CFD Analysis of Supercritical Water Reactor for Flow Back and Produced Water Treatment

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This thesis titled

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CFD Analysis of Supercritical Water Reactor for Flow Back and Produced Water Treatment

Director of Thesis: Jason Trembly

Shale deposits have the potential of unlocking a vast reserve of fuel across the United States. However, the current high water usage of the horizontal drilling and hydraulic fracturing techniques used to develop shale resources needs to be addressed. OHIO is developing the Integrated Precipitative Supercritical Process (IPSC), with the aim of reusing flowback and produced water (F/P) from shale wells to reduce the water intensity of shale development activities. Of the components in the IPSC process, the Supercritical Water Reactor (SCWR) will be responsible in the treatment of the major salt constituents in F/P water. The purpose of this thesis was to utilize CFD analysis, using ANSYS Fluent (Fluent), to investigate the heat transfer and fluid flow in the SCWR, at different inlet temperatures (350° C and 390° C) and operating pressures (23 MPa and 26 MPa).

A user-defined material representing Supercritical Water (SCW) was developed in Fluent, which was later compared to existing experimental data from literature and implemented to evaluate SCWR operation. Temperature and density contours along with flow patterns within the SCWR are presented. The estimated TDS solubility in the lower half of the SCWR were estimated based upon SCW density. It was observed that
at higher operating pressures, SCW could be heated to a higher temperature compared to pressures around the supercritical point ($P_{\text{Supercritical}} = 22.064$ MPa). However, the minimum SCW density increases as the operating pressure increases, resulting in an increase of TDS solubility. As a result, the ideal conditions would need to be a balance between the inlet temperature of F/P water and the operating pressure of the system.
DEDICATION

To my parents
ACKNOWLEDGEMENTS

I would like to thank my advisor Dr. Jason Trembly for giving me the opportunity to work on this intriguing and challenging area of research. I am especially appreciative for the time and resources that he invested in the completion of this thesis.

I would also like to thank my committee members Dr. David Bayless, Dr. Natalie Kruse- Daniels and Dr. Ben Stuart for their valuable input in improving the quality of this research and document.

The staff at ANSYS technical support also had a role in improving my understanding of Fluent and CFD, and I would like to thank them for their prompt feedback with all of my queries. A special mention also goes to Sayali Pathak, for helping me through many aspects of this research throughout its duration.

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CHAPTER 1: INTRODUCTION

1.1 Introduction

Shale deposits possess significant potential to provide the U.S. with abundant reserves of oil and natural gas (NG). Until recently, no economical methods of extracting oil and NG from shale deposits existed. However, recent advancements in horizontal drilling and hydraulic fracturing have made extraction of oil and NG from shale reserves economical.

Although promising, hydraulic fracturing raises concerns regarding its sustainability and impact on the surrounding environment due to its high water intensity and the chemical additives used to stimulate fracture production. On average U.S. shale wells require between 4-5 million gallons of water for the hydraulic fracturing process alone [1]. In addition, several compounds, such as acids, inhibitors, and biocide, are used to enhance the fracturing process. These compounds compose up to 0.5% by weight of the hydraulic fracturing fluid [1]. Furthermore, after fracturing and during operation shale gas wells generate wastewater, which contains a host of constituents from the hydraulic fracturing fluid and shale reservoir. Due to these constituents, the wastewater cannot be discharged and can be costly to treat or dispose of, increasing operating costs. The objective of this thesis is to evaluate super critical water (SCW) treatment as a method of producing a reusable product for shale well development and reducing hydraulic fracturing’s water intensity [2].
1.2 Shale Deposits and Reserves

Shale can be defined as a fine-grained sedimentary rock that occurs beneath a vast portion of the earth’s surface [3]. Shale is formed due to the compression of silt and other minerals over a long period of time. Shale formations are characterized by their laminated (formed of multiple layers) and fissile (readily splitting along the layers) nature [4].

Oil shale, on the other hand, is defined as any shale rock that contains more than 5% by volume of kerogen [5]. This kerogen has not thermally matured at high pressures and has not been converted into conventional oil [1], [6]. Shale deposits can be found at a variety of geological locations, ranging from freshwater and salt water bodies to continental basins and coastal swamp regions [7].

Shale deposits are spread across North America, South America, parts of Africa, and Europe. A breakdown of major shale deposits is shown in Table 1. In all, the minimum estimated global shale oil reserves total 3 trillion bbl. [6].

<table>
<thead>
<tr>
<th>Country</th>
<th>Total Recoverable Reserves (Bbbl)</th>
</tr>
</thead>
<tbody>
<tr>
<td>USA</td>
<td>626</td>
</tr>
<tr>
<td>Brazil</td>
<td>300</td>
</tr>
<tr>
<td>Russia</td>
<td>41</td>
</tr>
<tr>
<td>Democratic Republic of Congo</td>
<td>38</td>
</tr>
<tr>
<td>Australia</td>
<td>17</td>
</tr>
<tr>
<td>Canada</td>
<td>16</td>
</tr>
<tr>
<td>Italy</td>
<td>13</td>
</tr>
</tbody>
</table>
As seen in Table 1, the U.S. has the largest reserves of shale deposits. The distribution of U.S. shale deposits is shown in Figure 1.

Figure 1: U.S. shale deposits [8]

The major reserves based on the predicted deposits are the Marcellus and Utica shale in the Appalachian basin, the Eagle Ford in the U.S. Gulf Coast region and the Bakken formations in the Williston basin located within the Dakotas and Montana [9], [10]. With the use of hydraulic fracturing, the U.S. has the opportunity to meet its energy demands with domestic shale resources while lowering its total CO$_2$ emissions by
supplementing existing coal-fired power generation with natural gas combined cycle power plants.

1.3 Horizontal Drilling and Hydraulic Fracturing

Until recently, vertical drilling was the only available technique for the extraction of oil and gas from shale formations. This technique has two major drawbacks. First, a vertical well has very limited access to the shale formation since most shale formations are relatively thin along the vertical direction compared to its expansive area along the horizontal. As a result, a vertical well has diminished area of coverage, thereby reducing its productivity. This requires further vertical wells to be drilled to increase field production resulting in higher development costs and greater impact to the surface environment. Second, the tightness of the shale formation results in reduced hydrocarbon production, which diminishes the economic attractiveness of developing shale plays. However, with innovative horizontal drilling and hydraulic fracturing, a single well can access an expansive area with significant production rates, which makes shale formation development economically attractive. In addition, multiple horizontal wells can be drilled from a single well pad reducing surface disturbance.

1.3.1 Horizontal Drilling

The drilling of any oil and gas well, vertical or horizontal, is an intricate operation and takes up to a month to complete. Drilling is completed using industrial drill bits in several stages, starting with large diameter drill bits successively followed by smaller diameter bits. To protect the ground water and to maintain the integrity of the well,
steel casings are cemented into place after every stage of drilling. Typically, the well is lined with multiple casings in order to prevent contact of the drilling fluids with surrounding freshwater aquifers that are present near the well site. In the first 50-80 ft. length of the well, a large diameter hole is drilled and a conductor casing is placed in the hole, which helps stabilize the ground surrounding the drilling site. Next, air drilling is used until the well depth is below the deepest freshwater aquifer, which can extend an additional 200-800 ft. depending upon location. Air drilling is used in this initial region to prevent the freshwater aquifer from contacting drilling fluids. A series of compressors and boosters are used, which lift the water and the rock cuttings up to the surface. After air drilling is complete, the drilling equipment is retracted to the surface and a second layer of protection casing is installed around the surface of the well. Next, a series of high-pressure safety valves and seals called the blowout preventer is installed at the top of the casing, which controls well pressure and prevents surface releases [11].

Drilling is resumed after installation of the surface casing, but this method of drilling uses drilling mud, which mainly comprises of a mixture based on bentonite clay or other synthetic thickeners. The drilling mud plays a vital role as it lifts the rock cuttings, cools the drill bit, and controls down-hole pressure, thereby stabilizing the well. A few hundred feet above the target shale, the drilling assembly is stopped and retracted from the well. In the case of horizontal drilling, at this point a horizontal drilling tool is introduced. This tool gradually turns the drill bit, until a horizontal plane is reached. The later horizontal stages of the drilling are completed in the target shale formation.
Horizontal drilling continues in this manner at lengths greater than 4000 ft. This process requires a considerable volume of water and is dependent upon the shale formation [12]. The amount of water required for the drilling of major shale formations is shown in Table 2.

<table>
<thead>
<tr>
<th>Shale Type</th>
<th>Water (gallons)</th>
</tr>
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<tbody>
<tr>
<td>Barnett</td>
<td>250,000</td>
</tr>
<tr>
<td>Marcellus</td>
<td>85,000</td>
</tr>
<tr>
<td>Eagleford</td>
<td>125,000</td>
</tr>
<tr>
<td>Haynesville</td>
<td>600,000</td>
</tr>
<tr>
<td>Fayetteville</td>
<td>65,000</td>
</tr>
<tr>
<td>Niobrara</td>
<td>300,000</td>
</tr>
</tbody>
</table>

Lastly, a final layer of casing called the production casing is installed throughout the entire length of the well. Through this casing the fuel is extracted after the well has been hydraulically fractured [12].

1.3.2 Hydraulic Fracturing

Hydraulic fracturing has been used over the past 60 years and has produced over 600 trillion ft$^3$ of NG and about 7 billion barrels of oil [13]. The average water consumption during the hydraulic fracturing process for representative shale reserves is provided in Table 3 [2], [8], [12].
Table 3: Estimated water consumption numbers for horizontal drilling and hydraulic fracturing process in various shale plays [2], [8], [12]

<table>
<thead>
<tr>
<th>Shale Type</th>
<th>Drilling Process Water Consumption</th>
<th>Fracturing Process Water Consumption (gal/well)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eagle Ford</td>
<td>125,000</td>
<td>6,000,000</td>
</tr>
<tr>
<td>Marcellus</td>
<td>85,000</td>
<td>5,500,000</td>
</tr>
<tr>
<td>Haynesville</td>
<td>600,000</td>
<td>5,000,000</td>
</tr>
<tr>
<td>Fayetteville</td>
<td>65,000</td>
<td>4,900,000</td>
</tr>
<tr>
<td>Barnett</td>
<td>250,000</td>
<td>3,800,000</td>
</tr>
<tr>
<td>Niobrara</td>
<td>300,000</td>
<td>3,000,000</td>
</tr>
</tbody>
</table>

Figure 2 illustrates hydraulic fracturing with the use of horizontal drilling for the extraction of hydrocarbons from the Marcellus shale formations. The hydraulic fracturing process is initiated with the creation of perforations in the horizontal portion of the well. This is achieved with the help of a perforating gun. The perforating gun uses explosive charges to create the initial connection between the production casing of the well and the shale formation. These perforations are created at an interval of 50-80 ft. from each other. These perforations provide pathways for the fracturing fluid to increase shale formation porosity [12].
Figure 2: Illustration of hydraulic fracturing and horizontal drilling [14]

Fracturing fluid is composed of three components: water (90.0 wt. %), proppant (9.5 wt. %), and modifiers (0.5 wt. %) [13]. The composition of the fracturing fluid can vary slightly depending upon the driller and shale formation characteristics [15]. The function of proppant is to maintain the created fractures, providing a flow path for the produced hydrocarbons. Coarse sand grades are the most popular proppants in most wells due to their abundance in nature. In addition, some engineered ceramic materials are also used. Fracturing fluid modifiers are comprised of many chemicals that are necessary to enable efficient shale fracturing [16]. The hydraulic fracturing process is
completed through a number of substages in which fracturing fluid mixed with specific modifiers is injected sequentially. These substage sequences are initiated with acid treatment to remove the drilling mud and the casing cement from the pores and pore throats. Next the slickwater pad, which is a mixture of water-based fluid and a friction reducing agent, is used to fill the well bore in order to facilitate better flow and proppant placement in the fractures. Subsequently, the first proppant substage is initiated, in which a large amount of water with fine mesh sand is pumped into the well. The proppants used in the later stages are typically coarser in size, which further aids fracture propagation. After the final substage, the complete system is flushed with freshwater to remove any excess proppants from the wellbore and equipment [16]. The produced fluid is then diverted through a manifold into storage tanks where the fluid is contained until treatment or disposal.

1.4 Produced Water Treatment & Disposal Techniques

One of the biggest concerns about the implementation of the hydraulic fracturing process for shale extraction is the large volume of water it requires. For the hydraulic fracturing of an average depth horizontal well, around 4-5 million gallons of water is required [17]. This could also have an impact on local water availability and the local watersheds from which the water is extracted. On the other hand, the transportation of water from other distant sources will be a major economic drawback and could significantly impact local road infrastructure. The transportation costs may
extend further if the produced water generated is to be disposed of or treated at a location distant from the well site.

Secondly, the wastewater itself contains very high concentrations of components and properties that make it unfit for discharge. These components include but are not limited to suspended solids, dissolved solids, bacteria, hydrocarbons, and radioactivity. Currently, to address this issue, the following methods are being used to either dispose of or treat the wastewater.

1.4.1 Evaporation Pits and Ponds

Typically wastewater is stored in open pits or ponds at the well site and the water is evaporated using evaporative spraying and solar energy. This process is effective only in reducing total wastewater volume. As a result the remaining wastewater actually contains a higher concentration of problematic components than before. In addition, the evaporative spraying can result in the emission of volatile hydrocarbons contained within the wastewater.

1.4.2 Direct Reuse

The wastewater can be reused in the hydraulic fracturing process, but the presence of the dissolved solids can lead to major pipe scaling and hence can damage the equipment or result in frequent breakdowns. Furthermore, the presence of sulfate-reducing bacteria can lead to the production of hydrogen sulfide, which can result in well souring.
1.4.3 Public Owned Treatment Works (POTW)

POTWs have been used as a treatment option for wastewater generated from traditional oil and gas development sites. POTWs can remove suspended solids and other biodegradable materials. This method, although convenient, does have some drawbacks and issues. The first disadvantage is its inability to treat Total Dissolved Solids (TDS) as well as Naturally Occurring Radioactive Material (NORM) present in the produced water. Another major drawback is the increased volume of produced water generated at current treatment facilities. POTWs in Pennsylvania, where there has been an increase in the plant effluent from 400 ppm to 3000 ppm of dissolved solids, are perfect examples [18]. Finally, the transportation of the wastewater from the well pad to the POTW is not cost-effective over large distances and is also time-consuming.

1.4.4 Disposal Wells

Another option is the disposal of wastewater in Class II deep injection wells. Class II wells are typically used for disposal of fluids associated with oil and natural gas production, such as brine and other fluids. The U.S. has approximately 144,000 Class II wells in operation in the U.S. that inject over 2 billion gallons of brine every day [19]. Although regularly used throughout the U.S., this option has limited usage. The transportation and treatment costs make it infeasible to use the well injection method as a possible permanent solution for managing wastewater generated by shale wells. Consider the case of Bakken shale plays in the Williston region. The transportation costs for delivering the wastewater to the disposal wells were between $0.63-$5/bbl. This
large variation was due to fluctuations in the trucking charges ($110-$150/hour), the wait time, and the hauling distance. On the other hand, the cost of deep well injections ranged from $0.75-$1.75/bbl with injection costs increasing on a regular basis. The average total cost for water disposal was $2.00-$16.80/bbl, out of which 54-80% was attributed to transportation [20]. Another point to be noted here is that the scope for development of new well pads is immense due to the large reserves of shale plays available. As a result, wastewater injection wells will no longer be a realistic disposal option. Hence, treatment is the most suitable and sustainable option for the foreseeable future. Existing treatment technologies available for shale-generated wastewater include membrane separation and thermal processes.

1.4.5 Membrane Separation

The Membrane Filtration Guidance Manual defines membrane filtration as a pressure- or vacuum-driven separation process in which particulate matter larger than 1 μm is rejected by an engineered barrier primarily through a size exclusion mechanism. The four most used membrane separation processes are Microfiltration (MF), Ultrafiltration (UF), Reverse Osmosis (RO), and Electrodialysis (ED) [21]. MF and UF processes are very effective in removing suspended and colloidal particles as well as bacteria and other microorganisms present in the water. In MF and UF, the water is transported across a microporous membrane using the pressure gradient that is generated across the membrane, which helps separate the suspended particles from the water. The pore sizes of the membranes used in MF are in the range of 0.1-0.2 μm.
The UF process, on the other hand, is capable of straining out smaller-sized particles, typically between the size ranges of 0.01-0.05 µm. The transmembrane pressure (TMP) required for MF and UF is considerably lower than the other membrane separation processes. The TMP is the difference between the feed pressure and the backpressure. Normally, the TMP ranges from 3-40 psig [21]. Another point to be noted is that the operating costs are lower for microfiltration (around $3-$4/ft$^2$) compared to ultrafiltration (as high as $200/ft^2$ if ceramic-based membranes are used) and reverse osmosis [21], [22]. RO separates the soluble materials from produced water using pressure difference to force the solute through the filtering membrane. These membranes have the smallest pore sizes ranging from 0.5 to 1.5 µm. One major advantage of using RO is the ability to remove salinity up to 50,000 mg/L. On the other hand, RO requires pre-treatment and regular cleaning and it is not suitable for most shale generated waste water since its salinity is much higher than 50,000 mg/L [21], [22].

Lastly, ED uses the principle of membrane separation and ion exchange technology. The particles are forced through the membranes using electric current. The ions are removed from the produced water and pass through the membrane due to the force of attraction between the opposite electric charges on the other side of the membrane. Concentrations as high as 15,000 mg/L can be treated using ED [22], [23]. The one major advantage of this process is its continuity. This is due to the residence time, which controls the particles filtered from the water. For ED to function properly,
the water must be a conductor of electric current. But the purer the water becomes, the less current it conducts. This results in the rise in operating costs [21].

Membrane separation methods are ineffective in treating the NORM present in produced water. The maximum level of salinity that can be treated using membrane separation is 50,000 mg/L [23], [24]. There is also a high tendency of membrane fouling, resulting in short membrane life and/or regular maintenance at a high cost. Lastly, there is still the issue of the treatment or disposal of the brine concentrate product. Consequently, there still remain implications from transportation, treatment, and disposal costs.

1.4.6 Thermal Water Treatment Processes

In this type of treatment process, the wastewater is treated using the principle of evaporation and condensation. Current thermal treatment systems used by industry include humidification-dehumidification (HD), distillation, evaporation, and crystallization.

In the HD process, hot air is humidified using the wastewater in the humidifier or the evaporator. The humidified air is then cooled and dehumidified in the condenser and the freshwater is extracted in a collection tank [22], [24], [25]. The distillation process is useful to get purified water free of TDS by heating produced water to vapor and then condensing it and collecting it free of the precipitate that remains. However, the volatile inorganics cannot be removed using this process [25]. In the evaporation
process, the water is stored in pits and is heated using solar energy, and the salt concentrate that remains is collected for temporary storage and eventually disposal.

The above-mentioned methods of treatment are able to remove TDS up to values of 650,000 ppm. These processes are also capable of treating the TSS, volatiles and semi-volatile organics yielding a high quality water output. Lastly, these methods are well suited for sites having zero discharge requirements [23]. However, thermal treatment processes are unable to treat NORM that could be present in wastewater. Hence, additional processing methods are necessary. In addition, thermal treatment systems possess little thermal efficiency and are quite large and not suitable for mobile applications.

1.5 Integrated Precipitative Supercritical Process (IPSC)

To address the water intensity and wastewater management issues associated with shale development, Ohio University (OHIO) is developing the integrated precipitative supercritical process (IPSC), shown in Figure 3. This process applies a combination of solid filtering, ultraviolet, precipitation, adsorption, and supercritical water treatment steps to remove constituents present in the produced water.
1.5.1 **Supercritical Water Reactor (SCWR)**

The Supercritical Reactor (SCWR) is one of the main components of the IPSC process. With the help of the SCWR, the dissolved solids are precipitated using supercritical water properties. At these conditions, water loses its polarity and no longer acts as a solvent. As a result, the dissolved solids present in the water can be easily extracted. Prevention of precipitation of dissolved solids on the internal vessel wall (scaling) is critical for optimal thermal performance of the SCWR, as scaling would cause formation of an insulating layer, thereby reducing the rate of heat transfer. To prevent scaling, sufficient heat transfer will be necessary to cause the incoming water to reach target conditions before contacting internal wall surfaces with minimal heat flux at the wall.
1.6 Research Objectives

The purpose of this research was to conduct CFD analysis of the SCWR system to analyze and predict system heat transfer and flow patterns at select operating conditions. This required the completion of a set of objectives, which would help in ensuring that the conclusions and recommendations derived from this work could serve as a foundation for understanding SCWR operation. This study includes three objectives, which are described in the following sections.

1.6.1 Objective 1: Develop Supercritical Water CFD Model

The first objective was to develop ANSYS Fluent supercritical water CFD model, including a 3-D SCWR CAD model, user-defined functions for supercritical water properties, and conductive and convective heat transfer relationships. The CFD model will provide insights regarding SCWR operation and implications of design changes on SCWR performance. ANSYS Fluent was selected to complete this work as it is the industry standard for CFD modeling and contains a built-in energy equation subroutine and the ability to incorporate user-defined functions for fluid properties.

1.6.2 Objective 2: Comparison of Supercritical Water CFD Model Results with Experimental Results

The second objective is to compare supercritical CFD model results to experimental results found in peer-reviewed literature. As the SCWR geometry is unique and no experimental information is available to complete such a comparison, the CFD model geometry was modified to a straight tube configuration allowing for
comparison with data available from peer-reviewed literature. Completion of this comparative study will be used to provide a comparative range for results generated by the SCWR CFD model.

1.6.3 Objective 3: Analyze SCWR System Sensitivity

The third objective is to perform sensitivity analyses on major process variables including water inlet temperature and operating pressure using the SCWR CFD model. To evaluate the effect of inlet water temperature, simulations were conducted at 350 and 390°C as they span the pseudo-critical temperature at 24.5 MPa. As operating pressure has a significant impact on water’s heat capacity at pseudo-critical conditions, simulations were completed at 23 and 26 MPa with an inlet temperature of 350°C. SCWR fluid temperature contour plots from the simulations were used to evaluate potential for TDS removal and scaling at the SCWR wall.
CHAPTER 2: LITERATURE REVIEW

2.1 Introduction

This chapter provides a review of work conducted by previous investigators that is applicable to the objectives and recommendations of this thesis. The chapter is divided into four sections: SCW thermophysical properties, SCW heat transfer, SCW CFD simulations, and SCW solvent properties. The first three sections provide important background information used in the development, validation, and application of SCW in CFD. The final section provides an overview of inorganic compound solubility in SCW used to support recommendations discussed in Chapter 9.

2.2 SCW Thermophysical Properties

In order to develop a SCW CFD model, which can be used to evaluate the performance of a SCW reactor to treat F/P water, the thermophysical properties of water under operating conditions must be well understood. This chapter provides an overview of the definition of SCW and SCW thermophysical properties. As described in Chapter 3, mathematical functions of pertinent SCW thermophysical properties were developed from the information presented in this section and were incorporated in the SCW CFD model.

Water at a temperature of 373.096°C (T_c) and pressure of 22.064 MPa (P_c) is said to have reached supercritical state, and the point at these conditions is defined as the critical point (CP). Below P_c, the fluid is comprised of finely dispersed water droplets in a vapor of almost the same density [26]. Beyond this point, the water exists without a
distinct phase [27]. The variation of water phases with temperature and pressure is shown in Figure 4 [28].

![Figure 4: Water phase diagram [28]](image)

Supercritical fluids (SCF), including SCW, are widely used in industry for applications such as cooling, separations, and power production. The reason behind the favorability of SCF for these applications is due to their thermophysical properties, which drastically change at the CP [27]. The variation of important SCW thermophysical properties is shown in Figure 5.
Figure 5: Variation of SCW thermo-physical properties with temperature and pressure

From Figure 5, it can be observed that there is a sudden variation in SCW thermophysical properties beyond the CP. As pressure increases beyond CP, there is a temperature at which SCW specific heat reaches a maximum. This point is known as the pseudocritical point and the corresponding temperature is known as the pseudocritical temperature. It is also evident that the specific heat capacity magnitude decreases as pressure extends beyond CP. The variations in the properties are observed due to variations in the operating pressure and the temperature of the fluid. Using these two parameters, it is possible to vary the properties of SCW with relative ease. Keeping the operating pressure above 25 MPa can significantly reduce the heat load required on the
system. As seen in Figure 5, the heat capacity values reduce rapidly once the water reaches pressure values close to 25 MPa. Density of SCW also reduces rapidly at supercritical conditions. Since this variation in density is observed throughout the operating range of the SCWR, it is necessary to consider the fluid as a compressible fluid. The thermal conductivity also decreases in the operating range. This decrease is subtle compared to the rapid variations in the density and specific heat.

2.3 Heat Transfer in SCW

Heat transfer and fluid dynamics in SCW have received significant attention and have resulted in significant data and provided a wide scope for future investigations in this field. The data available includes numerous papers on the experimental as well as numerical methods to estimate heat transfer coefficients and other parameters at supercritical conditions [29]. Furthermore, due to the advancements in the field of CFD coding and software packages, simulations and validations have been attempted to understand how fluids interact with other materials at supercritical conditions. The following sections discuss the more significant and applicable results with regard to this thesis. These results include the validation aspects in addition to the most accurate and consistent turbulence models and mass transfer models to predict heat transfer and fluid flow in SCW.
2.3.1 Review of SCW Heat Transfer Studies

Pioro et al. developed a comprehensive list of over one hundred trials conducted to understand heat transfer phenomena in SCW [30]. Despite the large number of trials available, the variation of test section geometry is very limited, since the majority of the trials evaluated heat transfer in steel tubes of diameters ranging from 5-25 mm [30]. However, Licht et al. completed trials evaluating heat transfer within tube annuli and bundles to replicate the geometry sections implemented in Supercritical Water Reactors (SCWR) [29]. SCWR are a group of next generation nuclear reactors that are currently in the research and initial design phase. These reactors would use SCW as the coolant fluid, at temperatures of around 500° C and at operating pressures of 25 MPa. Theoretically, SCWR have been estimated to achieve efficiencies of close to 44% compared to the average efficiencies of 34% that current generation Light Water Reactors (LWR) provide [29], [31]. This section gives an overview of the most relevant SCW heat transfer phenomena works with respect to the objectives of this thesis.

Yamagata et al. conducted experiments with SCW flowing in SS-304 tubes. A comprehensive analysis was conducted involving horizontally and vertically oriented tubes with the effect of gravity taken into consideration. The operating pressures varied from 22.6-29.4 MPa. A complete test matrix is provided in Table 4 [32].
Table 4: Yamagata et al. experimental test matrix [32]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Operating Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>230-540°C</td>
</tr>
<tr>
<td>Pressure</td>
<td>22.6-29.4 MPa</td>
</tr>
<tr>
<td>Heat Flux</td>
<td>116-930 kW/m²</td>
</tr>
<tr>
<td>Diameter</td>
<td>7.5-10 mm</td>
</tr>
</tbody>
</table>

The authors presented the wall temperature and the Heat Transfer Coefficient (HTC) profiles with respect to the bulk fluid temperature as shown in Figure 6. Yamagata et al. used the wall temperatures measured by the thermocouples and the bulk fluid temperature at the corresponding locations along the test section to calculate the HTC. The relation is provided below.

\[ H = \frac{q}{T_w - T_b} \]  \hspace{1cm} (2.3)

Where,

\[ H = \text{Heat Transfer Coefficient, (W/m}^2\cdot\text{K)} \]
\[ q = \text{Heat flux applied on the wall, (W/m}^2\) \]
\[ T_w = \text{Wall temperature, (K)} \]
\[ T_b = \text{Bulk fluid temperature, (K)} \]
The experimental heat transfer coefficient values obtained by Yamagata et al. were also compared with a set of numerically calculated values using Nusselt correlations developed by the authors, shown in Equation 2.3, a variation of the Dittus-Boelter equation [33], [34].

\[
N_u_b = 0.023 Re_b^{0.8} Pr_b^{0.4} \begin{cases} 
Re_b \geq 10,000 \\
0.7 \leq Pr_b \leq 160 \\
\frac{L}{D} > 10
\end{cases} 
\] (2.4)

Where,

* $Re_b$ = Bulk Reynolds Number
* $Pr_b$ = Bulk Prandtl Number
* $L$ = Length of the pipe test section, (m)
\[ D = \text{Diameter of the pipe test section, (m)} \]

Yamagata et al. developed the following version of the Dittus-Boelter equation for calculation of the Nusselt number for heat transfer of SCW in vertical tubes.

\[ Nu_b = 0.0135 Re_b^{0.85} Pr_b^{0.8} F_c \]  \hspace{1cm} (2.5)

Where,

\[ F_c = \begin{cases} 
1 & \text{for } E > 1 \\
0.67 P_r^{-0.05} \left( \frac{\bar{c}_p}{c_{pb}} \right)^{n_1} & \text{for } 0 \leq E \leq 1 \\
\left( \frac{\bar{c}_p}{c_{pb}} \right)^{n_2} & \text{for } E < 0
\end{cases} \]

\( E \) is defined as the Eckert number defined by:

\[ E = \frac{T_m - T_b}{T_w - T_b} \]  \hspace{1cm} (2.6)

\( T_b = \text{Bulk temperature, (K)} \)
\( T_m = \text{Pseudocritical temperature, (K)} \)
\( T_w = \text{Wall temperature, (K)} \)
\( \bar{c}_p = \text{Integrated average specific heat equivalent to:} \)

\[ \bar{c}_p = \frac{h_w - h_b}{T_w - T_b} \]  \hspace{1cm} (2.7)

\( h_w = \text{Enthalpy of SCW at wall region, (kJ/kg)} \)
\( h_b = \text{Bulk enthalpy of SCW, (kJ/kg)} \)

In addition, the values of \( n_1 \) and \( n_2 \) at various operating pressures of the experiments are provided in Table 5 [32].

<table>
<thead>
<tr>
<th>Pressure (MPa)</th>
<th>( n_1 )</th>
<th>( n_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>22.6</td>
<td>0.71</td>
<td>0.93</td>
</tr>
<tr>
<td>24.5</td>
<td>0.66</td>
<td>1.01</td>
</tr>
<tr>
<td>29.4</td>
<td>0.56</td>
<td>1.21</td>
</tr>
</tbody>
</table>

Table 5: Values of \( n_1 \) and \( n_2 \) used in Eq. (2.5) by Yamagata et al. [32]
In addition to the Yamagata correlation, three more correlations worth discussing were implemented in this investigation. The Swenson et al. correlation developed for heat transfer in subcritical and supercritical water is defined in Equation 2.7.

\[ Nu_w = 0.00459 Re_w^{0.923} \left( \frac{\bar{c}_p}{\bar{c}_{pb}} \right) \mu_w \left( \frac{\rho_w}{\rho_b} \right) \tag{2.8} \]

Where,

\[ \mu_w = \text{Dynamic viscosity at the wall, (Pa} \cdot \text{s)} \]
\[ k_w = \text{Thermal conductivity at the wall, (w/m} \cdot \text{K)} \]
\[ \rho_w = \text{Fluid density at the wall, (kg/m}^3 \] \]
\[ \rho_b = \text{Bulk fluid density, (kg/m}^3 \] \]

Another important correlation used in Yamagata et al. and other works of Licht et al. is the Krasnoshchekov et al. correlation. This equation is applicable over 2000 data points which include CO\textsubscript{2} as well as SCW as the working fluid [29], [35], [36]. The Krasnoshchekov et al. equation is as follows [33].

\[ Nu_b = 0.023 Re_b^{0.8} Pr_b^{0.33} \left( \frac{\bar{c}_p}{\bar{c}_{pb}} \right)^n \left( \frac{\rho_w}{\rho_b} \right)^{0.3} \tag{2.9} \]

Where,

\[ n = \begin{cases} 0.4 \text{ for } \frac{T_w}{T_{pc}} < 1 \text{ or } \frac{T_b}{T_{pc}} \geq 1.2 \\ n_1 = 0.22 + 0.18 \left( \frac{T_w}{T_{pc}} \right) \text{ for } 1 \leq \left( \frac{T_w}{T_{pc}} \right) \leq 2.5 \\ n_2 = n_1 + (5n_1 - 2) \left( 1 - \left( \frac{T_b}{T_{pc}} \right) \right) \text{ for } 1 \leq \left( \frac{T_b}{T_{pc}} \right) \leq 1.2 \end{cases} \]

The HTC values using the various correlations were plotted and compared with the experimental results as shown in Figure 7 [32].
The Yamagata et al. correlation was able to predict the HTC with the most accuracy, followed by Styrikowitsch et al., although it was unable to predict the HTC peak at pseudocritical point. The Swenson et al. correlation underestimates the values throughout the test section [32].

Shitsman et al. conducted tests on heat transfer in SCW flowing in tubes and their data has been used to analyze the accuracy of a number of Nusselt correlations
available to calculate HTC [37][38]. Figure 8 shows various Nusselt correlations applied to the experimental data.

![Heat Transfer Coefficient vs. Bulk Temperature](image)

**Figure 8: Shitsman et al. data and Nusselt correlations [38]**

The Shitsman et al. correlation for flow in tubes is based on the bulk fluid temperature and is defined by the following Nusselt equation.

\[
Nu_b = 0.023Re_b^{0.8} Pr_{min}^{0.8}
\]  

(2.10)

Where, \( Pr_{min} \) is the minimum Prandtl value of \( Pr_w \) and \( Pr_b \) [38].
The Kitoh et al. correlation is also worth mentioning. The equation was developed in 1999 and is valid for mass flux ranging from 1000-1750 kg/m$^2$s and a temperature range of 20-550° C with maximum heat flux of 1800 MW/m$^2$ [39].

$$Nu = 0.015 Re^{0.85} Pr^{z}$$ \hspace{1cm} (2.11)

$$z = 0.69 - \frac{81000}{q} + f_c \times q$$ \hspace{1cm} (2.12)

$$f_c = \begin{cases} 
\text{Low Enthalpy} & \left(0 - 1.5 \frac{MJ}{Kg}\right): f_c = 29e^{-8} + \frac{0.11}{q} \\
\text{Intermediate Enthalpy} & \left(1.5 - 3.3 \frac{MJ}{Kg}\right): f_c = -8.7e^{-8} - \frac{0.65}{q} \\
\text{High Enthalpy} & \left(3.3 - 4.0 \frac{MJ}{Kg}\right): f_c = -9.7e^{-7} + \frac{1.30}{q}
\end{cases}$$

Finally, the Bishop et al. correlation is another Nusselt correlation widely used to calculate HTC based on the bulk fluid properties as well as on taking the properties at near wall into consideration [33], [40].

$$Nu_b = 0.0069 Re_b^{0.9} Pr_b^{0.66} \left(\frac{c_p}{c_{pb}}\right)^{0.66} \left(\frac{\rho_w}{\rho_b}\right)^{0.43} \left(1 + 2.4 \left(\frac{D}{L}\right)\right)$$ \hspace{1cm} (2.13)

Mokry et al. have conducted experiments on SCW flowing in vertical tubes (d=10mm) at pressures around 24 MPa and at a wide range of mass flux (200-1500 kg/m$^2$s) to study various heat transfer regimes within the test section [41]. The authors also attempted to understand the range of applicability of the standard Dittus-Boelter equation and the Bishop et al. correlation. An illustrative data plot from their study is shown in Figure 9 [41].
One of the most discussed phenomena observed in SCW flowing in tubes is the variation of HTC with mass flux of the fluid and heat flux applied to the system [29], [35], [36], [42]–[44]. Jackson et al. attribute this phenomenon to the sudden variation in the specific heat of SCW at the pseudocritical point, resulting in wide variations in the wall and the bulk temperature of the fluid [34], [35]. Another factor contributing to the drastic change in the HTC values is the buoyancy and acceleration effects due to the supercritical fluid density variation in the wall and bulk regions [29], [35], [42]. The variation of the HTC can mainly be characterized by three zones: the improved heat transfer (IHT) zone, the deteriorated heat transfer (DHT) zone and the normal heat transfer (NHT) zone [37].

The following relation defines the HTC,

\[
H = \frac{q}{\dot{W}_{w} - \dot{W}_{b}}
\]  

(2.14)
Where,

\[ H = \text{Heat Transfer Coefficient, (W/m}^2\text{K)} \]

\[ T_w = \text{Temperature at the wall region, (°C)} \]

\[ T_b = \text{Bulk temperature of the fluid, (°C)} \]

Figure 10 gives a better illustration of the different heat transfer regimes in SCW flow [28], [37].

As seen in Figure 10, the NHT region is evident at the inlet since it has not reached the pseudocritical point. As a result, the HTC values can be estimated using the conventional Dittus-Boelter equation [37]. However, as the temperature nears the pseudocritical point, the specific heat values start to increase drastically and as a result there is a larger temperature gradient between the bulk and the wall temperature of the fluid. As a result, the HTC values rapidly decrease, which is not taken into...
consideration by the Dittus-Boelter correlation and is known as the DHT region of the fluid. Once temperature moves beyond the pseudocritical point, specific heat rapidly decreases and there is a noticeable drop in the temperature gradient between the wall and bulk regions, which is indicative of the IHT region. As the temperature increases beyond the pseudocritical point, the specific heat value stabilizes and consequently the NHT region may be observed. Mokry et al. later developed a variation of the Nusselt correlation applicable at SCWR operating conditions (10-25 MPa; 320-625°C) [37][41]. It used the comparatively new set of thermophysical data sets available from the National Institute of Standards and Technology (NIST 2007), which could improve the accuracy of the Nusselt correlation in the pseudocritical region of SCW [45]. The process involved a dimensional analysis to obtain a general form of the Nusselt correlation. Functions such as the flow diameter, thermal conductivity, viscosity and specific heat were taken into consideration. The density values at bulk as well as at the wall regions of the flow, were included in the general equation to obtain a relation capable of giving the most accurate prediction of HTC values along the entire range of the supercritical conditions of water [45]. The final equation that was derived is as follows:

$$Nu_b = 0.0061Re_b^{0.904}Pr_b^{0.684} \left(\frac{\rho_w}{\rho_b}\right)^{0.564}$$  \hspace{1cm} (2.15)

To summarize, a number of experiments have been conducted to understand heat transfer in SCW. However, the flow geometry is mainly in the form of small cylindrical tubes, and as a result, the Nusselt correlations are applicable in these corresponding domains. The general observation is that these correlations are not able
to predict HTC in the pseudocritical region to the level of accuracy that is required. Pioro et al. have completed a survey of the most accurate correlations for calculating HTC in SCW flow [37]. The accuracy of these equations is observed to vary with the change in the phase of SCW, as shown in Table 6 [37]. The table provides a list of popular correlations that are available, along with their accuracy at predicting the HTC values at the sub regions of SCW. It can be seen that the correlation by Mokry et al. yields the lowest Root Mean Square percentage error at all sub regions of the supercritical phase.

Table 6: Overall weighted average and RMS errors in sub regions of supercritical phase [37]

<table>
<thead>
<tr>
<th>Correlation</th>
<th>Liquid-like region</th>
<th>Gas-like region</th>
<th>Pseudocritical region</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Errors (%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Average</td>
<td>RMS</td>
<td>Average</td>
</tr>
<tr>
<td>Bishop et al. (1965)</td>
<td>6.3</td>
<td>24.2</td>
<td>5.2</td>
</tr>
<tr>
<td>Swenson et al. (1965)</td>
<td>1.5</td>
<td>25.2</td>
<td>-15.9</td>
</tr>
<tr>
<td>Krasnoshchekov et al. (1967)</td>
<td>15.2</td>
<td>33.7</td>
<td>-33.6</td>
</tr>
<tr>
<td>Jackson et al. (2002)</td>
<td>13.5</td>
<td>30.1</td>
<td>11.5</td>
</tr>
<tr>
<td>Mokry et al. (2009)</td>
<td>-3.9</td>
<td>21.3</td>
<td>-8.5</td>
</tr>
<tr>
<td>Dittus &amp; Boelter (1930)</td>
<td>32.5</td>
<td>46.7</td>
<td>87.7</td>
</tr>
<tr>
<td>Cheng et al. (2009)</td>
<td>1.3</td>
<td>25.6</td>
<td>2.9</td>
</tr>
<tr>
<td>Kuang et al. (2008)</td>
<td>6.6</td>
<td>23.7</td>
<td>2.9</td>
</tr>
</tbody>
</table>

For this research, the experiments conducted by Yamagata et al. [32] will be used as the means of validation. The range of operating parameters in their work coincides with those expected in the operation of the SCR and will provide a good means of gauging the ability of the CFD model to predict the heat transfer phenomena,
as seen in their test results. One point to note after this discussion is that the abovementioned correlations were developed and derived with a specific geometry of flow in mind. These correlations were most relatable to internal flow in long thin tubes, and as a result, are relatively limited to those specific type of geometrical test sections. Due to the complex geometry and flow patterns expected in the SCR, none of the above correlations are expected to predict the HTC values in the SCR. As a result, the bulk fluid and wall temperatures will be required to calculate the HTC values at individual locations on the reactor wall using Equation 2.14.

2.3.2 CFD Simulations of SCW

This section provides a review of SCW CFD simulations in the field of heat transfer and fluid flow analysis using Fluent and other CFD codes. The majority of the literature corresponds to simulations conducted on a specific set of geometry, mainly involving long tubes and annular cavities. However, despite the lack of geometrical similarity to the SCWR, the simulations’ findings in regards to turbulence models used for simulation of SCW flow can be applied to this thesis. The majority of the prior research in CFD analysis of SCW was completed using FLUENT [34], [43], [44], [46]–[50]. However, other software packages such as Star CCM [27], CD-Adapco [51]–[54], and ANSYS CFX [33] were also used. A complete list of the works conducted on CFD analysis in supercritical fluids, mainly SCW and CO₂, has been provided by Yoo et al. [42] and De Rosa et al. [55].
The most important aspect when simulating heat transfer of SCW flow is taking the variation of the thermophysical properties of SCW into consideration, since the properties play a pivotal role in determining the accuracy of the results obtained. There are a number of options available, such as the use of piecewise linear and piecewise polynomial methods to define the variation of properties with respect to temperature [34], [56]. Other methods include the direct implementation of the data sets into the software; however, this is possible only using Star CCM [27]. Farah et al. [47] have provided a detailed discussion of the application of these methods along with the inbuilt option of including the IAPWS set of equations for defining the thermophysical properties of SCW as a function of temperature and pressure. The authors studied the accuracy of the \( k-\epsilon \) and \( k-\omega \) solver with sub model variations, by calculating the HTC for SCW water flow in vertical bare tubes used as a cooling medium in nuclear reactors. The results obtained using the \( k-\omega \) Shear Stress Transport (SST) turbulence model were able to predict within ±10% for the wall temperatures in the DHT region of flow and under ±5% for the NHT region. It was concluded that the results were significantly more accurate than any of the empirical correlations used to predict HTC [47]. The results from Sharabi et al. [57] also indicate that the \( k-\omega \) and \( k-\epsilon \) models are more accurate at lower heat and mass flux values [47]. The \( k-\omega \) model with “swirl imposed” flow was shown to be the most accurate at predicting the temperature values; however, there was an average overestimation of the values by 15% [56]. These same conclusions were obtained by Moussiere et al. when conducting 2-D as well as 3-D simulations using the
k-\( \Omega \) solver with swirl flow [48]. Masuda et al. used an in-house developed CFD code called STREAM to simulate SCW flow in a T-junction using the k-\( \varepsilon \) solver, claiming that the results show it to be the best turbulence model for simulating SCW flow in complexly shaped geometry [58]. However, due to the software limitations, the density and the specific heat were considered constant at a temperature of 637 K. The variation of the viscosity and the thermal conductivity of SCW were defined with the use of fourth order polynomials based on the International Association for Properties of Water and Steam (IAPWS) data sets. Similar conclusions were drawn in other works regarding the applicability of the k-\( \Omega \) and k-\( \varepsilon \) solver to model SCW flow with the use of temperature-dependent thermophysical properties to obtain the most accurate results [27], [33], [34], [43], [44], [46], [49], [51]–[54], [59].

Other important conclusions included the effect of the mass flux on the accuracy of the simulation. Withag et al. mention buoyancy playing a role in the accuracy of the results. It is expected that the results would be more accurate at high mass flux due to the reduced effect of buoyancy in the flow [50]. The authors also mentioned that recirculation near the inlet was observed in the simulations at low mass flux values due to the effect of buoyancy, resulting in a more complex flow field [50].

In addition to the selection of the turbulence model and the accurate variation of thermophysical properties, the mesh settings also play an important role in determining the accuracy of the solution. Roelofs et al. [46] have explained that the wall \( y^+ \) number plays a big role in the accurate resolution of the boundary layer along the
tube wall, resulting in more accurate flow conditions. The wall $y^+$ is a dimensionless number that is a measure of the mesh refinement at the wall region of the fluid flow and is defined by the following equation:

$$y^+ = \frac{\rho \nu y}{\mu}$$

Where,
- $\nu$ = Normal distance to the wall
- $\rho$ = Fluid density
- $\nu$ = Fluid velocity
- $\mu$ = Dynamic viscosity

According to Roelofs [46], due to the high Prandtl number of the flow, the thermal boundary layer is much thinner than the momentum boundary layer. In order to fully resolve the thermal and the momentum boundary layers in the pipe, a wall $y^+$ value close to 1 is desirable.

Roelofs et al. conducted a sensitivity analysis using various $y^+$ values and the results of one of the studies conducted using experimental data from Yamagata et al. is provided in Figure 11 [46].
The k-ε solver with enhanced wall treatment was used for the simulation and the results show considerable variation in the temperature values based on the wall $y^+$ values. The maximum deviation from the experimental results observed was 24% using $y^+$ values of 40, while 11% deviation was observed using mesh refined to $y^+$ values of less than 1 [46]. Results from a mesh with $y^+ \leq 1$ resulted in the most accurate results. A similar approach was adopted by Shang et al. [52] in their experiments to model SCW in fuel rod bundles. A mesh sensitivity using three wall $y^+$ values was conducted and the results proved that $y^+ \leq 1$ gave the best results [54].

A point to be noted, however, is that the computational costs for conducting simulations using highly refined mesh with low $y^+$ are very high. In addition to this fact, the boundary layer refinement that is necessary to obtain low $y^+$ values has been
attempted only in the case of simple 2-D geometries involving axisymmetric sections of long cylindrical pipes, and applying the same methodology to the SCWR could be difficult at certain geometric locations of the model, according to Roelofs et al. [46].

To conclude, a large amount of literature available dealing with the physical and computational experimentation on SCW flow was reviewed to aid in the selection of the most appropriate turbulence models to ensure accurate results. Based on the articles reviewed, the Reynolds Averaged Navier Stokes (RANS) model, which includes the k-ε and k-Ѡ models, has been widely used and has provided satisfactory results. However, the main differentiation between these studies and the current project is the complex geometry of the SCWR. The majority of past work has been based on simple geometry involving long cylindrical pipes, with most variations being within the flow parameters and the heat flux applied to these systems. But in the case of the SCWR, there is the possibility of a more complex flow in contrast to the relatively simple flow fields observed in the cylindrical pipes. This has the potential to affect the heat transfer occurring in the reactor, which would consequently affect the temperature profiles in the various regions of the SCWR. Due to this complication, the second objective of this thesis is to determine which simulation model, k-ε or k-Ѡ, is best suited for the SCWR application.

The application of piecewise polynomials and piecewise linear polynomials has proved to be a good measure for modeling the variation of the thermophysical properties of SCW [27], [34], [46], [50] and can be applied in this research. Finally, the
results of the simulation are very sensitive to the quality of the mesh and the wall $y^+$ values, with $y^+$ values close to 1 having proved to give the most accurate results in the previous works. However, due to the large and complex domain of the SCWR, this may not be attainable, and a balance between the computational costs and the accuracy has to be struck in CFD simulations.

2.4 Supercritical Water as a Solvent

Although not directly incorporated into this work, SCW solvent properties will be needed to further refine the CFD model developed as part of this work. This section provides a review of inorganic compound solubility in SCW. Information from this section is used to support recommendations made in Chapter 9.

Water is a very good solvent for inorganic salt compounds at ambient temperature and pressure. Common examples of inorganic salts include sodium chloride (NaCl), calcium chloride (CaCl$_2$), potassium chloride (KCl), sodium sulfate (NaSO$_4$), and many other common salts. The scientific principle explaining ambient water’s excellent inorganic salt solvent properties is its high polarity. This is due to its high dielectric constant [60], [61] at an ambient temperature and pressure of 25° C and 0.1 MPa respectively. However, due to the large reduction in the density of the fluid at supercritical conditions, this number drops from 78.5 to around 6 [60], [61]. Bröll and Galli et al. [60]–[62] explain that this reduction is caused by the reduced hydrogen bonds at supercritical conditions, which in turn can be ascribed to the reduction in the density of the SCW. An important aspect of dissolution is the compensation for the
lattice energy of the crystals by the enthalpy of hydration of the ions in the solvent. But as the density decreases, the hydrogen-bonding network begins to break down. This causes a decrease in the permittivity of the network to accommodate a solute within its structure. As a result, there is an increase in the association levels of the oppositely charged ions (for example Na\(^+\) and Cl\(^-\)). However, due to the significant reduction in the density of water, the associated ions are not hydrated well enough compared to the individual ions [63]. This eventually results in the precipitation of the solute from the SCW. Contrarily, the solubility of organic compounds is significantly higher in SCW compared to that at ambient conditions.

It is evident after this discussion that the density of SCW has a pivotal role in deciding its properties as a solvent. The reduction in density that leads to its the loss of permittivity [63], [64] and a drop in its dielectric constant, which consequently leads to a reduction in its polarity. Therefore, at high densities, ionic bonds can be easily dissolved in SCW, while at low densities, SCW acts a good solvent for non-polar organic compounds [60].

Although F/P water contains a wide range of inorganic salts, four major cationic species are of particular interest, including sodium (Na\(^+\)), calcium (Ca\(^{2+}\)), magnesium (Mg\(^{2+}\)), and potassium (K\(^+\)). The cations are typically found in the form of chlorides, carbonates, and sulfates. Typical concentrations of these ions found in F/P water are shown in Table 7 [65], [66].
Table 7: Concentration levels of ions of interest in SCWR [65], [66]

<table>
<thead>
<tr>
<th>Ions</th>
<th>Concentration Levels (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na⁺</td>
<td>23,000-57,300</td>
</tr>
<tr>
<td>Cl⁻</td>
<td>46,100-141,000</td>
</tr>
<tr>
<td>Ca²⁺</td>
<td>2,530-25,800</td>
</tr>
<tr>
<td>Mg²⁺</td>
<td>530-4,300</td>
</tr>
<tr>
<td>K⁺</td>
<td>130-3,100</td>
</tr>
<tr>
<td>CO₃²⁻</td>
<td>2,310-5,838</td>
</tr>
<tr>
<td>SO₄²⁻</td>
<td>35-134</td>
</tr>
</tbody>
</table>

Significant work has been completed to determine, experimentally and analytically, the solubility of inorganic salts in SCW throughout the past fifty years [67]. In particular, the solubility of NaCl in SCW has been studied extensively. The solubility of NaCl in SCW at 500° C is shown in Figure 12 [67].

Figure 12: NaCl solubility in SCW [67]
Bischoff et al. and Andreko et al. have developed a cubic equation to fit the solubility of NaCl in SCW. The operating conditions for this study ranged from 12 MPa at 380° C to 40 MPa at 600° C [63]. The equation 2.17 is valid up to the melting point of NaCl (801° C).

\[ x_{NaCl\text{ satd.}} = 0.090 + 1.1183 \times 10^{-7} \times T^2 + 1.16643 \times 10^{-9} \times T^3 \]  \hspace{1cm} (2.17)

Where,

\[ x_{NaCl\text{ satd.}} = [\text{NaCl}], \% \]

\[ T = \text{Temperature, (° C)} \]

DiPippo et al. have also investigated the solubility of NaCl and NaSO₄ in SCW over the temperature range of 450-550° C and at pressures varying from 10-25 MPa and salt concentration levels of 5, 10, 15 and 20 wt.% [63], [68], [69]. The experimental results of the solubility of NaCl by DiPippo et al. are provided in Figure 13 [68].
The solubility of NaCl was then predicted using Equation 2.18. The range of applicability of this equation however is limited to a density value of < 100 kg/m³[63][67].

\[
\log C_{NaCl} = 7.772 + 3.866 \log(\rho_w) - \frac{1233.4}{T} \tag{2.18}
\]

Where,

\( C = \) Concentration, (ppm)  
\( \rho_w = \) SCW density, (g/cm³)  
\( T = \) SCW temperature, (K)

Based on the data provided by Tester et al., Savage et al. obtained the solubility of common inorganic compounds at 25 MPa [70]. Data from Savage et al. is shown in Figure 14.
Leusbrock et al. have conducted a comprehensive study on the solubility of common inorganic salts in SCW [71]–[74], [75]. The authors studied the solubility of phosphate and sulfate salts in water at a pressure range of 18.8-23.2 MPa and temperatures of 382-417° C [74]. More importantly, the solubility of chloride salts was also investigated at conditions of 18.5-23.5 MPa and 387-417° C [73]. The solubility of NaCl and KCl salts increases with SCW density, as explained in relation to the dielectric constant and hydrogen bonding by Bröll et al. and Galli et al. [60], [61], [63].

Figure 14: KCl, NaCl, and CaCl₂ solubility with temperature at 25 MPa [70]
Figure 15: NaCl, KCl, MgCl$_2$, and CaCl$_2$ solubility with water density [72], [73]
CHAPTER 3: PLAN OF WORK

3.1 Introduction

This chapter provides a reiteration of thesis objectives and a short summary of the deliverables to fulfill each objective.

3.2 Objectives and Deliverables

The purpose of this research was to conduct CFD analysis of the SCWR system to analyze and predict system heat transfer and flow patterns at select operating conditions. This required the completion of a set of objectives, which would help in ensuring that the conclusions and recommendations resulting from this work could serve as a foundation for understanding SCWR operation. This study includes three objectives, which are described in the following sections.

3.2.1 Objective 1: Develop a Supercritical Water CFD Model

The first objective was to develop an ‘ANSYS Fluent SCW CFD’ model including a 3D SCWR CAD model, user defined functions for supercritical water properties, and conductive and convective heat transfer relationships. The CFD model will provide insights regarding SCWR operation and implications of design changes on SCWR performance. ANSYS Fluent was utilized to complete this work as it is the industry standard for CFD modeling and contains a built-in energy equation sub-routine and ability to incorporate user defined functions for fluid properties.

The deliverable to fulfill this objective was a completed ANSYS Fluent SCW CFD model to be used to fulfill Objectives 2 and 3. As Fluent does not contain thermo-
physical properties for SCW, user defined property functions for SCW density; specific heat, thermal conductivity, and viscosity were incorporated. In addition, a 3D CAD drawing and mesh for the SCWR prototype are to be developed and integrated into ANSYS Fluent to fulfill Objective 3.

3.2.2 Objective 2: Compare Supercritical Water CFD Model Results with Experimental Results

The second objective was to compare supercritical CFD model results to experimental results found in peer-reviewed literature. As the SCWR geometry is unique and no experimental information is available to complete such a comparison, the CFD model geometry was modified to a straight tube configuration allowing for comparison with data available from peer-reviewed literature.

Plots comparing SCW CFD results with data from experimental results from literature were provided to fulfill this objective. Experimental data from Yamagata et al. was used for this comparison [48]. Plots provided for comparison include tube wall temperature with bulk fluid enthalpy and HTC with bulk fluid enthalpy.

3.2.3 Objective 3: Analyze SCWR System Sensitivity

The third objective was to perform sensitivity analyses on major process variables, including water inlet temperature and operating pressure using the SCWR CFD model. To evaluate the effect of inlet water temperature, simulations were conducted at 350 and 390° C, as they span the pseudocritical temperature at 24.5 MPa. As operating pressure has a significant impact on water’s heat capacity at pseudocritical
condition, simulations were completed at 23 and 26 MPa with an inlet temperature of 350° C. SCWR fluid temperature contour plots from the simulations were used to evaluate potential for TDS removal and scaling at the SCWR wall.

Temperature contours, velocity contours, flow lines, density contours, and estimated TDS solubility in the lower half of the SCWR were provided as deliverables to fulfill this objective. Temperature contours along the center of the SCWR, and SCWR wall aided in evaluating TDS solubility and SCWR mechanical integrity. Velocity contours and flow lines throughout the SCWR are provided to evaluate fluid turbulence and flow through the reactor. Density contours throughout the SCWR are provided to support velocity and flow line analysis and to estimate TDS solubility in the lower half of the SCWR. TDS solubility estimates for the lower half of the SCWR are provided based upon the density contours in this region in order to evaluate, the ability of SCWR in removing TDS from F/P water.
CHAPTER 4: OBJECTIVE 1

4.1 Introduction

The purpose of this chapter is to discuss the theory behind the governing mathematical equations and turbulence models used in Fluent to model SCW flow. In addition, a description of the model is provided, including SCWR CAD model and Fluent solver settings. In addition, the simulation setup including the development of SCWR geometry using ANSYS Design Modeler (DM), the generation of a grid for the control volume of the SCWR using ANSYS Meshing (AM), and the application of boundary conditions and material properties are provided.

4.2 CFD Model Methodology

Fluent is finite volume software that has been widely used to simulate, predict, and analyze fluid flow and heat transfer in real world problems. The Fluent solver uses basic governing equations to predict the variation of the dependent variables, such as fluid density, velocity, and other thermophysical properties, under the influence of internally or externally applied energy sources. For any basic fluid flow, the equations for the conservation of mass and momentum are solved. However, since applied heat flux is critical to achieving operating conditions, the equation for the conservation of energy is also solved in Fluent.

4.2.1 Conservation of Mass

The equation for the conservation of mass, also known as the continuity equation, is shown in Equation 4.1 [76].
\[
\frac{\delta \rho}{\delta t} + \nabla \cdot (\rho \vec{v}) = S_m
\] (4.1)

Where,
- \(\rho\) = Density of working fluid, \((kg/m^3)\)
- \(\vec{v}\) = Velocity vector of the working fluid, \((m/s)\)
- \(S_m\) = Source terms, \((kg/m^3 \cdot s)\)

The above governing equation is applicable to any three-dimensional compressible flow, which holds true for the case of the SCWR model. However, for the validation study, Equation 3.1 is reduced to a simplified form for an axisymmetric geometry. An axisymmetric geometry, is a 2D model which is entirely symmetrical around any one of the axes. The simplified 2D equation for the conservation of mass is given in Equation 3.2. The directional vectors are reduced to the longitudinal \((\delta x)\) and the radial \((\delta r)\) components, respectively.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial r}(\rho v_r) + \frac{\rho v_r}{r} = S_m
\] (4.2)

4.2.2 Conservation of Momentum

The equation for the conservation of momentum (Navier-Stokes equation) for a compressible fluid in a three-dimensional system is provided in Equation 3.3.

\[
\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\vec{t}) + \rho \vec{g} + \vec{F}
\] (4.3)

Where,
- \(\rho\) = Fluid density, \((kg/m^3)\)
- \(\vec{v}\) = Velocity vector of the working fluid, \((m/s)\)
- \(p\) = Pressure, \((kg/m \cdot s^2)\)
- \(\vec{F}\) = External forces, \((kg \cdot m/s^2)\)
- \(\vec{g}\) = Gravitational forces, \((kg \cdot m/s^2)\)

The stress tensor, \(\vec{t}\) is given by the following relation [76].
\[
\bar{\tau} = \mu \left[ (\nabla \bar{v} + \nabla \bar{v}^T) - \frac{2}{3} \nabla \cdot \bar{v} \right] I
\]
(4.4)

Where,
\( \mu \) = Molecular viscosity, (kg/m\cdot s)
\( I \) = Unit tensor

The above equation is directly applicable to the case of the SCWR, since it is a three dimensional model. For the case of the validation model, which is an axisymmetric geometry, the continuity equation can be reduced to the axial (\( \delta x \)) and the radial directions (\( \delta r \)). This is provided in Equations 3.5 and 3.6, respectively [76].

\[
\frac{\partial}{\partial t} (\rho v_x) + \frac{1}{r} \frac{\partial}{\partial x} (\rho rv_x v_x) + \frac{1}{r} \frac{\partial}{\partial r} (\rho rv_x v_r) = - \frac{\partial p}{\partial x} + \frac{1}{r} \frac{\partial}{\partial x} \left[ r \mu \left( \frac{2}{3} \nabla \cdot \bar{v} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( 2 \frac{\partial v_x}{\partial r} + \frac{\partial v_r}{\partial x} \right) \right] + F_x
\]
(4.5)

\[
\frac{\partial}{\partial t} (\rho v_r) + \frac{1}{r} \frac{\partial}{\partial x} (\rho rv_x v_r) + \frac{1}{r} \frac{\partial}{\partial r} (\rho rv_r v_r) = - \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial x} \left[ r \mu \left( \frac{2}{3} \nabla \cdot \bar{v} \right) \right] - 2 \mu \frac{v_r}{r^2} + \frac{2\mu}{3r} (\nabla \cdot \bar{v}) + \rho \frac{v_r^2}{r} + F_r
\]
(4.6)

Where,
\( \nabla \cdot \bar{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r} \)
(4.7)

The last term is valid only if swirl-dominated flows are to be experienced. This was not the case in the validation experiments, since the diameter of the flow was very small (d=10 mm) and the mass flux was considerably large (G=1,260 kg/m\(^2\)\cdot s), preventing any appreciative swirl flow in the flow geometry. However, due to low mass flow rates in the SCWR, the effect of swirl is expected to be dominant at the center of
the reactor, where the incoming fluid discharges from the inlet tube and into the main reactor vessel.

4.2.3 Turbulence Models

Turbulence is characterized by the random and chaotic behavior of a fluid, which is influenced by fluid velocity, pressure, and flow field [77]. The turbulence of a flow is dependent upon the ratio of the fluid viscosity and the flow inertia. This ratio is defined as the Reynolds number (Re). Re is used to determine flow turbulence regime and is shown in Equations 3.8 and 3.9.

\[ Re = \frac{\text{inertial forces}}{\text{viscous forces}} \]  

(4.8)

The general correlation for the Reynolds number is

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

(4.9)

Where,

\[ \rho = \text{Fluid density, (kg/m}^3) \]
\[ v = \text{Average flow velocity, (m/s)} \]
\[ L = \text{Characteristic length, (m)} \]
\[ \mu = \text{Dynamic viscosity, (kg/m} \cdot \text{s)} \]

4.2.4 Internal Flow in a Pipe

For an internal flow through a pipe or a duct, Re can be calculated using the correlation shown in Equation 3.10.

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

(4.10)

Where, \( d_h \) is the hydraulic diameter, calculated using the following relationship.

\[ d_h = \frac{4 \times A}{p} \]  

(4.11)
Where,
\[ A = \text{Cross sectional area, } (m^2) \]
\[ P = \text{Wetted perimeter, } (m) \]

For a fluid in a cylindrical geometry, the flow is considered laminar when \( Re \leq 2,300 \). Within this region of flow, the adjacent fluid layers slide past each other in an orderly pattern \[77\]. The flow is considered fully turbulent when \( Re \geq 4,000 \). In the turbulent regime, the fluid flow patterns are random and chaotic, resulting in large variations in the fluid velocity. Experiments conducted on fluid flow through pipes indicated that initially, at Reynolds numbers less than 2,300, any accidental disturbances to the flow are quickly muffled and the flow continues in a uniform path. However, as the Reynolds number approaches values beyond 2,300, the fluid flow becomes more sensitive to any disturbances occurring in the flow, resulting in sudden changes in the flow patterns and the generation of turbulence in the flow regime. This region where the Reynolds number is between 2,300 and 4,000 is known as the transitional flow regime (\( 2,300 \leq Re \leq 4,000 \)) and the Re value is often indicated as the Critical Reynolds Number.

A turbulent flow has the capability to enhance heat, mass, and momentum transfer. The chaotic behavior of fluid motion will promote effective mixing and result in high values of diffusion coefficients for mass, momentum, and heat \[77\]. Therefore, the role of turbulence is of prime importance in the functioning of the SCWR. Since the heat is being supplied from the outer walls of the reactor vessel, a lack of turbulence would result in overheating of the reactor walls.
4.2.5 Turbulence Models Applicable to SCW Flow

Three approaches may be used to model fluid flow, including Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and Reynolds Average Navier Stokes (RANS) approaches. The first, and the most computationally expensive method, is the Direct Numerical Simulation (DNS). This approach solves the Navier Stokes equation numerically without any turbulence model [76], [78].

Conversely, LES is not as computationally expensive and is useful for resolving large scales of turbulence [78]. Although this method is able to provide better accuracy compared to the RANS method, this approach is applicable only for flows with very low Reynolds numbers [78]. Furthermore, based on previous literature reviewed on SCW, the LES model has not been applied or recommended for modeling SCW flow. In terms of the mesh requirements, the LES approach can be used on relatively coarse mesh as compared to the DNS method, since large eddies are expected in the simulations. However, the mesh refinement is still higher compared to the RANS approach [76]. Another important factor to be considered is that LES is applicable only to transient simulations [76], [77].

The most widely used approach in CFD simulation of industrial applications is the Reynolds Average Navier Stokes (RANS) approach [76], [78]. As its name suggests, the RANS approach involves the application of the mean flow properties for the solving of the Navier Stokes equation and for the closure of any transport equations used to model turbulence [77]. This makes it the most computationally feasible method out of
the three models. Due to its computational feasibility and its applicability in complex geometries, the RANS method is applicable to a wide range of control volumes involving wall bounded flows of varying velocities [76], [78], [79].

The two turbulent models that have been known to give reasonably accurate results are the k-ε and the k-ω. These are discussed in the following sections.

4.2.5.1 RANS k-ε Model

The k-ε model solves two additional transport equations for turbulent kinetic energy (k) and the turbulence dissipation rate (ε) [76]. The turbulent kinetic energy is the measure of intensity of turbulence in a fluid flow. As the term suggests, it is the measure of the kinetic energy contained within the turbulent region of a fluid flow [76].

The turbulence dissipation rate, on the other hand, is defined as the rate at which the turbulent kinetic energy is dissipated in the form of internal energy within the system, such as thermal energy. These two parameters are the basis of the k-ε turbulence modeling [44], [54], [76], [80].

\[
\begin{align*}
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) &= \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon & (4.12) \\
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon u_i) &= \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} \left( G_k + C_{3\varepsilon} G_b \right) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} & (4.13)
\end{align*}
\]

Where, \( \mu_t \) is the turbulent viscosity, calculated using the following equation:

\[
\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon} & (4.14)
\]

The terms \( G_k \) and \( G_b \) denote generation of turbulent kinetic energy due to mean velocity and buoyancy, respectively [76].
As explained in the ANSYS Theory Guide [76], the model constants were derived from experiments conducted on fundamental fluid flows such as boundary layers, mixing layers and jets, in addition to wall bounded flows, which are frequently encountered in nature and consequently in various engineering applications. These constants are as follows.

\begin{align*}
C_\mu &= 0.09 \\
C_{1\varepsilon} &= 1.44 \\
C_{2\varepsilon} &= 1.92 \\
\sigma_k &= 1.0 \\
\sigma_\varepsilon &= 1.3
\end{align*}

As cited in Chapter 2, this model has been widely used to simulate SCW flow in heated tubes and has provided accurate results. However, the accuracy of the simulation is contingent on the complete resolution of the boundary layer along the wall region. The solver has a number of options for incorporating wall treatment functions based on the wall \( y^+ \) values. Buoyancy is also expected to play a role in defining the flow patterns in the SCWR, since there are large variations in the density of SCW. The k-\( \varepsilon \) model has the ability to take these buoyancy effects into consideration, hence providing a more realistic flow and temperature profile. One disadvantage of the k-\( \varepsilon \) method is its poor solving capability at high-pressure gradients [78]. This, however, is not expected to be an issue for the SCWR simulation, since the variation of the pressure within the system is negligible compared to the operating pressures.
4.2.5.2 RANS k-ω Model

The k-ω model although similar to the k-ε, involves the transport equations for the calculation of turbulent kinetic energy (k) and specific dissipation rate (ω).

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

(4.15)

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

(4.16)

Where \( \Gamma_k \) and \( \Gamma_\omega \) represent the effective diffusivity of k and \( \omega \) due to turbulence, respectively. \( Y_k \) and \( Y_\omega \) are the dissipation rates of k and \( \omega \) due to turbulence. The effective diffusivities for the k-ω model are given by the following correlations.

\[
\Gamma_k = \mu + \frac{\mu_t}{\sigma_k}
\]

(4.17)

\[
\Gamma_\omega = \mu + \frac{\mu_t}{\sigma_\omega}
\]

(4.18)

Where \( \sigma_k \) and \( \sigma_\omega \) are turbulent Prandtl numbers for k and \( \omega \) [76].

Overall, the k-ω model is known for its robustness and accuracy [78]. A prime advantage of this method is its wall \( y^+ \) insensitivity, meaning wall refinement is not needed to resolve the boundary layer flow. As a result, the k-ω approach is much more numerically stable and is easier to implement [76], [78]. The k-ω model is also able to perform well under adverse pressure gradients. One major disadvantage of this method is its inability to take the buoyancy effects into consideration. Despite this drawback, the k-ω mode has been widely used to model SCW flows in the past. However, the accurate results could be credited to the lack of effects of buoyancy since the flow was in a very small cross sectional area (d=10 mm) and at extremely high flux (G>1,200 kg/m²·s).
In the case of the SCWR, the mass flux values will be at extremely low ranges (~10 kg/m²·s) compared to those evaluated in literature [8], [30], [32], [33], [37], [43], [45]. As a result, the effects of buoyancy in the flow were expected to be strong. At these conditions, the k-ω model would result in inaccurate flow patterns and temperature profiles in the SCWR due to its inability to include buoyancy effects. Due to this important factor, the k-ω model was not selected for this research and all simulations were conducted using the k-ε turbulence model.

4.3 SCWR Methodology

The SCWR geometry used for this research was based on a bench-scale design being developed at Ohio University (OHIO). The dimensions of the reactor are provided in Figure 16. The region of interest, also known as the control volume, is the space occupied by the fluid inside the SCWR. The governing equations of fluid flow, momentum, and heat transfer are applied and solved for this control volume. The size of the control volume, along with the number of discretized cells in a mesh, determines the computational cost of the simulations. The larger the size of the fluid domain, the larger the number of cells required to discretize it in order to obtain a mesh with a good enough quality to accurately represent and predict the temperature and flow patterns. As a result, a smaller control volume would require fewer cells in the mesh and, consequently, less time to solve a fluid flow problem. In this study, the symmetry of the SCWR vessel about the y-axis was used to reduce the mesh elements by 50%. This was achieved by modeling only half of the geometry and applying a symmetrical boundary
condition on the other non-modeled half of the geometry. Through this approach, it was possible to reduce the computational time in both the meshing process as well as in the solver time. More importantly, the integrity of the domain was not compromised since the symmetrical boundary condition would apply the same turbulence and heat transfer patterns on the non-modeled half of the reactor.

Figure 16: SCWR CAD Model (All dimensions are in inches)

The geometric dimensions of the SCWR model, which are required at the boundary conditions of Fluent solver, are provided in Table 8.
Finally, the named selections are generated, since these are required to supply the boundary conditions in the Fluent solver. In the case of the SCWR, the named selections required are the inlet, two outlets, and the heated surface. These are shown in Figure 17.

Table 8: SCWR size matrix

<table>
<thead>
<tr>
<th>Section</th>
<th>Dimensions (inches)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Diameter</td>
<td>0.5” (1.27 cm)</td>
</tr>
<tr>
<td>Outlet Diameter</td>
<td>0.25” (0.635 cm)</td>
</tr>
<tr>
<td>Wall Thickness</td>
<td>1.1” (2.8 cm)</td>
</tr>
</tbody>
</table>

![Figure 17: Named selections in SCWR geometry](image)
4.4 SCWR Mesh

To develop a computational grid for the SCWR, an inbuilt application ANSYS Meshing (AM) was used. Based on the literature review [46], [52], [54], [81], [82], the mesh along the walls has to be refined to ensure that complete resolution of the boundary layer is accomplished and accurate flow pattern and heat transfer predictions are achieved. This requires significant computational effort in developing a grid with wall $y^+ \leq 1$.

![Figure 18: Wall inflation in the case of Yamagata et al. validation experiment](image)

The computational grid generated for the SCWR vessel is shown in Figure 19.
One major limitation of boundary layer inflation is the significant rise in the computational time of the simulation. This is due to the greater number of cells in the computational grid. To ensure a balance between accuracy and computational effort, only walls with adjacent high-speed flows were implemented with mesh inflation settings. SCWR sections using mesh inflation included all the wall-bounded domains of the reactor vessel. Even though the walls of the reactor are the source of heat, the relatively low velocities at the walls will not result in sudden velocity changes, ensuring steady conjugate heat transfer that does not require mesh inflation. The mesh inflation applied on the SCWR inlet and outlet sections is shown in Figure 20.
To evaluate the effect of mesh settings on simulation results a mesh dependence study was completed. A set of independent grids ranging from 3 to over 11 million cells were generated and solved. The grid size matrix is provided in Table 9. Results from the mesh dependence study are discussed in Chapter 6.

<table>
<thead>
<tr>
<th>Mesh#</th>
<th>Nodes</th>
<th>Cells</th>
<th>Average Orthogonal Quality</th>
<th>Average Skewness</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>684,134</td>
<td>3,544,133</td>
<td>0.79</td>
<td>0.32</td>
</tr>
<tr>
<td>2</td>
<td>1,085,042</td>
<td>5,428,740</td>
<td>0.86</td>
<td>0.21</td>
</tr>
<tr>
<td>3</td>
<td>1,557,127</td>
<td>7,876,037</td>
<td>0.87</td>
<td>0.22</td>
</tr>
<tr>
<td>4</td>
<td>1,961,630</td>
<td>11,010,969</td>
<td>0.86</td>
<td>0.21</td>
</tr>
</tbody>
</table>
4.5 Fluent Solver Settings

After the mesh was generated, it was imported into the Fluent solver setup. A steady state solver method was selected; as these results would be the most appropriate to evaluate SCWR performance.

4.5.1 Material Properties

To define SCW properties, a set of user-defined functions was developed and implemented in ANSYS Fluent using a linear piecewise methodology. Using this approach, the various thermophysical properties of SCW were defined as a function of temperature. Since the SCWR operation was assumed to be an isobaric process, as previously discussed, the density, specific heat, thermal conductivity, and viscosity properties were defined as independent function sets based upon pressure. The data referenced to develop the function sets was provided by the National Institute of Standards and Technology (NIST) RefProp, which contains water properties ranging from 0-1,500° C and 0-100 MPa [83]. The complete list of data points selected for this study is provided in the appendix. For the material of the SCWR shell, stainless steel was selected with a fixed thermal conductivity of 18W/m²·k, from the default Fluent material database.

4.5.2 Boundary Conditions

Boundary conditions were applied to each named section of the SCWR. The simulation is initiated using a set of provided property values. In this thesis study, two inlet temperatures (350 and 390° C) were evaluated.
Table 10 & Table 11 present the simulation settings used for each inlet temperature study.

Table 10: SCWR test matrix at 350° C inlet

<table>
<thead>
<tr>
<th>Named Selection</th>
<th>Cell Zone Type</th>
<th>Material</th>
<th>Boundary Condition</th>
<th>Velocity (m/s)</th>
<th>Temperature (° C)/Heat Flux (W/m²)</th>
<th>Hydraulic Diameter (m)</th>
<th>Wall Thickness (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>Fluid</td>
<td>SCW</td>
<td>Velocity inlet</td>
<td>0.015</td>
<td>350° C</td>
<td>0.0127</td>
<td>N/A</td>
</tr>
<tr>
<td>Outlet(s)</td>
<td>Fluid</td>
<td>SCW</td>
<td>Outflow</td>
<td>N/A</td>
<td>N/A</td>
<td>0.00635</td>
<td>N/A</td>
</tr>
<tr>
<td>Heated Surface</td>
<td>Solid</td>
<td>Steel</td>
<td>Wall</td>
<td>N/A</td>
<td>15000 W/m²</td>
<td>N/A</td>
<td>0.02794</td>
</tr>
<tr>
<td>Inlet Tube</td>
<td>Solid</td>
<td>Steel</td>
<td>Wall interface</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>0.02794</td>
</tr>
</tbody>
</table>

Table 11: SCWR test matrix at 390° C inlet

<table>
<thead>
<tr>
<th>Named Selection</th>
<th>Cell Zone Type</th>
<th>Material</th>
<th>Boundary Condition</th>
<th>Velocity (m/s)</th>
<th>Temperature (° C)/Heat Flux (W/m²)</th>
<th>Hydraulic Diameter (m)</th>
<th>Wall Thickness (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>Fluid</td>
<td>SCW</td>
<td>Velocity inlet</td>
<td>0.05</td>
<td>390° C</td>
<td>0.0127</td>
<td>N/A</td>
</tr>
<tr>
<td>Outlet(s)</td>
<td>Fluid</td>
<td>SCW</td>
<td>Outflow</td>
<td>N/A</td>
<td>N/A</td>
<td>0.00635</td>
<td>N/A</td>
</tr>
<tr>
<td>Heated Surface</td>
<td>Solid</td>
<td>Steel</td>
<td>Wall</td>
<td>N/A</td>
<td>15000 W/m²</td>
<td>N/A</td>
<td>0.02794</td>
</tr>
<tr>
<td>Inlet Tube</td>
<td>Solid</td>
<td>Steel</td>
<td>Wall interface</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>0.02794</td>
</tr>
</tbody>
</table>

4.6 CFD Results Processing

CFD results are processed using CFD Post, which is an inbuilt application in ANSYS Workbench. Using CFD Post, high quality contours, streamlines, and vectors for analyzing and presenting flow patterns can be obtained. In addition, the inbuilt export option enables it to export a vast range of data points for various properties, such as
temperature, velocity, and density, to create high-definition plots. The post-processed results used in this research include a series of temperature, velocity, and density contours of the reactor. These parameters will play a major role in understanding and predicting the salt precipitation inside the reactor. The density of the fluid at a specific region can provide an estimate of the solubility of the salts at that region. Furthermore, the velocity contours can be used to determine if the turbulence is low enough at the bottom of the reactor to facilitate easy collection of the separated salt content. In addition to these contours, temperature plots were also created to estimate the heat transfer profile along the walls of the reactor in order to locate enhanced and deteriorated heat transfer regions with the help of HTC plots. With the aid of all these results, it was possible to come to conclusions on the applicability of the system and the safety of the operating conditions of the reactor.
CHAPTER 5: OBJECTIVE 2

5.1 Introduction

This chapter provides a comparison of supercritical water CFD model results with experimental data from peer-reviewed literature. A comparison of CFD model results with experimental data is necessary to demonstrate that the model is capable of predicting supercritical water system behavior. As the SCWR is a unique design with no existing experimental data available for comparison, the existing CFD model was modified to represent a heated vertical tube configuration for comparison with existing experimental data. The article titled “Forced convective heat transfer to SCW flowing in tubes” by Yamagata et al. was selected for comparison purposes.

The paper used the same materials for the operating fluid (SCW) and test section material, as the SCWR pilot plant being developed at OHIO. In addition, the paper included the use of operating pressure and inlet temperature, which were very similar to the operating conditions at in the SCWR. The experiment also used a range of heat flux values, which would help in understanding the applicability of the SCWR CFD model at a wide range of heat load conditions. Information discussed in this chapter includes the experimental/simulation setup and a comparison between experimental/simulation wall temperatures with bulk enthalpy, heat transfer coefficient behavior, and mesh refinement to improve CFD accuracy.
5.2 Objective 2 Methodology

The experimental setup from Yamagata et al. is shown in Figure 21 [32]. The test section was a 2 m long AISI type 316 stainless steel tube with a 7.5 mm internal diameter and a 2 mm thick wall.

![Diagram of Yamagata et al. experimental test apparatus](image)

Figure 21: Yamagata et al. experimental test apparatus [32]

This test section was operated in a vertically upright position. A series of 21 thermocouples was attached at various uniform intervals along the external wall of the test section. The test section was externally heated using resistive heating applied only to the surface of the test section, with insulated flanges located at the tube inlet/outlet.
The experimental test parameters and configurations used by Yamagata et al. are provided in Table 12 [32].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>22.6 MPa, 24.5 MPa, and 29.4 MPa</td>
</tr>
<tr>
<td>Bulk fluid temperature range</td>
<td>230-540°C</td>
</tr>
<tr>
<td>Heat flux</td>
<td>116-930 kW/m²</td>
</tr>
<tr>
<td>Mass flux</td>
<td>310-1830 kg/m²·s</td>
</tr>
<tr>
<td>Flow direction</td>
<td>Horizontal, vertically upward and downward</td>
</tr>
</tbody>
</table>

For comparison with the CFD model developed in this research, four tests were selected and replicated in Fluent. The results were compared with the corresponding test data. The experimental parameters of the comparative trials are provided in Table 13 [32]. Only vertical flow geometries were selected for this comparison, as these best represent SCWR flow orientation. To heat the SCW to the desired temperatures, the 1.5 m length test section was not sufficient. As a result, the outlet water was recycled to the inlet until the desired outlet temperatures were obtained. Plots were then constructed to present wall temperature with bulk fluid enthalpy, calculated based on the heat added to the system at the position of the respective thermocouple.
### Table 13: Comparison simulation parameters [32]

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Flow Orientation</th>
<th>Inlet Temperature (°C)</th>
<th>Mass flux (kg/m²⋅s)</th>
<th>Heat flux (kW/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Vertically upward</td>
<td>340</td>
<td>1260</td>
<td>233</td>
</tr>
<tr>
<td>2</td>
<td>Vertically upward</td>
<td>340</td>
<td>1260</td>
<td>465</td>
</tr>
<tr>
<td>3</td>
<td>Vertically upward</td>
<td>340</td>
<td>1260</td>
<td>698</td>
</tr>
<tr>
<td>4</td>
<td>Vertically upward</td>
<td>340</td>
<td>1260</td>
<td>930</td>
</tr>
</tbody>
</table>

The geometry of the comparative CFD model is shown in Figure 22. Here, \( d \) is the inner diameter of the test pipe section, and \( H \) is the effective height of the pipe. For each of the four cases, Yamagata et al. employed the same test section with a 1.5 m length [32]. In the case of the Fluent setup, the effective height \( (H_e) \) of the tube needed to reach the specified outlet temperature was calculated by using the inlet and outlet temperatures for each case as well as the applied heat flux. The inlet and outlet temperatures of each case were used to calculate the total enthalpy in the system and derive the height of the tube required for each of the four cases that were taken into consideration.
Details of $H_e$ calculation are provided in the appendix. $H_e$ values estimated for each case are presented in Table 14.

Table 14: CFD comparison case effective heights

<table>
<thead>
<tr>
<th>Case</th>
<th>$H_e$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>9.8</td>
</tr>
<tr>
<td>2</td>
<td>6.7</td>
</tr>
<tr>
<td>3</td>
<td>3.7</td>
</tr>
<tr>
<td>4</td>
<td>1.2</td>
</tr>
</tbody>
</table>

The CFD model geometry was designed such that it is axisymmetric about the x-axis. This helped in reducing the computational domain and, as a result, the time required to solve the simulation. The mesh section of the geometry is shown in Figure 23. The wall region of the pipe along the y-axis, was meshed with inflation layers to resolve the boundary layer flow. Since heat transfer initiates from the walls, it is
important to have a highly refined mesh in this region as the heat transfer dynamics are much greater at the wall surface compared to the table bulk fluid flow region.

Wall $y^+$ values $\leq 1$ were attained along the entire wall length for each of the four geometry models used in the simulations. Wall $y^+$ values $\leq 1$ are necessary for generating a mesh capable of producing high resolution temperature and flow field pattern profiles along the wall region [33], [46], [52], [81], [82].

Figure 24 presents the $y^+$ values along the wall for each simulation case and shows that each mesh will provide acceptable resolution.
SCW properties were derived from the NIST RefProp software, which is based on the IAPWS standards [83]. The simulation was solved using the steady-state k-ε solver with enhanced wall treatment to account for the refined mesh generated near the wall regions of the fluid flow. The wall was modeled as a stainless steel surface using conductivity values from the Fluent property database. The boundary conditions were applied as per the test matrix in Table 13. The simulations converged after approximately 800 iterations. The results were post-processed and are provided in the following section.

5.3 CFD Model Comparison with Experimental Data

To evaluate the supercritical CFD model’s capability of predicting supercritical water system behavior, results from the CFD model were plotted with experimental results from Yamagata et al. Figure 25 presents both model and experimental results plotted as tube wall temperature against bulk fluid temperature at the respective
location of the thermocouple. Model results are plotted as smoothed lines, while experimental results are shown as individual data points. The summed square of residuals SSR was calculated for each of the cases using the following equation.

\[
SSR = \sum_{i=0}^{n}(y_i - \hat{y}_i)^2
\]  

(5.1)

Where,

\( i \) = Number of data points; for this study, 55 data points were selected for each case
\( y_i \) = Experimental wall temperature at select bulk fluid enthalpy
\( \hat{y}_i \) = CFD wall temperature at corresponding bulk fluid enthalpy

In addition to the SSR, the Total Sum of Squares (SST) was also calculated using the following statistical correlation.

\[
SST = \sum_{i=0}^{n}(y_{mean} - y_i)^2
\]  

(5.2)

Finally, the SST and SSR were used to calculate the \( R^2 \) values for each case using the following equation.

\[
R^2 = \frac{SST - SSR}{SST}
\]  

(5.3)

The \( R^2 \) values for the four cases are shown in Table 15.
Figure 25: Comparison of CFD model results with experimental data from Yamagata et al [32].

Table 15: $R^2$ values between model and experimental results

<table>
<thead>
<tr>
<th>Case</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.98</td>
</tr>
<tr>
<td>2</td>
<td>0.98</td>
</tr>
<tr>
<td>3</td>
<td>0.82</td>
</tr>
<tr>
<td>4</td>
<td>0.89</td>
</tr>
</tbody>
</table>

The CFD model profiles of all four cases follow those of the experimental data, indicating that the CFD model can predict supercritical water behavior flowing vertically under externally heated conditions. The discrepancy between the model and experimental results can be largely attributed to the piecewise polynomials used to define fluid properties as a function of temperature, as ANSYS Fluent only allows 50
data points to be used to define the functions. Due to the dramatic change in physical properties near the pseudocritical point, the piecewise polynomials have inherent limitations in their ability to precisely model physical properties in this transition region.

As seen in Figure 25, the CFD model over-predicted wall temperatures in Cases 3 and 4. The greater error associated with Cases 3 and 4 is believed to be caused by the larger heat fluxes (698 and 930 kW/m$^2$, respectively) as compared to Cases 1 and 2. These larger heat fluxes at the same mass flux cause greater heating, resulting in more significant changes in fluid density, turbulence, and heat transfer along the tube wall surface. The larger errors observed in Cases 3 and 4 are a result of both user-defined property functions and meshing at the tube wall interface.

To determine if meshing at the tube wall interface limited the model’s capability of predicting Case 3 behavior mesh refinement was evaluated. Any additional refinement at the wall region would have resulted in large variation in cell sizes at the interface and the bulk fluid region. This would have resulted in poor mesh quality, leading to discretization errors and mesh check failure errors. Therefore, to further refine the mesh, the minimum cell size was decreased by two orders of magnitude. Details of the evaluated meshes are provided in Table 16. The simulations were completed with the same conditions as Case 3 in Table 13.
Table 16: Mesh refinement parameters

<table>
<thead>
<tr>
<th>Case</th>
<th>Minimum Cell Size</th>
<th>Cell Count</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard</td>
<td>0.25</td>
<td>275,000</td>
</tr>
<tr>
<td>Mesh 2</td>
<td>0.01</td>
<td>4,000,000</td>
</tr>
<tr>
<td>Mesh 3</td>
<td>0.005</td>
<td>12,000,000</td>
</tr>
</tbody>
</table>

The results of the simulations are shown in Figure 26 and maximum errors are provided in Table 17. It can be observed that the mesh refinements reduce model prediction error. However, mesh refinement does come at a cost of additional computation time, as shown in Table 17. Based on the results, Mesh 3 would not be considered efficient, as it provided minimal improvement in model accuracy while increasing computational time by over 650%.

Figure 26: Mesh refinement results for case 3 of Yamagata et al.
Table 17: $R^2$ values and computational time based upon model meshing

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$R^2$</th>
<th>Computation Time (hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard</td>
<td>0.82</td>
<td>1:50</td>
</tr>
<tr>
<td>Mesh 2</td>
<td>0.95</td>
<td>6:00</td>
</tr>
<tr>
<td>Mesh 3</td>
<td>0.96</td>
<td>15:00</td>
</tr>
</tbody>
</table>

Figure 27 shows the comparison of the HTC values obtained for all the 4 cases, using the CFD model and the corresponding experimental data points. The HTC calculations were a function of the bulk fluid and the wall temperature values along the length of the test section. The results show the developed SCW CFD model is able to adequately predict HTC behavior near the supercritical point under the various heat flux conditions.

Figure 27: Case 1 model and experimental HTC Values [48]
6.1 Introduction

The third objective of this thesis was to develop a prototype-scale SCWR simulation and investigate parameters such as inlet temperature and operating pressure on SCWR operation. The results presented in this chapter are used to fulfill this objective. First, SCWR results at inlet temperatures of 350° C and 390° C at 24.5 MPa are presented, followed by results at 23 MPa and 26 MPa at an inlet temperature of 350° C.

6.2 Objective 3 Methodology

Details regarding the CFD modeling methodology used in the completion of Objective 3 are provided in Chapter 4.

6.3 350° C Inlet Temperature Simulation Results

The first simulation evaluated water entering the SCWR at 350° C and 24.5 MPa, which is below the water’s pseudocritical point at 381° C. Three simulations were completed using 3M, 5M, and 8M cell meshes. Details of the simulations’ boundary conditions are provided in Table 10. Simulation results presented include temperature contour plots at the SCWR’s center and wall region, axial temperature profiles along the inlet tube, wall HTC contours, velocity contours, density contours, and estimated TDS solubility.
6.3.1 Temperature Contours

Fluid temperature contours were plotted on the surface of the SCWR labeled as 'symmetry. The wall temperatures from simulations containing 3M, 5M and 8M cells are shown in Figure 28-Figure 30. All meshes show similar patterns at the symmetry region and at the wall of the SCWR. Increasing mesh size gave marginally better temperature contour resolution but resulted in an approximately 400% increase in the computation time for the case of the 5M cell mesh and a 1,100% increase in the case of the 8M cell count mesh setting.

Figure 28: Temperature contours of the SCWR with 350°C inlet at 24.5 MPa along (a) Symmetry and (b) SCWR wall regions: 3M mesh settings
Figure 29: Temperature contours of the SCWR with 350° C inlet at 24.5 MPa along (a) Symmetry and (b) SCWR wall regions: 5M mesh settings

Figure 30: Temperature contours of the SCWR with 350° C inlet at 24.5 MPa along (a) Symmetry and (b) SCWR wall regions: 8M mesh settings
The temperature profile along the SCWR longitudinal axis is provided in Figure 31. The temperature rise of the water is gradual inside the inlet tube. However, a more rapid temperature rise is observed after the water exits the inlet tube and moves into the reactor vessel. This can be credited to the strong mixing, shown in Section 7.3.2, due to the effects of buoyancy forces. As the temperature increases, the density of SCW drops. This reduction in density is responsible for the large buoyancy effects, since the lighter fluid rises and the denser fluid descends, resulting in the flow patterns that are evident in this simulation. In addition, water within the inlet tube stays below the pseudocritical temperature, minimizing scaling of the inlet tube by precipitating TDS. In addition, the temperature of the water at the center of the reactor rises above pseudocritical temperature. Based on the literature from Savage et al. and Leusbrock et al. [73], [75], the solubility of the TDS can be expected to be significantly lower at the temperatures seen in the central portion of the reactor [70] as shown in Section 7.3.4.
The wall temperature profile along the longitudinal axis is provided in Figure 32. The maximum temperature along the wall approached 460° C in all cases. The temperature along the walls was considerably higher in the top half, while the wall temperature values were lower in the bottom half. This is due to the lack of turbulence and mixing in the top half of the reactor, as shown in Section 7.3.2. In the bottom SCWR region, the incoming flow from the inlet tube results in turbulence, causing a swirling vortex and diffusive forces and resulting in more mixing. In addition, as the water heats, its density decreases, causing further turbulence as the lighter fluid starts moving upwards (in positive y-axis direction). The residence time of the fluid in the bottom
portion of the SCWR will be lower due to the constant turbulence observed in this region.

Figure 32: Wall temperature profile of the SCWR at 350°C inlet at 24.5 MPa

Figure 33 shows calculated wall HTC values for the SCWR. The HTC values in the top half of the SCWR are significantly lower compared to the corresponding values in the lower half. This can be explained using the turbulence and fluid flow patterns shown in Figure 38. Since constant mixing is present in the bottom of the reactor, a lower temperature gradient, caused by turbulence, results in higher HTCs. However, above the inlet point of the fluid (y ≥ 0.1075 m), there is very little disturbance observed in the
fluid flow. As a result, this region is dominated by a high temperature gradient between the wall and the bulk temperature, leading to significantly lower HTC values.

![Figure 33: Wall HTC values for the SCWR with 350° C inlet at 24.5 MPa](image)

6.3.2 Turbulence Intensity

The turbulence intensity is defined as the ratio of the fluctuations of the turbulent velocities in a cell to the Reynolds Average velocity of the fluid domain. Figure 34 shows the variation in the turbulence, alongside the turbulence contours expected in the center of the SCWR at the 350° C inlet condition. Figure 35 is also provided to show the turbulence intensity plot with respect to the location on the y-axis, at the center of the SCWR. As the water enters the SCWR through the inlet tube the water transitions to
supercritical state. This heating results in a dramatic decrease in fluid density resulting in high turbulence at the outlet of inlet tube.

Figure 34: Turbulent Intensity in SCWR operating at 24.5 MPa at 350 °C inlet conditions using 5M cell mesh
Figure 35: Turbulence intensity along y-axis location in the SCWR operating at 24.5 MPa and 350°C inlet condition

6.3.3 Velocity Contours

Figure 36-Figure 38 present the velocity contours and flow lines for 350°C inlet at 24.5 MPa with meshes containing 3-8M cells. The greatest area of turbulence was located below the exit of the inlet tube. This turbulence was a result of the water being heated above its pseudocritical state, causing a large density decrease, from 600 kg/m$^3$ to 150 kg/m$^3$, as shown in Section 7.3.3. The buoyancy effects caused by the density decrease are evident and cause the swirling motion of the fluid immediately entering the center of the reactor.

It can be observed that there was a lot of variation in the velocity vectors among the 3 mesh settings. This was to be expected, due to the large variations in the
thermophysical properties of SCW before the pseudocritical point. As a result, the Fluent solver reached stagnation points during the iterations to resolve the continuity equation, causing the velocity profiles to vary at each of the three mesh settings. This can be seen more clearly using the velocity profile along the centerline of the SCWR, as shown in Figure 39. A point to be noted is that the variation in the velocity patterns indicates the instability of Fluent in converging the flow; however, the ranges of velocities in each of the three cases can be observed to be similar, which indicates that mesh independence was achieved by this point and that any further changes in mesh settings would not have resolved the flow any further.

Figure 36: (a) Velocity contours and (b) flow lines in the SCWR with 350° C inlet at 24.5 MPa conditions: 3 million cells mesh setting
Figure 37: (a) Velocity contours and (b) flow lines in the SCWR with 350° C inlet at 24.5 MPa conditions: 5 million cells mesh setting
Figure 38: (a) Velocity contours and (b) flow lines in the SCWR with 350° C at 24.5 MPa conditions: 8 million cells mesh setting
6.3.4  Density Contours

The density contours for 5-8M cell meshes are provided in Figure 40- Figure 42. A large decrease in fluid density from the tube inlet into the center of the SCWR can be observed, which corresponds with the fluid transitioning beyond its pseudocritical point. This results in strong buoyancy forces, consequently giving rise to swirling flow in the bottom half of the reactor, as shown in Section 7.3.2.
Figure 40: Density contours in the SCWR with 350° C at 24.5 MPa: 3M cells

Figure 41: Density contours in the SCWR with 350° C at 24.5 MPa: 5M cells
Density plots along the center of the SCWR vessel are provided in Figure 43. These plots provide a quantitative means of observing the density decrease of fluid. As seen in the plots for density and specific heat (Figure 5), a large reduction in density is expected along the pseudocritical region, with a density of between 600 kg/m$^3$ at the inlet to approximately 150 kg/m$^3$ at its lowest value observed in the reactor. The drop in SCW density results in large buoyancy effects. The fluid motion helps in the mixing of the fluid and results in a more diverse temperature pattern at the bottom of the SCWR as compared to its top half.
The density of the fluid along the centerline of the SCWR does show slight sensitivity to the mesh setting. Meshes with 5M and 8M cells are essentially converged, while the 3M mesh simulation shows some variation as the fluid traverses the pseudocritical point. It can be observed in the plots from Figure 31, Figure 32, Figure 33, Figure 39, and Figure 43 that the variation in the results observed between the 5M cell mesh and 8M cell mesh settings is not as high as that seen between the 3M cell and 5M cell mesh settings.

Figure 43: Density profile along the centerline of the SCWR for 350° C inlet at 24.5 MPa
6.3.5 Estimated TDS Solubility

Based on the temperature and density of the fluid in the reactor, it was possible to estimate TDS solubility using solubility data available from literature. However, the data available from Leusbrock et al. [72], [73], [75] is limited to the range of 20-175 kg/m$^3$. Such low densities were not achieved in this simulation. As a result, the expected solubility in the lower half of the SCWR vessel was estimated using the data from Savage et al. [70]. The solubility was estimated using the bulk temperature values in the lower section of the reactor, immediately below the inlet tube, as shown in Figure 44.

Figure 44: SCWR lower section for 350° C inlet at 24.5 MPa
Using FLUENT post-processing, the bulk temperature values were calculated along the centerline of the reactor and are provided in Figure 45. The values below the inlet tube (\(y \leq 0.1075\) m) were used to estimate the solubility of the TDS. These values are presented in Table 18. The results from this simulation indicate that the SCWR has the potential to remove a significant portion (~90%) of TDS contained in F/P water under the prescribed boundary conditions.

Table 18: Estimated TDS solubilities at the bottom half of the SCWR for 350° C inlet at 24.5 MPa

<table>
<thead>
<tr>
<th>Salt</th>
<th>Inlet Concentration (ppm)</th>
<th>Solubility at SCWR Bottom (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaCl</td>
<td>&gt;150,000</td>
<td>&gt;10,000</td>
</tr>
<tr>
<td>CaCl₂</td>
<td>30,000</td>
<td>&gt;10,000</td>
</tr>
<tr>
<td>KCl</td>
<td>50,000</td>
<td>&gt;10,000</td>
</tr>
<tr>
<td>MgCl₂</td>
<td>50,000</td>
<td>~1000</td>
</tr>
</tbody>
</table>
6.4 390° C Inlet Temperature Simulation Results

This section presents SCWR simulation results for an inlet temperature of 390° C at 24.5 MPa. The boundary conditions used in the simulation are provided in Table 11. Simulation results presented include temperature contour plots at the SCWR’s center and wall region, axial temperature profiles along the inlet tube, wall HTC contours, velocity contours, density contours, and estimated TDS solubility.

Figure 45: Bulk temperature profile for 350° C inlet at 24.5 MPa
6.4.1 Temperature Contours

Fluid temperature contours in the center of the SCWR and reactor wall temperatures from simulations containing 3-8M cells are shown in Figure 46-Figure 48. Simulation sensitivity to mesh size is more noticeable in the present case. This behavior is caused by the fluid entering the SCWR above the pseudocritical temperature, which results in a rapid decrease in the fluid’s specific heat. For the same amount of heat flux, a much larger temperature rise occurs, approximately 300° C, and there is a corresponding drop in density, resulting in greater velocity entering the center of the SCWR.

Figure 46: Temperature contours of the SCWR with 390° C inlet at 24.5 MPa along 
(a) Symmetry and (b) SCWR wall region: 3M mesh settings
Figure 47: Temperature contours of the SCWR with 390°C inlet at 24.5 MPa along (a) Symmetry and (b) SCWR wall region: 5M mesh settings

Figure 48: Temperature contours of the SCWR with 390°C inlet at 24.5 MPa along (a) Symmetry and (b) SCWR wall region: 8M mesh settings
The wall temperature profile for this case, Figure 50, indicates that the fluid will heat to a nearly uniform temperature along the walls of the reactor, with a very low temperature variation (~15° C). This was not the case at the 350° C inlet condition, where a temperature variation of approximately 75° C was observed. In addition, extreme heating over the entire area of the vessel is observed, which is expected as the specific heat of SCW decreases from 115 kJ/kgK to a range of 2-4 kJ/kgK.

Figure 49: Axial temperature profiles along the y-axis, for the SCWR for 390° C inlet at 24.5 MPa
6.4.2 Turbulence Intensity

The turbulence experienced in this system was much lower than in the previous case of 350 °C inlet condition. This can be explained due to lower drop in operating densities in this case. The contour for turbulence are provided in Figure 51 and Figure 52.
Figure 51: Turbulent Intensity in SCWR operating at 24.5 MPa at 350 °C inlet conditions using 5M cell mesh

Figure 52: Turbulence intensity with y-axis location in the SCWR operating at 24.5 MPa and 350 °C inlet condition
6.4.3 Velocity Contours

Figure 53-Figure 55 present the velocity contours and flow lines for this case. A large amount of agitation is observed in the inlet tube region of the SCWR, as opposed to the swirling vortex seen in the lower half of the SCWR in the case of a 350° C tube inlet. Ideally, the flow in the inlet tube must be stable and smooth, as any agitation, when combined with low density conditions at the inlet tube, would result in a large amount of precipitation in the inlet tube region. This could result in the clogging of the tube with precipitates and eventual backflow in the system. Additionally, a large difference between the 3M and 5M/8M mesh cases can be observed. In the 3M mesh case, the flow field is not as well developed compared to the other cases, which leads to differences in the temperature profiles as well. These differences are likely a result of the lower cell count within the tube, which does not allow for sufficient development of heat transfer within the inlet tube.
Figure 53: (a) Velocity contours and (b) Flow lines in the SCWR for 390° C inlet at 24.5 MPa: 3M mesh

Figure 54: (a) Velocity contours and (b) Flow lines in the SCWR for 390° C inlet at 24.5 MPa: 5M mesh
6.4.4 Density Contours

The density contours for the 390°C inlet condition are shown in Figure 56-Figure 58. In comparison with the 350°C inlet case, the decrease in density occurs within the inlet tube rather than in the center of the SCWR. The drop in the density of SCW is visible in Figure 59. In comparison with sub-pseudocritical conditions, the density drop is considerably low (60 kg/m³ compared to 420 kg/m³). As a result, the buoyancy effects are lower in this case.
Figure 56: Density contours along the center of the SCWR for 390° C inlet at 24.5 MPa: 3M mesh

Figure 57: Density contours along the center of the SCWR for 390° C inlet at 24.5 MPa: 5M mesh
Figure 58: Density contours along the center of the SCWR for 390° C inlet at 24.5 MPa: 8M mesh
6.4.5 Estimated TDS Solubility

Under this simulation’s boundary conditions, the SCW is able to reach a temperature that reduces the fluid’s density to below 200 kg/m$^3$. Temperatures found in the lower half of the SCWR for the 390° C inlet case using the 8M cell mesh are shown in Figure 60. Due to the SCW temperatures, a high level of TDS removal would take place. The bulk temperature profiles along the height of the reactor vessel are provided in Figure 61. Using the bulk temperature plots calculated for the three mesh settings, the solubility ranges were calculated with the help of solubility information available from Tester et al. [68]. The solubility ranges are provided in Table 19. The results from
this simulation indicate that the SCWR has the potential to remove nearly all TDS (> 99%) contained in F/P water under the prescribed boundary conditions.

Figure 60: SCWR lower section temperatures for 390° C inlet at 24.5 MPa
Table 19: Estimated TDS solubilities in the lower half of the SCWR for 390° C at 24.5 MPa

<table>
<thead>
<tr>
<th>Salt</th>
<th>Inlet Concentration (ppm)</th>
<th>Solubility at SCWR bottom (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaCl</td>
<td>&gt;150,000</td>
<td>200-1000</td>
</tr>
<tr>
<td>CaCl₂</td>
<td>30,000</td>
<td>2-10</td>
</tr>
<tr>
<td>KCl</td>
<td>50,000</td>
<td>150-900</td>
</tr>
<tr>
<td>MgCl₂</td>
<td>50,000</td>
<td>100-250</td>
</tr>
</tbody>
</table>

6.5 SCWR Sensitivity to Operating Pressure

The previous section evaluated the SCWR’s sensitivity to inlet temperature. The focus of this section is to evaluate the SCWR’s sensitivity to operating pressure, as this parameter has a role in defining several properties, of which specific heat shows the maximum variation. Operating pressures of 23 MPa and 26 MPa were evaluated at an inlet temperature of 350° C. The remainder boundary conditions were identical to those
of the previous simulations (see Table 10). Since the variation in the results was relatively stabilized at the 5M cell mesh setting, the sensitivity tests were conducted at this mesh setting in order to obtain efficiency in computational time.

6.5.1 Temperature Contours

The temperature contours for the SCWR’s operations at 23 and 26 MPa are provided in Figure 62 and Figure 63. Operating at 23 MPa resulted in lower overall temperatures within the SCWR as a consequence of the higher specific heat capacities of SCW at lower pressures, as previously noted in Figure 5. The maximum temperature observed in the 26 MPa case was approximately 50° C greater than that at 23 MPa. SCWR wall temperature contours are provided in Figure 63. Heating of the SCWR shell is more gradual at 23 MPa, which is again related to the higher SCW specific heat values at the lower operating pressure. Axial and wall temperature plots are provided in Figure 64 and Figure 65, respectively. These results further show increased heating of both the SCW and the SCWR shell at higher pressures due to lower fluid specific heat values.
Figure 62: Temperature contours for 350° C inlet with 5M mesh at operating pressures of (a) 23MPa and (b) 26MPa
Figure 63: Wall temperature contours for 350° C inlet conditions with 5M cell mesh at operating pressures of (a) 23MPa and (b) 26MPa
Figure 64: Axial temperature plots for the SCWR at 350°C inlet temperature with 5M mesh at 23 MPa and 26 MPa

Figure 65: Wall temperature plots for the SCWR at 350°C inlet temperature with 5M mesh at 23 MPa and 26 MPa
HTC plots for the two operating pressure cases are provided in Figure 66. HTC values along the entire wall are lower at the higher operating pressure due to the slight variations in the flow velocities observed in the two cases (see Figure 69 below). At the higher operating pressure, the SCW along the wall region is easily heated to high temperatures, but the bulk temperature values are relatively lower. This creates a larger temperature gradient, which in turn results in lower HTC values. This appears to be the case along the entire region of the SCWR wall in the case of 26 MPa, as denoted by the relatively flat HTC profile.

Figure 66: HTC plots for SCWR at 350° C inlet with 5M mesh at 23 MPa and 26 MPa
6.5.2 **Turbulence Intensity**

The turbulence intensity contours and comparison plots for the two operating pressure cases are shown in Figure 67 and Figure 68, respectively. Since the inlet temperature for both the cases was 350° C, the turbulence observed was similar in the lower half of the SCWR. However, since the decrease in the density was steeper in the case of 23 MPa, there were instances where turbulence intensities were higher in the top half of the reactor as well.

![Figure 67: Turbulence intensity comparison in the SCWR operating at 350° C inlet condition: (a) 23 MPa (b) 26 MPa](image)
6.5.3 Velocity Contours

The velocity plots along the center of the SCWR are provided in Figure 69. The velocity plots indicate that both cases share a similar velocity variation trend. However, the 26 MPa case has a slightly higher velocity as the fluid exits the inlet tube, which is again attributed to the lower specific heat values. Both profiles show a rapid rise in the velocity at the inlet tube exit. This is due to the rapid temperature increase in this region, resulting in a significant decrease of fluid density. This creates strong buoyancy effects in the region, generating higher velocities in the bottom half of the reactor (i.e. $0 \leq y \leq 0.11$ m). This is indicated with respect to the density variations shown in Figure 70.
Figure 69: Velocity plots for 350° C inlet with 5M mesh at 23 MPa and 26 MPa

Figure 70: Density plots for 350° C inlet with 5M mesh at 23 MPa and 26 MPa
However, the vector contours, as shown in Figure 71, reveal an aspect that is not visible in the plots (Figure 69). In the case of the 23MPa pressure setting, the velocity intensity appears to be higher at a select region near the wall, due to the variation in the local densities, which may have resulted in larger buoyancy forces. This is a potential explanation for the reduction in the temperature gradient at that cross section of the SCWR, which in turn caused the spike in the HTC plots shown in Figure 66. Despite its advantage of better heat distribution, the higher agitation observed at the lower operating pressure could cause an obstacle to the collection of precipitated TDS within the SCWR.

Figure 71: Velocity vectors for 350° C inlet with 5M mesh at operating pressures of (a) 23MPa and (b) 26MPa
6.5.4 Estimated Solubility of TDS

TDS solubility estimates were made using the bulk fluid temperature and/or density of the SCW at the lower half of the SCWR section. A comparison of TDS solubility is provided in Table 20. It can be noted that the solubility of TDS increases with operating pressure. The lower TDS solubility in the 23 MPa case is a result of the decreased SCW density at the lower pressure, which leads to lower salt solubility. These results demonstrate that SCW density is the dominant parameter controlling TDS solubility.

Table 20: Estimated TDS solubilities in the lower half of the SCWR for 350° C inlet at 23 MPa and 26 MPa

<table>
<thead>
<tr>
<th>Salt</th>
<th>Inlet Concentration (ppm)</th>
<th>Solubility at SCWR Bottom (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>23 MPa</td>
</tr>
<tr>
<td>NaCl</td>
<td>&gt;150,000</td>
<td>~ 6500</td>
</tr>
<tr>
<td>CaCl₂</td>
<td>30,000</td>
<td>750</td>
</tr>
<tr>
<td>KCl</td>
<td>50,000</td>
<td>~ 10,000</td>
</tr>
<tr>
<td>MgCl₂</td>
<td>50,000</td>
<td>500-1000</td>
</tr>
</tbody>
</table>
CHAPTER 7: CONCLUSIONS

7.1 Introduction

This chapter provides conclusions drawn from the simulations completed for this thesis. The chapter is composed of two sections, the first providing a summary of the results from Chapters 6 and 7 and the second providing conclusions for each thesis objective.

7.2 Summary

7.2.1 Objective 1 Summary

In order to evaluate operation of OHIO’s SCWR reactor a SCW CFD model was developed. User defined functions were developed for important SCW properties including density, specific heat, thermal conductivity, and viscosity. A SCW CFD model was developed in ANSYS Fluent which included the continuity, Navier-Stokes, and energy equations; while, the RANS k-ε model was used for fluid turbulence modeling. In addition, a 3-D SCWR geometry was created using DM and meshed using AM. The user defined SCW properties and developed CFD model were applied to the meshed 3-D mesh to evaluate SCWR operation.

7.2.2 Objective 2 Summary

To determine the capability of the developed SCW CFD model to predict supercritical water system behavior, results from the model were compared with experimental data from literature. As the SCWR is a unique design with no existing experimental data available for comparison, the existing CFD model was modified to
simulate a heated vertical tube configuration for comparison with existing experimental data from Yamagata et al. Four experimental cases from Yamagata et al. were simulated using the SCW CFD model with the k-ε turbulence solver and enhanced wall inflation treatment [32].

Model results compared to experimental data showed the SCW CFD model was able to adequately predict wall temperatures to within 5% of the experimental data. Model accuracy at higher heat fluxes (> 698 kW/m$^2$) was found to decrease due to rapid thermophysical property variation and turbulence at the tube wall interface. Mesh refinement at the tube wall interface was shown to increase model accuracy at the cost of computational efficiency.

An important point of distinction between this simulation and the SCWR system is the magnitude of the applied heat and mass flux. Unlike the system used by Yamagata et al., the SCWR system will not use such intense heat and mass fluxes [32]. This should result in better prediction of flow and heat transfer patterns because lower fluxes should not cause drastic changes in thermophysical properties. Due to the relatively slow mass fluxes, the SCWR fluid will experience greater natural convective flows and buoyancy effects. However, results from this comparative study indicate that the developed supercritical CFD model may be used to adequately predict the temperature, density and flow patterns of fluid in the SCWR at any pre-defined operating pressures and inlet temperature conditions ranging from 350-390° C. Additional pressure values
can also be implemented into the model using the thermophysical database available from NIST.

7.2.3 Objective 3 Summary

The objective of the sensitivity analyses was to evaluate the effect of inlet fluid temperature and operating pressure on SCWR operation. Simulations with fluid inlet temperatures of 350° C and 390° C at 24.5 MPa were completed. Results from the simulations showed greater SCWR temperature rise in the 390° C inlet case. This was because 390° C is above water’s pseudocritical point at 24.5 MPa, resulting in significantly lower specific heat values and greater temperature rise at the same heat and mass flux conditions. Based on the limited solubility data available, it can be concluded that lower SCW densities result in lower TDS solubility. As SCW density decreases with increasing temperature, the 390° C inlet temperature showed lower TDS solubility in the bottom half of the SCWR. However, operating the SCWR with water entering the vessel above its pseudocritical temperature will be problematic as the inlet tube will likely scale and could therefore be blocked by precipitating TDS. In addition, the SCWR shell temperature for the 390° C inlet temperature was found to be too high to maintain the mechanical integrity of the vessel and would pose a significant safety risk.

The operating pressure sensitivity analysis evaluated SCWR operation at 23 MPa and 26 MPa at an inlet temperature of 350° C. Operating pressure had a measurable effect on fluid temperatures in the SCWR with a direct relationship between operating
pressure and fluid temperature. TDS solubility also showed a direct relationship with operating pressure. Unlike the temperature sensitivity results, lower TDS solubility was found in the 23 MPa case even though SCWR fluid temperatures were measurably lower than in the 26 MPa case. The lower TDS solubility at 23 MPa was a result of lower SCW densities than those existing at 26 MPa.

7.3 Conclusions

7.3.1 Objective 1 Conclusions

The deliverable to fulfill this objective was a CFD model that would allow evaluation of SCWR operation. In this work, a SCW CFD model utilizing the k-ε turbulence model with enhanced wall treatment and user-defined thermophysical property functions for SCW density, specific heat, thermal conductivity, and viscosity was developed. In addition, a 3-D CAD model of the SCWR was developed, meshed, and imported into ANSYS Fluent where it was solved using the SCW CFD model. This SCW CFD model was successfully used in modeling activities under Objectives 2 and 3, fulfilling the deliverable for Objective 1.

7.3.2 Objective 2 Conclusions

To fulfill the second objective, results from the SCW CFD model were to be compared with experimental results found in peer-reviewed literature. A publication by Yamagata et al. was selected for comparison [32]. To complete the comparison, a vertical tube 3-D CAD drawing was developed, meshed, and imported into ANSYS Fluent. CFD simulations based on four experimental cases provided in the publication
were completed. The model and experimental results were compared by plotting tube wall temperature with bulk fluid enthalpy and HTC with bulk fluid enthalpy as provided in the publication. The SCW CFD model showed adequate prediction of experimental results in cases with heat flux values below 465 kW/m²; however, the model under predicted wall temperature values at heat fluxes greater than 698 kW/m². The under prediction at higher heat fluxes was attributed to an under-refined mesh at the tube wall/fluid interface. Mesh cell size was reduced by two orders of magnitude and demonstrated better prediction of experimental results at a heat flux of 698 kW/m². Increasing mesh size provided better prediction of rapidly changing thermophysical properties near the pseudocritical point. The SCW CFD model also demonstrated adequate simulation of heat transfer behavior, predicting wall temperature values within 5° C of the experimental results. Using the results, it may be concluded that the SCW CFD model is best suited for predicting SCW behavior at heat fluxes of less than 465 kW/m². As the SCWR will be operated using heat fluxes of less than 465 kW/m², the developed SCW CFD model will provide an adequate means of predicting SCWR behavior. The comparison results provided in Chapter 6 fulfill the deliverables for Objective 2.

7.3.3 Objective 3 Conclusions

To fulfill the third objective, an SCWR sensitivity analysis was to be completed, evaluating the effects of inlet temperature and operating pressure. SCWR temperature contours, velocity contours, fluid flow lines, density contours, and TDS solubility
estimates in the lower half of the SCWR were to be provided. Inlet temperatures of 350° C and 390° C at 24.5 MPa were evaluated. It may be concluded from the inlet temperature sensitivity analysis that operating the SCWR with an inlet fluid temperature below its pseudocritical point is best, as it will prevent scaling and blockage of the inlet tube and will preclude high SCWR shell temperatures, as was predicted in the 390° C case. Temperature, density, and flow lines from the 350° C case demonstrated turbulence at the exit of the inlet tube caused by heating and subsequent decrease in fluid density, resulting in a significant buoyancy effect. This buoyancy effect is important as it allowed the water to transition to supercritical state within the center of the reactor, which would cause TDS precipitation and minimize scaling at the SCWR wall.

An operating pressure sensitivity analysis at 23 MPa and 26 MPa at an inlet temperature of 350° C was also completed. As in the previous 350° C inlet case at 24.5 MPa, the 26 MPa case showed water transitioning to supercritical state as it exited the inlet tube. This result was expected due to the lower specific heat values at the higher operating pressure. TDS solubility was found to be lower in the 23 MPa case due to lower SCW density, which is directly related to TDS solubility. From these results it may be concluded that operating the SCWR at a pressure slightly above water’s supercritical pressure (22.06 MPa) is best, as this will minimize SCW density, providing greatest TDS removal potential. In addition, operating the SCWR at a lower pressure also increases
process safety and its cost effectiveness, as this will limit the SCWR shell temperature and its thickness. Results provided in Chapter 7 fulfill the requirements of this objective.
CHAPTER 8: RECOMMENDATIONS

The CFD modeling of the SCWR yielded important information regarding the operation of the system. To further refine an operating envelope for the SCWR, additional sensitivity analyses are necessary to evaluate the effect of further operating parameters, including but not limited to inlet velocity, mass flux, and heat flux. The focus of these additional sensitivity analyses on the thermophysical properties of SCW should be to minimize TDS solubility within the lower section of the SCWR as well as to minimize scaling, all while maintaining the mechanical integrity of the SCWR.

The next recommendation is to validate the SCW CFD model with experimental data from a prototype system. The prototype system should be equipped with multipoint thermocouples located within the inlet tube and near the side of the SCWR wall. Temperature data from the SCWR may then be plotted with model results to determine prediction accuracy. Based on validation criteria, the SCW CFD model may then be further refined to improve prediction accuracy. Validation experiments should be completed with TDS-free water as the thermocouple sheaths will likely provide a nucleation site for precipitating TDS and interfere with SCW temperature measurement. Once validated, the SCW CFD model could then be used to support commercial-scale SCWR system design with a known level of confidence.

The final recommendation is to increase the fidelity of the existing SCW CFD model by incorporating a discrete phase model (DPM) to evaluate precipitation and subsequent transport of TDS particles within the SCWR. The DPM will account for TDS
precipitation chemistry including population balance based upon TDS solubility at the local temperature, precipitated particle size ranges/densities, and endothermic enthalpy of the precipitation reactions. Information regarding TDS solubility, precipitated particle size ranges, and reaction enthalpies may be found in peer-reviewed literature. TDS precipitation and solid interactions within the system are quite complex, TDS precipitation may take place through homogeneous nucleation throughout the fluid or on existing particles within the fluid. Additionally, the precipitation’s endothermic enthalpy will result in localized cooling which will need to be understood to effectively control heat flux for efficient TDS removal. Finally, once precipitated the particles may agglomerate or undergo attrition which will effect particle settling. Little to no information regarding agglomeration/attrition of salt particles in supercritical media is available in literature and experimental testing would be required to acquire such data. As a first pass, it is recommended a module be added to the existing SCW CFD model which accounts for TDS solubility, precipitation enthalpy, precipitated particle size range, and DPM to evaluate particle settling within the SCWR.

An additional recommendation is to incorporate TDS, TDS precipitation enthalpy, and precipitated TDS particle sizes into the CFD model to create a more realistic simulation of F/P water and the precipitation process of the four major TDS. Since the ANSYS Fluent material database does not include the TDS components for this research, creation of new materials based on existing databases will be required. Incorporation of TDS precipitation enthalpies will be critically important as the precipitation reactions are
strongly endothermic and F/P water contains high levels of TDS, which will cause cooling of the SCW at the precipitation sites. Incorporation of these properties into the existing SCW CFD model will allow for the prediction of the additional heat flux required to maintain the precipitated TDS from dissolving again in the SCW. In addition, incorporation of precipitated TDS particle size distributions into the model will allow particle settling and separation techniques to be evaluated.
REFERENCES


APPENDIX A: Hₑ APPROXIMATION METHODOLOGY

The mathematical approach is provided with the help of following correlations.

\[ Q = \Delta h = m \times C_p (T_{out} - T_{in}) \]  \hspace{1cm} (A.1)

Where,
\( Q \) = Heat load on the system, [W]
\( C_p \) = Specific heat at constant pressure [J/kg·K]
\( m \) = mass flow rate, [kg/s]

However,
\[ \Delta h = C_p (T_{out} - T_{in}) \text{ [J/kg]} \]  \hspace{1cm} (A.2)
\[ m = G \times A_{cross} \]  \hspace{1cm} (A.3)

\( G \) = Mass flux [kg/m²·s]
\( A_{cross} \) = Cross sectional area of the water flow [m²]

This gives us the effective height, \( H \) of the pipe

\[ Q = q \times 2 \times \pi \times r \times H \]  \hspace{1cm} (A.4)

\( q \) = Heat flux supplied at the wall [W/m²]

The constants in these sets of equations are:

\( d = 7.5 \times 10^{-3} \text{ m} \)
\( G = 1260 \text{ kg/m}^2 \cdot \text{s} \)