaged normalized temperature and velocity magnitude maps. Comparing a and b, it was interesting to note that the standard Rayleigh case had a more uniform temperature distribution. There was also a dramatic difference in the velocities between c and d.
Figure 45  Changing Ra, 3D temperature, velocity magnitude, and vector maps
The standard reactor geometry is used and standard fluid properties are used unless otherwise specified. Double averaged and normalized. a) temperature map - standard reactor b) temperature map - Ra increased an order of magnitude c) velocity magnitude map - standard reactor d) velocity magnitude map - Ra increased an order of magnitude e) legend for scaling.
Figure 46  Changing Rayleigh, 3D NPDF of velocity magnitude
Double averaged velocity magnitude as input.  a) standard case b) $Ra$ increased an order of magnitude.
Figure 47  Changing Rayleigh, 3D boundary layer thickness and velocity Double averaged. aa) and bb) respectively. a) standard case b) $Ra$ increased an order of magnitude.
Examining Figure 46 shows that the 3D NPDF of the double averaged velocity magnitude does not correlate well with Figure 24, the 2D time averaged velocity magnitude NPDF. This shows the reason for conducting a separate Rayleigh magnitude study in 3D. This figure will be referenced with examining how a parameter effects the magnitude of the Rayleigh number.

The boundary layer thickness and velocities shown in Figure 47, conform to the trends explained in Section 5.1.1.

The velocity vectors are presented imposed on temperatures for completeness, they show nearly identical flow between the standard case (baseline) and case with $Ra$ increased an order of magnitude.

5.2.2 Changing aspect ratio

The following results investigate the effects of changing the length and diameter of the reactor. Unlike in the 2D study of aspect ratio, they are presented together because only five simulations were conducted for this specific study. Similar to the previous section, the results presented show time averaged and or double averaged variables. When a variable is double averaged it condenses the entire flow field from a 3D cylinder into a single plane or a single image or set of images if it is spatially averaged. The time averaged cross-sections are shown at important locations to detail how the 3D simulations transfer fluid through the insulator region. Finally, instantaneous cross-sectional videos are referenced to show the 3D nature of fluid. All of the simulations used standard water properties, given in Table 4 and standard bound conditions, given in Section 4.1.3. Table 19 details the important features of each simulation. Again, bolded signifies values different from the standard italicized case.
Table 19  Changing aspect ratio, 3D, setup for Figures 48-53.

<table>
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<tr>
<th>Fig letter Parameter</th>
<th>a)</th>
<th>b)</th>
<th>c)</th>
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<td>10:1</td>
<td>5:0.5</td>
<td>5:2.15</td>
</tr>
<tr>
<td>( \bar{h} )</td>
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<td>2.59</td>
<td>10.36</td>
<td>10.36</td>
<td>2.40</td>
</tr>
<tr>
<td>Ra ( \frac{L}{4} )</td>
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<td>8.80E6</td>
<td>8.80E6</td>
<td><strong>1.10E6</strong></td>
<td><strong>8.08E7</strong></td>
</tr>
<tr>
<td>Ra L</td>
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<td><strong>9.78E9</strong></td>
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<tr>
<td>Ra D</td>
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<td>5.63E8</td>
<td>5.63E8</td>
<td><strong>7.04E7</strong></td>
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<td>Figures</td>
<td>48-53</td>
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Figure 48  Changing aspect ratio, 3D reactor without scaling for Figures 49-51
The green, red, yellow, and blue represent the center of the geometry, sidewall heating of Th, insulator, and sidewall cooling of Tc, respectively. a) aspect ratio 5:1, standard case b) aspect ratio 2.5:1 c) aspect ratio 10:1 d) aspect ratio 5:0.5 e) aspect ratio 5:2.15.

The double averaged normalized temperature maps, Figure 49, revealed a surprising feature; case b showed an inversion of temperature inside the core region. The temperature inversion is defined as the lower core section colder than the upper core section. By examining the core temperature differences, it appeared that smaller aspect ratio cases, b and e, showed uniform or inverted temperature profiles. While higher aspect ratio cases, c and d, showed distinct normal temperature differentials in the cores.
Figure 49  3D temperature & vector maps.
All use the standard water properties and boundary conditions. Double averaged and normalized. a) baseline case – aspect ratio 5:1 b) aspect ratio 2.5:1 c) aspect ratio 10:1 d) aspect ratio 5:0.5 e) aspect ratio 5:2.15.
Figure 50  Changing AR, 3D velocity magnitude maps
All use the standard water properties and boundary conditions. Double averaged and normalized. a) baseline case – aspect ratio 5:1 b) aspect ratio 2.5:1 c) aspect ratio 10:1 d) aspect ratio 5:0.5 e) aspect ratio 5:2.15.
Figure 51  Changing aspect ratio, 3D velocity vectors.
Note: not scaled between cases. All use the standard water properties and boundary conditions. Double averaged. a) baseline case – aspect ratio 5:1 b) aspect ratio 2.5:1 c) aspect ratio 10:1 d) aspect ratio 5:0.5 e) aspect ratio 5:2.15.
Figure 52  Changing aspect ratio, 3D NPDF of velocity magnitude. All have standard water properties and boundary conditions. Double averaged velocity magnitude as input. a) baseline case – aspect ratio 5:1 b) aspect ratio 2.5:1 c) aspect ratio 10:1 d) aspect ratio 5:0.5 e) aspect ratio 5:2.15.
Figure 53  Changing AR, 3D boundary layer thickness and velocity. Double averaged. aa) and bb) respectively. a) baseline case – aspect ratio 5:1 b) aspect ratio 2.5:1 c) aspect ratio 10:1 d) aspect ratio 5:0.5 e) aspect ratio 5:2.15.
The double averaged normalized velocity magnitude maps, Figure 50, showed that the max fluid speed is similar for each simulation. There appears to be no trends of where high-speed flow occurs in the reactor with respect to aspect ratios. In all 3D simulations, the fastest moving fluid was found to be in the boundary layer.

The double averaged velocity vectors, Figure 51, showed that the flow was not axisymmetric because the vectors cross the axis of symmetry (shown in red). This indicated that the flow exhibited strong 3D characteristics. The double averaged swirling contours are shown in Appendix B. From the temperature maps and velocity vectors, Figures 49 and 51 respectively, it became apparent that the 3D study needed to determine how the fluid was passing through the insulator region.

The NPDF, Figure 52, indicated that increasing the length, case c caused the greatest increase in overall fluid flow speed. However, the opposite did not prove true, as decreasing the length, case b, did not significantly change the overall flow speed inside the reactor. Increasing the diameter did increase the overall flow speed inside the reactor, case e; however, decreasing the diameter also increased the overall flow speed inside the reactor, case d. From these results it appears that no discernable trend relating changing length, diameter, or aspect ratio can be linked to changing the magnitude of the Rayleigh number. This is farther evidenced by comparing Figures 46 and 52 alongside Table 19.

The boundary layer thicknesses were almost identical for every 3D simulation, Figure 53 aa. Again, the oscillations occur where the cold and hot boundary layers impinge in the insulator region thus the boundary layer is destroyed; these oscillations should be ignored. Figure 53 bb does show differences in the velocity of the boundary layer. An increase in length, case c allowed for the boundary layer to develop longer which
increased the overall velocity of the boundary layer. Also increasing the diameter moved the shearing core flow farther from the boundary layer, which allowed for a faster moving boundary layer in case e as well. The opposite occurred when the length was decreased or the diameter was decreased, cases b and d, respectively.

The time averaged cross sections of multiple variables for each reactor is presented below. It should be noted that for the cross sections presented below that letters b-f refer to locations inside the reactor were the cross section was taken. Locations are always placed in the same general areas of each reactor: b is located centrally in the upper cooled section, c is always just above the insulator, d is always inside the insulator, e is always just below the insulator, and f is located centrally in the lower heated section of the reactor. Letter a refers to the diagram detailing the reactor and where the cross-sections are. In a, the green lines represent the cross-section locations, red lines indicate lower lateral wall heating, blue lines indicate upper lateral wall cooling, and the yellow line indicates the insulator (near d).
Figure 54  3D temperature cross-sections, AR 5:1
Time averaged, standard fluid properties, and standard boundary conditions. Shows important cross-sections away and near the insulator.
Figure 55  3D axial velocity cross-sections, aspect ratio 5:1
Positive is towards the top cap, negative towards the bottom cap, time averaged, standard fluid properties, and standard boundary conditions. Shows important cross-sections away and near the insulator.
Figure 56  3D temperature cross-sections, aspect ratio 2.5:1  
Time averaged, standard fluid properties, and standard boundary conditions. Shows important cross-sections away and near the insulator.
Figure 57  3D axial velocity cross-sections, aspect ratio 2.5:1
Positive is towards the top cap, negative towards the bottom cap. Time averaged, standard fluid properties, and standard boundary conditions. Shows important cross-sections away and near the insulator.
Figure 58  3D temperature cross-sections, aspect ratio 10:1
Time averaged, standard fluid properties, and standard boundary conditions. Shows important cross-sections away and near the insulator.
Figure 59  3D axial velocity cross-sections, aspect ratio 10:1
Positive is towards the top cap, negative towards the bottom cap. Time averaged, standard fluid properties, and standard boundary conditions. Shows important cross-sections away and near the insulator.
Figure 60  3D temperature cross-sections, aspect ratio 5:0.5
Time averaged, standard fluid properties, and standard boundary conditions. Shows important cross-sections away and near the insulator.
Figure 61  
3D axial velocity cross-sections, aspect ratio 5:0.5
Positive is towards the top cap, negative towards the bottom cap. Time averaged, standard fluid properties, and standard boundary conditions. Shows important cross-sections away and near the insulator.
Figure 62  3D temperature cross-sections, aspect ratio 5:2.15
Time averaged, standard fluid properties, and standard boundary conditions. Shows important cross-sections away and near the insulator.
Figure 63  3D axial velocity cross-sections, aspect ratio 5:2.15
Positive is towards the top cap, negative towards the bottom cap. Time averaged,
standard fluid properties, and standard boundary conditions. Shows important cross-
sections away and near the insulator.
Figure 64 3D temperature cross-sections Rayleigh increased an order of magnitude, time averaged, standard fluid properties, and standard boundary conditions. See Section 5.2.1 for details. Shows important cross-sections away and near the insulator.
Figure 65  3D axial velocity cross-sections, Rayleigh increased an order
Positive is towards the top cap, negative towards the bottom cap., aspect ratio 5:1, time
averaged, standard fluid properties, and standard boundary conditions. See Section 5.2.1
for details. Shows important cross-sections away and near the insulator.
The time averaged cross sections showed an interesting feature difference between cases with uniform or inverted core temperatures (aspect ratios 5:1, 2.5:1, and 5:2.15) to standard core temperature differences (aspect ratios 10:1 and 5:0.5). All cases with uniform or inverted core temperatures exhibited a symmetrical pattern found in Figures 54-57, 62, and 63. The symmetry is most apparent in aspect ratio 2.5:1. It seems that when the core begins to invert in temperature a unique flow pattern begins to appear through the insulator region, whereas cases with the standard temperature differential, no apparent flow pattern through the insulator is discernable, Figures 58-61. To confirm this, the instantaneous cross-sections should be examined, to determine if this is the result of averaging or if this is a steady pattern of fluid flow. The swirling velocity is shown in Appendix B and an investigation determining if this unique pattern was a numerical artifact of the mesh. Appendix B figures show that the unique flow pattern through the insulator region is real and independent of the mesh.

The instantaneous cross-sections are in [50], [51], [52], [53], and [54]. The direct links 2.5:1, 5:1, 10:1, 5:2.15, and 5:0.5 are provided for ease of access. The instantaneous cross sections showed that there is a huge difference between how the boundary layers interacted near and inside the insulator. Higher aspect ratios showed chaotic flow of the boundary layer passing through the insulator region, while lower aspect ratios showed uniform more steady transfer of fluid through the insulator region. Vertical cross-sections showing the entire reactor are in [55], detailing the instantaneous temperature and velocity magnitude contours (3D).

The inversion is explained by a feature not found in the 2D simulations, the ability of the fluid to swirl. This allowed more fluid from the boundary layers to pass through the
insulator and reach the opposite core regions. The steady flow of cases with uniform or inverted temperatures was a result of buoyancy forces. In cases that were uniform or inverted, the core did not generate buoyancy forces opposing the cores motion, as the core was already at the lowest energy potential. In cases with the normal temperature differential, the core generated opposing buoyancy forces to the movement of the core. This caused the insulator to become very unsteady in nature because the boundary layers are pushing the core of the fluid towards the caps, whereas buoyancy wants the core to move towards the insulator.

5.3 2D 3D comparisons

The previous sections compared the trends that resulted from 2D and 3D simulations. They were analyzed independently without comparisons; now direct comparisons will made to see if the trends they implied were the same. The similarities and differences were explained and shown in the following sections. There was also the introduction and comparison between a 2D and 3D laminar simulation. The laminar simulation was held until last to show fundamental differences that occur when the axisymmetric assumption was used compared to the full 3D simulation.

5.3.1 Turbulent

Direct comparisons between 2D and 3D simulations were made by comparing circumferentially averaged 3D simulations to instantaneous 2D simulations. This was shown in [56] and individual 2D to 3D case comparisons were shown with direct links of 2.5:1, 5:1, 10:1, 5:2.15, 5:0.5. There were clear differences in temperature and overall fluid flow in low aspect ratio cases. The higher the aspect ratio the more similar the results between 2D and 3D simulations.
5.3.2 Laminar

The comparison between the 2D and 3D laminar simulation is now introduced to better understand the physical phenomena occurring inside the reactor. The length, height, and insulator were the same as aspect ratio 5:1; however, the fluid properties and boundary conditions were changed to induce laminar flow. The setup differences for the 2D and 3D laminar simulations were as follows: \( \Delta T = 20K \), \( \beta = 7.58027e-09 \), 2D mesh of 42k elements, and 3D mesh of 4,540k elements.

The 3D simulation had not yet reached thermal convergence; however, it was simulated for almost 5 hours of numerical time, about 2 months of CPU time. During the 3D simulation, the fluid proceeded to move in a very 2D manner, with almost no swirl, and no fluid crossing the centerline. As the simulation continued eventually the fluid began to swirl and the strength of the swirl grew until it became significant enough to greatly affect the thermal distribution near the insulator. It was shortly after this point that the simulation was stopped. The 3D transient simulation was also compared to a 3D steady state simulation. The steady state 3D simulation also showed evidence of the swirling fluid, however would never able to completely converge to a steady state. The comparison was not presented as the results are almost identical, only the final transient 3D results are shown.

The 2D simulation was conducted by Hooman Enayati. This simulation was conducted transiently and compared to a steady state simulation, with nearly identical results. The comparison of 2D transient to 2D steady state is not presented here.
Figure 66  2D and 3D laminar temperature and velocity magnitude maps
a) spatially averaged 3D normalized temperature  b) spatially averaged 3D normalized velocity magnitude  c) 2D normalized temperature  d) 2D normalized velocity magnitude  e) legend for scaling 3D and 2D normalized temperatures and velocity magnitudes.
Figure 66 shows the 2D (c and d) and spatially averaged 3D (a and b) normalized temperature and velocity magnitude maps. Comparing a and c shows how fluid in the 3D simulation penetrates through the insulator region much more than the 2D. It is noteworthy to mention that even the laminar 3D reactor has an aspect of an inverted core temperature, at least near the insulator shown in a. There also is cool fluid that has reached the lower cap and stagnated in the 3D reactor (a). Also note that the fastest velocity occurs inside the core region by the insulator.

Because the 3D laminar reactor indicates fluid that is traveling in the circumferential direction, cross-sections of this reactor are presented. From the cross-sectional details it is evident that the 3D flow is very different from the 2D flow. In Figure 69 c-e, the fluid of the boundary layer beings to swirl into two main sections. In Figure 68 c-e the fluid that has now left the boundary layer is moving through the insulator region. It is apparent that the fluid is not recirculating without passing through the insulator region. The 2D simulation shows that the fluid is purely recirculating without passing through the insulator region. This results in a significant difference in the thermal distribution inside the 2D and 3D reactors.

Inspecting the maximum velocity occurring inside the reactors, refer to Figure 66 b and d, show that the 3D had significantly faster flow inside the core region. This is because the core region near the insulator in the 3D simulation has an inverted temperature. This results in the core generating a buoyancy force that corresponds with the forced motion of the core region. The 2D reactor, Figure 66 c has a core with the standard temperature profile near the insulator. This core generates buoyancy forces opposing the forced direction of flow, hence resulting in a slower fluid speed.
Figure 67  3D laminar temperature cross-sections, aspect ratio 5:1. Shows important cross-sections away and near the insulator.
Figure 68  3D laminar axial velocity cross-sections, aspect ratio 5:1. Positive is towards the top cap, negative towards the bottom cap. Shows important cross-sections away and near the insulator.
Figure 69  3D laminar axial velocity cross-sections, aspect ratio 5:1. Positive is counter clockwise, negative is clockwise. Shows important cross-sections away and near the insulator.
5.3.3 Inversion

From reviewing Sections 5.3.1 and 5.3.2 it is clear that the inversion was the greatest difference between 2D and 3D simulations. Notably due to the 3D nature of fluid flow through the insulator region, even the laminar simulation with extremely slow fluid speeds showed the aspects of inverted temperature. For turbulent simulations it is important to know if the inversion occurs, as the temperature differential will greatly affect the chemistry in a real reactor.

Table 20 below presents the values of specific parameters that are important to predicting the temperature inversion. These values are from the 2D simulations and their results, and were used for determining a dimensionless inversion characteristic (IC).

Aspect ratio 5:1* was the 2D case with the Rayleigh number increased an order of magnitude.

<table>
<thead>
<tr>
<th>AR</th>
<th>D</th>
<th>L</th>
<th>ρ</th>
<th>δ _μ</th>
<th>δ_δ</th>
<th>A</th>
<th>A_δ</th>
<th>I.C.</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5:1</td>
<td>0.15875</td>
<td>0.41105</td>
<td>8.5384e-4</td>
<td>997.1</td>
<td>.011</td>
<td>2.2e-3</td>
<td>0.0198</td>
<td>1.082e-3</td>
</tr>
<tr>
<td>5:1</td>
<td>0.15875</td>
<td>0.82210</td>
<td>8.5384e-4</td>
<td>997.1</td>
<td>.012</td>
<td>2.6e-3</td>
<td>0.0198</td>
<td>1.275e-3</td>
</tr>
<tr>
<td>10:1</td>
<td>0.15875</td>
<td>1.64419</td>
<td>8.5384e-4</td>
<td>997.1</td>
<td>.0125</td>
<td>2.6e-3</td>
<td>0.0198</td>
<td>1.275e-3</td>
</tr>
<tr>
<td>5:2.15</td>
<td>0.34202</td>
<td>0.82210</td>
<td>8.5384e-4</td>
<td>997.1</td>
<td>.014</td>
<td>2.6e-3</td>
<td>0.0919</td>
<td>2.772e-3</td>
</tr>
<tr>
<td>5:0.5</td>
<td>0.079375</td>
<td>0.82210</td>
<td>8.5384e-4</td>
<td>997.1</td>
<td>.011</td>
<td>2.4e-3</td>
<td>0.0049</td>
<td>5.804e-4</td>
</tr>
<tr>
<td>5:1*</td>
<td>0.15875</td>
<td>0.82210</td>
<td>8.5384e-4</td>
<td>997.1</td>
<td>.032</td>
<td>1.7e-3</td>
<td>0.0198</td>
<td>8.632e-4</td>
</tr>
</tbody>
</table>

\[
I.C. = \frac{D \ A \ \mu}{L \ A_\delta \ \rho \ \delta_\delta} = \frac{1}{\overline{h}} A \ \frac{1}{Re_\delta}
\]

\[A \text{ – cross section area of the reactor}\]

\[A_\delta \text{ – cross sectional area of the boundary layer}\]

The definition of the inversion characteristic is shown above. It is a combination of the aspect ratio, \(\overline{h}\), which was related to the overall scale of the reactor. The cross-
sectional areas, $\bar{A}$, corresponding to the boundary layer and its relationship to the reactor. Finally, the boundary layer modified Reynolds number, $Re_\delta$, which was a measure of the strength of the boundary layer in the respective reactor. Higher IC numbers indicated a reactor that was more likely to show uniform or inverted temperatures, while lower IC numbers indicated a greater standard temperature differential. The purpose of calculating the IC was to determine if inversion was likely from only a 2D simulation. From the table above an IC value greater than 0.08 predicted uniform or inverted temperature, when compared to the 3D simulations the table correctly predicted the temperature differentials. The table also successfully predicted 5:1*, which corresponds to the higher order Rayleigh case, shown in Section 5.1.1. This specific 3D case did not show uniform or inverted temperatures, which the IC from the 2D simulation was able to predict.
CHAPTER VI

CONCLUSION

The laterally heated cylindrical natural convection reactor was studied in different aspects than literature previous covered. The parameters of study included, length, diameter, aspect ratio, insulator, and heating ratios. The simulations conducted were both 2D and 3D; the results were then analyzed as instantaneous, time averaged, circumferentially averaged, or double averaged. The variables studied included velocity vectors, velocity magnitude, temperature, and boundary layers (thickness and velocity). The analysis covered 2D and 3D independently and then compared their differences and similarities. Lastly a 2D and 3D laminar simulation was conducted.

The study presented here has deficiencies which need to be addressed. Foremost is no time step convergence test was performed for 3D simulations. It is assumed that the 2D timestep convergence is sufficient. Real fluid properties were assumed constant by using the Boussinesq assumption. All of the reactors simulated did not contain internal features such as a baffle, porous media, rack, and seeds. All turbulence was modeled using a RANS model.

For future studies the deficiencies need to be addressed. More three-dimensional simulations are needed to confirm the results. Experimental data will be crucial for
determining which turbulence modeling provides the most accurate results. The inversion characteristic can be modified to account for internal geometry such as baffles, seeds, and a rack. Most importantly, a clearer definition of the characteristic length needs to be determined. This study was not able to determine a specific definition but clearly shows that the length scales used in literature governing the reactor studied are improper.

The study has shown that the reactor layout studied is insufficiently modeled by a 2D simulation. The flow is shown to be inherently three-dimensional in nature, even though the boundary conditions are axisymmetric, and applies to both laminar and turbulent flow regimes. The 2D axisymmetric assumption yields incorrect thermal environments because the flow is inherently 3D in nature. The thermal environment is the most important feature of a reactor because the thermal environment drives the fluid inside the reactor. Without the correct thermal-field it is impossible to generate the correct fluid flow patterns. The validity of the 2D assumption is worst in low aspect ratio reactors, as shown by aspect ratio 2.5:1. It appears that higher aspect ratios are more properly modeled by the 2D assumption, but it still generates a significant thermal error.

No internal configurations for real reactors were examined in this study; however, the results shown provide useful guidance for designing a laterally heated reactor. Firstly, it is important to design from the 3D simulation as the 2D is completely insufficient. Secondly, aspect ratio of the reactor is the most important factor that affects the environment inside the reactor. At least when the diameter is significantly larger than \( \delta \). Small diameter to \( \delta \) ratios were not studied. Designs involving a high aspect ratio reactor will generate a thermal environment more similar to current designs that incorporate a baffle; higher temperatures inside the lower core and cooler temperatures inside the upper
core of the reactor. Lower aspect ratio reactors result in more uniform or inverted thermal environments inside the reactor. The lower aspect ratios present a unique design with potential advantages not yet investigated thoroughly.

The simulations conducted do not consider a baffle inside the reactor; however, there are important advantages to eliminating the baffle inside the reactor for low aspect ratio reactors. Firstly, the thermal environment is more likely to show an inverted temperature difference inside the core. The stronger the inversion the greater the temperature difference which will thus increase the rates of deposition or etching of species if designed properly. Secondly, the temperature inversion generates a more stable flow inside the reactor. This means that internal configurations will see repeated fluid flow, temperatures, and concentrations of species which promotes increase growth rates. Lastly, when a baffle is incorporated into the design the transfer of fluid from the top section to the lower section becomes limited. This means that baffles decrease the amount of fluid that circulates throughout the entire reactor and a baffle-less reactor increases dramatically the total amount of fluid that circulates throughout the reactor, evidenced by the thermal inversion. This implies that there is a greater potential of mass transfer inside a baffle-less reactor.

There are difficulties in studying these specific reactors, as the length scale is not properly defined which hinders potential scalability of reactors. From the results presented a conceivable length scale is $\delta$, the thickness of the momentum boundary layer. From the 3D boundary layer thickness results (Figure 53), it appears that the thickness is independent of the length, diameter, and aspect ratio. It also appears independent of heating ratios as presented in the 2D results (Figure 44). This signifies that the length
scale is functionally a definition of the fluid and temperature differential applied to the sidewalls and implies there is no clear external definition of the characteristic length for this specific reactor.


https://www.youtube.com/watch?v=0ZeAcaFcaM&list=PLSoFI1TSrZYshCAyt-9fzgayKz6QNeff. [Accessed Aug 2017].

https://www.youtube.com/watch?v=lyBL3a6QNMY&list=PLSoFI1TSrZYTbWpbnPJlcUmqVIJKmw2N. [Accessed Aug 2017].

https://www.youtube.com/watch?v=IucOcCCKPjo&list=PLSoFI1TSrZYSKQQF64Jc0fODJf8rEFZol. [Accessed Aug 2017].

https://www.youtube.com/watch?v=zVg_aDcXYIk&list=PLSoFI1TSrZYQGPjRIJryGe3FB3X6BjRHJ. [Accessed Aug 2017].

https://www.youtube.com/watch?v=fmflAj29shU&list=PLSoFI1TSrZYRcI4azQvFgM8WZIyE2zsnt. [Accessed Aug 2017].

151

APPENDICES
APPENDIX A. NPDF CONVERGENCES

2D

Converging 5:1 80k NPDF

Converging 5:1 40k NPDF

Converging 10:1 120k NPDF

Converging 10:1 80k NPDF
APPENDIX B. 3D EXTRA

161

Corresponding Mesh and Contour.
AR 2.5:1 Mesh Flow Independence. Finer mesh 853k. Time averaged axial velocity.

Corresponding Mesh and Contour.
APPENDIX C. NOMENCLATURE

\( \phi_{rz} \) - scalar at similar r,z locations
\( m \) - number of samples
\( \phi_{xyz} \) - scalar at similar x,y,z locations
\( n \) - number of samples
\( Th \) - temperature of heated wall
\( Tc \) - temperature of cooled wall
\( Lh \) - length of lower heated wall
\( Lc \) - length of upper cooled wall
\( Li \) - length of insulator
\( L \) - length of the reactor
\( L^* \) - normalized length
\( D \) - diameter of the reactor
\( D^* \) - normalized diameter
\( R \) - radius of the reactor
\( R^* \) - normalized radius
\( AR \) - improper aspect ratio of the reactor L:D
\( \bar{h} \) - proper aspect ratio of the reactor L/D
\( g \) - gravitational constant
\( Ra \) - Rayleigh number
\( Pr \) - Prandtl number
\( Gr \) - Grashof number
\( \beta \) - coefficient of thermal expansion
\( \Delta T \) - temperature difference between \( Th \) and \( Tc \)
\( \mu \) - dynamic viscosity of the fluid
\( c_p \) - specific heat of the fluid
\( \rho \) - density of the fluid
\( k \) - thermal conductivity of the fluid
\( \frac{L}{A} \) - volume to lateral surface ratio
\( X \) - characteristic length
\( \delta_t \) - thermal boundary layer thickness
\( \delta \) - momentum boundary layer thickness
\( \phi \) - scalar quantity
\( t \) - time
\( T \) - temperature
\( \bar{T} \) - time/space averaged temperature
\( \bar{\bar{T}} \) - double averaged temperature
\( T^* \) - normalized temperature
\( |V| \) - velocity magnitude
\( |\bar{\bar{V}}| \) - time/space averaged velocity magnitude
\( |\bar{V}| \) - double averaged velocity magnitude
\( |V|^* \) - normalized velocity magnitude
\( N_{faces} \) - number of faces enclosing cell
\( \phi_f \) - scalar value convected through face f
\( \rho_f \phi_f \cdot \hat{A}_f \) - mass flux through the face
\( \hat{A}_f \) - area of face f
\( \nabla \phi_f \) - gradient of \( \phi \) at f
\( \mathbf{V} \) - cell volume
$S_\phi$ - source of $\phi$ per unit volume
$\nabla \phi$ - gradient of $\phi$
$\Gamma_\phi$ - diffusion coefficient for $\phi$
$\hat{A}$ - surface area vector
$\hat{v}$ - velocity vector
$S_h$ - volumetric heat sources
$k_t$ - turbulent thermal conductivity
$k$ - thermal conductivity
$G_k$ - generation of turbulent kinetic energy
$\sigma_k$ - turbulent Prandtl number for $k$
$\sigma_\omega$ - turbulent Prandtl number for $\omega$
$\Gamma_k$ - effective diffusivity of $k$
$\Gamma_\omega$ - effective diffusivity of $\omega$
$G_\omega$ - generation of $\omega$
$Y_k$ - dissipation of $k$
$Y_\omega$ - dissipation of $\omega$
$S_k$ - source of $k$ per unit volume
$S_\omega$ - source of $\omega$ per unit volume
$Pr_t$ - turbulent Prandtl number
$G_b$ - generation of $k$ due to buoyancy
$Y_m$ - compressible generation of $k$
$k$ - turbulent kinetic energy
$\mu_t$ - turbulent viscosity
$\epsilon$ - turbulent dissipation
$\phi$ - instantaneous scalar quantity
$\bar{u}_i$ - time averaged velocity vector
$\bar{\phi}$ - time averaged scalar quantity
$\hat{u}_i$ - instantaneous velocity vector
$\bar{\tau}$ - stress tensor
$\rho \hat{g}$ - gravitational body force
$F$ - external body source
$S_m$ - mass source term

**CONSTANTS**

$\sigma_{k,1}, \sigma_{k,2}, \sigma_{\omega,1}, \sigma_{\omega,2}, \alpha_1, \beta_{i_1}, \beta_{i_2}, \beta_i, \alpha_\omega, \alpha_0, \sigma_k, \sigma_\omega, R_k, a_0^\omega, C_{1\epsilon}, C_{2\epsilon}, C_{3\epsilon}, \sigma_\epsilon, \sigma_k, C_\mu, \zeta^*, R_\beta,$

$\beta_\omega^*, F(M_t)$