COMPUTATIONAL FLUID DYNAMICS MODELING OF A CONTINUOUS TUBULAR HYDROTERMAL LIQUEFACTION REACTOR

BY

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THESIS
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ABSTRACT

Fossil fuels are long known for its unsustainability and environmental impact. Therefore, the search for renewable energy resources has been a persistent effort in both academia and industry. Amongst a wide variety of candidates, Environmental-Enhancing Energy (E²-Energy) receives special attention due to the incorporation of energy production, carbon dioxide capture, and wastewater treatment. Hydrothermal liquefaction (HTL) is the key component in the technology. It involves the conversion of biowaste and algae into hydrocarbon fuels at elevated temperature and pressure. However, E²-Energy is not yet commercially feasible due to a lack of reliable, up-scaled HTL equipment despite its promising prospective. Improving the efficiency of the hydrothermal conversion is an effective way of increasing the economic viability and benefits of the technology. Tubular continuous reactors are generally considered to be favorable for HTL due to the continuous production and the aptitude for scale-up. Recently, a bench scale tubular continuous reactor system has been developed at the University of Illinois.

As HTL is sensitive to the reacting environment, it is crucial to understand the velocity and temperature distributions, heating uniformity, and heat transfer efficiency within the reactor. However, the high pressure and temperature of HTL process make it difficult to conduct direct measurements of these parameters. A numerical investigation is an appropriate alternative. The objective of this study is to develop a computational fluid dynamics (CFD) model using commercial code ANSYS FLUENT to examine the adequacy of the current design. The model takes inputs of operating temperature of the reactor, temperature of the feedstock reservoir, and residence time, and outputs various parameters including the velocity and temperature profiles and Nusselt number.
The flow regime is best characterized as a turbulent mixed convection. Therefore, shear stress transition $k-\omega$ model with low-Reynolds-number correction is chosen because it is able to resolve the turbulence features and at the same time preserve the buoyancy-induced flow pattern. A representative test is run using water as the feedstock with the input parameters being 300 °C, 25 °C, and 30 min, respectively. Typical mixed convection characteristics are observed: symmetric secondary vortex within the cross-section perpendicular to the tube axis and temperature stratification. In addition, Nusselt number in the fully developed region is significantly higher than that of Poiseuille flow, indicating an enhanced heat transfer rate. The residence time distribution is also found to noticeably deviate from typical laminar flow. The mean retention time is shortened by about 60 seconds for a total of 300 seconds due to the variation of velocity in the heated zone. A correction method is proposed to account for this accelerating effect.

Finally, the model is validated by virtually replicating Mori’s experiment (Mori et al. 1966). The computational prediction and experimental measurement show satisfactory agreement.
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Nomenclature

Gr = Grashof number, \( \frac{g \beta (T_w - T_m) D}{\nu^2} \)

Re = Reynolds number, \( \frac{w_m D}{\nu} \)

Ri = Richardson number, \( \frac{Gr}{Re^2} \)

Pr = Prandtl number, \( \frac{\nu}{\alpha} \)

Ra = Rayleigh number, \( Gr \cdot Pr \)

Pe = Peclet number, \( Re \cdot Pr \)

Nu = Nusselt number, \( \frac{hD}{k} \)

\( g \) = gravitational acceleration, m/s²

\( \beta \) = thermal expansion coefficient, 1/K

\( T \) = temperature, °C

\( \nu \) = kinematic viscosity, m²/s

\( \alpha \) = thermal diffusivity, m²/s

\( D \) = tube diameter, m

\( r \) = radial distance, in

\( R \) = tube radius, in

\( w \) = axial velocity, m/s

\( h \) = heat transfer coefficient, W/(m²·K)

\( k \) = thermal conductivity, W/(m·K)
\[ \theta = \text{dimensionless temperature, } \frac{T_w - T}{T_w - T_c} \]

\[ W = \text{dimensionless axial velocity, } \frac{w}{w_c} \]

\[ \dot{m} = \text{mass flow rate, kg/s} \]

\[ \dot{q}_s = \text{surface heat flux, W/m}^2 \]

\[ \tau = \text{residence time, s} \]

\[ z = \text{axial distance from the inlet, in} \]

\[ \eta = \text{energy recovery ratio of the heat exchanger} \]

**Subscripts**

\[ w = \text{value at the tube wall} \]

\[ c = \text{value at the tube center} \]

\[ m = \text{mean value of the cross section} \]
CHAPTER 1
Introduction

1.1. Energy

In 2010, the U.S. annual energy consumption was 98.0 quadrillion Btu. Fossil fuels accounted for 83.0% of the total consumption, with petroleum 36.7%, natural gas 25.1%, and coal 21.2%. Meanwhile, 30.6% of the total energy consumption and 49.2% of petroleum consumption were imported, respectively (USDOE 2011). The reliance on import leads to a potential threat on energy security. Also, fossil fuels are known for being subject to limited amount of reserves and thus not sustainable. Moreover, the environmental impact of fossil fuels, such as increased greenhouse gas levels, raises a global concern about their usage. Therefore, it is of great importance to seek alternative (renewable and carbon-neutral) energy resources.

1.2. Microalgae biomass

Biomass refers to all organic matter that stems from plants, including aquatic and terrestrial. As a result of photosynthesis by these plants, biofuels derived from biomass have significantly reduced net carbon dioxide emission. Due to the capability of mitigating greenhouse gas emission, conversion of biomass has been given great research attention worldwide.

First generation biofuels have been based on extraction from sugar and starch crops (ethanol) and oilseed crops (biodiesel) (FAO 2008). The production of first generation biofuels, however, brought great controversy, due to the competition with food production for the use of arable land. For this reason, the potential of replacing fossil fuels by first generation biofuels remains limited. Currently, the production of first generation biofuels only contributes to 1% of global transport fuels (Brennan and Owende 2010).
The development of second generation biofuels has focused on lignocellulosic biomass derived from whole plant matter of designated energy crops or agricultural, forest, and wood processing residues (Moore 2008). Although it resolve the conflict between food production and fuel generation, second generation biofuels are still far from commercial-scale exploitation because cellulosic biomass is more resistant to being broken down than starch, sugar and oils, which makes the conversion into liquid fuels more expensive (FAO 2008).

From the first and second generation biofuels, we can abstract the ideal characteristics for a technically and economically feasible biofuel resource: it should demand minimum amount of arable land; should produce abundant biomass within short duration of time; should mitigate global warming; and, should be competitive to fossil fuels in price. Successful employment of microalgae can meet these requirements.

Microalgae consist of a wide range of unicellular and simple multi-cellular microorganisms, including cyanobacteria (*Chloroxybacteria*), green algae (*Chlorophyta*), red algae (*Rhodophyta*), and diatom (*Bacillariophyta*) (Brennan and Owende 2010). The advantages of using algae as a biofuel feedstock are: (1) microalgae have a higher photosynthetic efficiency and faster growth rate than terrestrial plants, they can double the biomass in as short as 3.5h during exponential growth period (Chisti 2007; Singh and Dhar 2011); (2) microalgae can be grown and harvested all year round; (3) the lipid content in microalgae typically ranges from 20% to 50% on a dry weight basis, exceeding 80% in some species (Spolaore et al. 2006; Metting Jr. 1996), consequently, biodiesel yield per area of microalgae is much higher than that of rapeseed (Schenk et al. 2008); (4) microalgae can be cultivated on non-arable lands, minimizing the impact on food production (Searchinger et al. 2008); (5) algal biofuels are carbon neutral, as producing 1kg of algae biomass fixes about 1.83kg of carbon dioxide (Chisti 2007);
(6) microalgae can remove nitrogen and phosphorus from wastewater, therefore, microalgae cultivation can be coupled with wastewater treatment (Cantrell et al. 2008); (7) microalgae biomass also produces valuable co-products such as protein, in addition, the residue after oil extraction can be used as animal feed and fertilizer (Spolaore et al. 2006), or generate ethanol and methane by fermentation (Hirano et al. 1997).

1.3. Hydrothermal liquefaction

Currently, microalgae are most commonly utilized as the feedstock of biodiesel production. The process involves the extraction of triglycerides from algal biomass and the subsequent conversion (via transesterification) into biodiesel. This approach requires drying of the algal biomass and extraction using organic solvents. These steps add considerable cost to the process. An alternative method that needs no drying or organic solvents is hydrothermal conversion. The approach converts moist microalgae paste in aqueous media at elevated temperature and pressure. Liquefaction is performed at temperatures below the critical point of water and liquid bio-crude oil that primarily consists of hydrocarbons is the desired product. Studies of hydrothermal liquefaction have been conducted under various parameters with a number of microalgae species (Dote et al. 1994; Sawayama et al. 1995; Kishimoto et al. 1994; Yang et al. 2004). It was conclude that the oil yield and quality vary significantly with respect to temperature, retention time, catalyst, and microalgae strains. Typically, hydrothermal liquefaction is carried out at temperatures between 200–300 °C for 30–60 minutes with or without alkali catalyst. Oil yields range from 33 to 64 wt %. Heating values of the bio-crude are usually 28–50 MJ/kg. In addition, Minowa et al. (1995) and Sawayama et al. (1999) analyzed the ratio of energy input and output of microalgae liquefaction and suggest that the process is a net energy producer.
1.4. **Reactor design**

Bench scale hydrothermal liquefaction experiments are typically conducted in batch autoclaves. One of the shortcomings of autoclaves is relatively low heat transfer rate and high thermal inertia (Knezevic 2009). As a result, considerable amount of reactions occur during the prolonged heating/cooling time (Fang et al. 2004; Watanabe et al. 2005). Therefore conventional autoclave reactors are not suitable for HTL kinetics and mechanism studies. Additionally, elongated heating and cooling period severely limit their application in commercial scale production. Continuous systems, on the other hand, enjoy several advantages including high throughput, steady state operation, and easy scale-up. Considering the benefits, we recently developed a bench-scale, continuous, tubular hydrothermal liquefaction reactor. Generally, three assumptions are made in most studies on tubular reactors: ideal plug flow and no axial mixing; complete radial mixing; and uniform velocity and temperature profiles across the radius. Various parameters may then be readily derived. The assumptions, however, may not be applicable to all applications, especially those with such extreme operating conditions as hydrothermal liquefaction. Consequently, a closer examination is warranted.

1.5. **Objectives**

It is of great interest to understand the hydrodynamic and thermal characteristics of the new-designed tubular plug-flow reactor, since oil yield and quality are directly influenced by reaction temperature and retention time. However, due to the difficulty of directly measuring the temperature and velocity within the tube, computational fluid dynamic analysis is employed. Therefore, this study intends to investigate the heat transfer performance of the reactor using a commercially available computational fluid dynamic code ANSYS-FLUENT. The detailed objectives are proposed:
1. Examine the effectiveness of the designed length of the heat exchanger and find out the heat recovery ratio;

2. Define the flow regime within the reactor and apply appropriate model to discover the velocity and temperature profiles;

3. Study the effect of tube orientation on the flow field and heat transfer;

4. Analyze the residence time distribution.
2.1. Mixed convection heat transfer

Laminar convective heat transfer is encountered in a wide variety of engineering application and thus is very well studied both analytically and experimentally. Most studies, however, are limited to pure forced convection where constant properties of fluid are assumed. Since the density of most fluids is dependent on temperature, the assumption is valid only when the temperature change is sufficiently small so that the magnitude of natural convection is negligible compared to that of forced convection. As a matter of fact, both mechanisms are of comparable order of magnitude in many practical situations. Such flow is usually termed mixed convection or combined convection flow.

The relative magnitude of free and forced convection may be obtained from a study of dimensionless parameters. Richardson number describes the importance of buoyancy force in a mixed convection flow. It is the ratio of Grashof number to the square of Reynolds number.

\[
Ri = \frac{Gr}{Re^2} = \frac{g \beta (T_w - T_m) L}{u^2}
\]  

(2.1.1)

where \( g \) is the gravitational acceleration, \( \beta \) is the thermal expansion coefficient, \( T_w \) is the wall temperature, \( T_m \) is the mean temperature, \( L \) is the characteristic length, and \( u \) is mean velocity.

Typically, forced convection is predominant whereas natural convection is negligible when \( Ri < 0.1 \); natural convection is predominant whereas forced convection is negligible when \( Ri > 10 \); and neither is negligible when \( 0.1 < Ri < 10 \). Still, it is sometimes difficult to draw a clear distinction between the two effects and arbitrary criteria are necessary. For instance, Metais and
Eckert (1964) arbitrarily defined mixed convection as the actual heat flux deviated more than 10 percent from that by either pure forced convection or pure free convection.

Strong influence of buoyancy force can be expected in the current system due to the low velocity and the high heat flux.

2.1.1. Effect of buoyancy force

A number of studies investigated the effect of buoyancy force with various configurations, including working media, tube orientation, dimensionless numbers, etc. It is generally concluded that the velocity and temperature profiles are markedly different from their counterpart for pure forced convection. A significant increase of Nusselt number is also typically observed. This section summarizes the relevant literature studies on this topic.

2.1.1.1. Velocity and temperature profile

Velocity and temperature profiles at cross-sections perpendicular to tube axis can be readily derived by solving governing equations for laminar flow and energy balance. The results are independent of tube orientation when gravity is ignored. In mixed convection, however, the inclination of tube axis significantly influences motion and heat distribution, two limiting cases being: vertical tube and horizontal tube. In vertical tubes buoyancy force is parallel to the direction of flow; thus it is still possible to analytically solve the governing equations for momentum and energy and the solution remains axisymmetric about the tube axis. In horizontal tubes, on the other hand, buoyancy force and externally forced flow are perpendicular to each other; the absence of axial symmetry considerably increases the mathematical difficulty in solving the fluid motion. Therefore, various attempts were made using experimental, analytical, and numerical methods.
Mori et al. (1966) experimentally studied the effect of buoyancy force on the velocity and temperature fields of the fully developed flow of air in a uniformly heated horizontal tube. Velocity and temperature were measured by calibrated, cylindrical yaw probes and T-shaped thermocouples traversing the tube, respectively. They concluded that because wall temperature was higher than the bulk fluid temperature, the fluid near the wall was heated and moved upward along the wall due to buoyancy, while the fluid in the center was cooler and thus descended. As a result, a secondary flow that was symmetric about the vertical plane passing through the tube axis was formed. Due to this effect, velocity and temperature distributions were found to evidently differ from those of Poiseuille flow. Instead of the parabolic shaped, velocity and temperature profiles were concave downward in vertical direction whereas remained symmetric in horizontal direction. In the follow-up report (Mori and Futagami 1967), they observed the secondary flow described above by injecting NH_{4}CL smoke in a transparent tube. It was also pointed out that the dimensionless velocity profile was relatively independent of $Ra$, while the dimensionless temperature profile concaved further downward with increasing $Ra$.

Siegwarth and Hanratty (1970) investigated the stream function and velocity and temperature distributions of a high Prandtl number fluid – ethylene glycol – in a heated horizontal tube by experimental and computational methods. The measured and calculated temperature profile showed good qualitative accordance with Mori’s data. Stream functions computed by finite difference method also agreed well with Mori’s visualization. However, velocity profile remained close to a parabolic shape due to large Prandtl. In addition, maximum velocity appeared above the horizontal axis in contrast to Mori’s observation. The trend was attributed to the decrease of viscosity with height in the tube due to the increase in temperature, whereas the viscosity of air stayed relatively constant with temperature.
Given the fact that no exact solution exist for mixed convection flow in horizontal tubes, perturbation method is a common approach in theoretical studies. The method starts from the exact solution of pure forced convection, and adds natural convection as a perturbation term to it to obtain an approximate solution. Morton (1959) hypothesized that the motion due to buoyancy can be regarded as a secondary flow that modified the main flow by creating a circulation of the fluid in a direction normal to the tube axis. He then obtained the solutions for the velocity and temperature in the fully developed region as power series of $Ra \cdot Re$. The solutions had the following general form:

$$\psi = A\psi_0 + A^2\psi_2 + ... \quad (2.1.2)$$

$$W = W_0 + AW_1 + A^2W_2 + ... \quad (2.1.3)$$

$$\theta = \theta_0 + A\theta_1 + A^2\theta_2 + ... \quad (2.1.4)$$

where $\psi$, $W$, and $\theta$ are stream function, axial velocity and temperature, respectively, and $A$ is Rayleigh number. $W_0$ and $\theta_0$ represent the case of pure forced convection.

Faris and Viskanta (1969) used $Gr / Re^2$ as the perturbation parameter to study a laminar combined free and forced convection flow within a horizontal circular tube subject uniform heat flux at the wall. Flow was assumed fully developed and fluid properties were considered constant except for density in the body force term of momentum equation. The predictions of velocity and temperature profiles agreed well with the experimental data by (Mori et al. 1966). The perturbation approximation, however, is restricted to low Rayleigh number flows and gives unrealistically high estimate of Nusselt number for $ReRa > 3000$ (Bergles and Simonds 1971; Mori et al. 1966; Mori and Futagami 1967).

Mori and Futagami (1967) employed the boundary layer theory to derive analytical expression of flow and temperature fields in a mixed convection flow at high $Ra$ values. A
boundary layer sufficiently thin compared to the tube radius was assumed. Solutions were then solved in the core region where secondary velocity was assumed to be uniformly downward and the boundary layer separately. The results were concluded to be applicable in the range of $Re \cdot Ra \geq 10^4$ and showed good consistency with their previous report (Mori et al. 1966).

A numerical analysis was carried out by (Wang et al. 1994). The governing equations of continuity, momentum and energy with the Boussinesq approximation were solved by finite difference method. Various combinations of $Pr$ and $Ra$ were tested and it was discovered that flow reversal would happen near the top of tube wall with low $Pr$ and high $Ra$. A $Pe - Ra$ coordinate was given to predict regime of reverse flow occurrence. Similar backflow phenomenon was also observed by Mikesell for flows with $\frac{NuGr}{PrRe^2} > 150$ (Mikesell 1963).

2.1.1.2. Nusselt number correlation

Nusselt number indicates the relative importance of convective and conductive heat transfer. For fully developed laminar flow in circular tubes with uniform surface heat flux, it is well known that $Nu = \frac{48}{11}$ (Cengel 2007). This prediction is limited to pure forced convection and is found to be inaccurate as buoyancy has a significant impact on the heat transfer rate even at very low temperature gradient (Morton 1959; Mori et al. 1966). In many studies, the heat transfer coefficient was found to be considerably higher than indicated in elementary theory due to the secondary flow. Plenty of efforts have been devoted to establishing a correlation of Nusselt number and the degree of natural convection.

In his perturbation model (Morton 1959), Morton also gave a prediction to Nusselt number. As with the velocity and temperature fields, solution was given as power series of the perturbation parameter $RaRe$: 
\[ Nu = 6 \left\{ 1 + \left( 0.0586 - 0.0852 Pr + 0.2686 Pr^2 \right) \left( \frac{RaRe}{4608} \right)^2 + \ldots \right\} \]  

(2.1.5)

Ede (1961) published one of the earliest reports about the effects of natural convection on laminar flow of water under uniform heat flux boundary condition. Seven pipes of inner diameter ranging from 0.5 to 2.0 inches were tested, with Reynolds number and Grashof number varying from 300 to $10^5$ and $10^4$ to $10^7$, respectively. Thermocouples were attached to a series of positions along the tube with each position having five thermocouples around the periphery. Calculations were based on the average value at each distance. The correlation was given as:

\[ Nu = 4.36 \times (1 + 0.06 Gr^{0.3}) \]  

(2.1.6)

However, the absence of Reynolds number and Prandtl number in Ede’s correlation was questioned (Kupper et al. 1969). It was suggested that Nusselt number be a function of Reynolds, Prandtl and Grashof numbers. A correlation was presented based on a series of experiments of similar setup:

\[ Nu = \frac{48}{11} + 0.048 Pr^{\nu/3} (ReRa)^{\nu/5} \]  

(2.1.7)

Mori (1966) calculated local Nusselt number based on measurements of velocity and temperature at a cross-section and proposed the following correlation:

\[ Nu = 0.61 (ReRa)^{\nu/5} \left( 1 + \frac{1.8}{(ReRa)^{\nu/5}} \right) \]  

(2.1.8)

The prediction agreed very well with their experimental data. However, this formula was applicable to fluids of Prandtl number around unity as air was used as the working fluid.

Alternative to correlation formulae, correlation plots of various variables were also reported. Shannon and Depew (1968) carried out an experimental investigation of free convection effect. Water was introduced into the test system at ice point. Nusselt number,
Reynolds number, and Grashof number were calculated based on local average. Reynolds numbers ranged from 120 to 2300, and Grashof number reached as high as $2.5 \times 10^5$. A correlation plot of $(Nu - Nu_{Gc})$ vs. $\frac{(GrPr)^{1/4}}{Nu_{Gc}}$ was obtained, where $Nu_{Gc}$ is the theoretical value for Poiseuille flow.

Newell and Bergles (1970) solved the governing equations for two limiting cases by central finite difference scheme: infinite-conductivity tube wall and glass tube wall. They represented the upper and lower bound to the average Nusselt number estimate, respectively. The correlation of fully developed Nusselt number with Grashof-Prandtl number product was presented. In the follow-up study (Bergles and Simonds 1971), the data were combined with the analysis of transition region to derive a comprehensive prediction of Nusselt number along the tube axis ($\frac{x/L}{RePr}$) at various Rayleigh and Prandtl numbers.

2.1.2. Laminar to turbulent transition

It is necessary to examine the transition in convective heat transfer flow as the heat transfer coefficient of turbulent flow differs significantly from that of laminar flow. While the criterion for transition of forced convection flow from laminar to turbulent is universally agreed (Cengel 2007), that for mixed convection is much less understood.

In their report (Mori et al. 1966), critical Reynolds number was proposed as a measurement of turbulence level. The authors concluded that when the turbulence level at the entrance was high, the secondary flow suppressed the turbulence. As a result, critical Reynolds number increased with Rayleigh number. In contrast, when the flow at the inlet was laminar, the secondary flow acted as turbulence. Therefore, critical Reynolds number decreased with Rayleigh number. The formulae for the above two cases were give as, respectively:
\[ Re_{cr} = 128(ReRa)^{\frac{1}{4}} \]  

\[ Re_{cr} = \frac{7700}{1 + 0.14Re \cdot Ra \times 10^{-5}} \]  

Nagendra (1973) investigated the interaction of combined natural and forced convection in the transition regime of a horizontal tube under uniform heat flux using water. Velocity, temperature, and pressure drop across the test section were recorded over time to detect fluctuations as an indicator of turbulence. The effects of velocity and heat flux on the transition were studied separately by fixing the heat input while changing velocity and keeping the velocity constant while varying heat flux, respectively. It was found that hydrodynamic and thermal turbulence occurred separately. These two regimes merged at sufficiently high Reynolds and Rayleigh number, resulting in turbulent mixed convection. A plot of boundaries of laminar, transition, and turbulent flow regimes were given.

El-Hawary confirmed Nagendra’s hypothesis by applying similar method to air (El-Hawary 1980). The author found that the transition due to hydrodynamic effects occurred at values of \( GrPr \) that were little dependent on \( Re \). Similarly, laminar flow became thermally disturbed at a relatively constant value of \( RaPr \) for all Reynolds number. The author also noticed that there was a disturbed regime that was practically similar to laminar flow. Further increasing the flow rate, the wall heat flux, or both would cause the flow to enter a short transition period and then turbulent regime. Unlike Nagendra, however, El-Hawary concluded that both thermal turbulence and hydrothermal turbulence were of the same nature in a sense that they were characterized by similar velocity and temperature fluctuations and markedly increased Nusselt number than laminar flow. Consequently, no subdivision was intended for the turbulent flow zone in the flow regime map presented.
2.2. Residence time distribution

In ideal tubular reactors, where plug-flow is assumed, all molecules of species reside within the reactors for exactly the same amount of time. In reality, however, nonideal flow patterns widely exist, resulting in a distribution of residence time of materials within the reactors. It is of great importance to investigate the residence time distribution (RTD) to understand the mixing characteristics in a chemical reactor.

Historically, RTD is determined experimentally by injecting a pulse of inert tracer into the reactor at time $t = 0$, and then monitoring the tracer concentration in the effluent as a function of time $C(t)$. A series of parameters may then be derived from $C(t)$ (Fogler 1999):

Residence time distribution function $E(t)$:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t) \, dt} \quad (2.2.1)$$

Cumulative distribution function $F(t)$:

$$F(t) = \int_0^t E(t) \, dt \quad (2.2.2)$$

Mean residence time $t_m$:

$$t_m = \int_0^\infty t E(t) \, dt \quad (2.2.3)$$

Variance $\sigma^2$:

$$\sigma^2 = \int_0^\infty (t - t_m)^2 E(t) \, dt \quad (2.2.4)$$

Skewness $s^3$:

$$s^3 = \frac{1}{\sigma^3} \int_0^\infty (t - t_m)^3 E(t) \, dt \quad (2.2.5)$$
Residence time distribution function describes in a quantitative manner how much time different fluid elements have spent in the reactor; cumulative distribution function measures the fraction of the exit stream that has resided in the reactor for a period of time shorter than a given value $t$; mean residence time quantifies the average time the effluent molecules spent in the reactor; the magnitude of variance is an indication of the spread of the distribution; and the magnitude of skewness assesses the extent that a distribution is skewed in one direction or another in reference to the mean.
CHAPTER 3
Materials and methods

3.1. Computational fluid dynamics

Computational fluid dynamics utilizes numerical methods and algorithms to solve equations governing fluid flow and heat and mass transfer. Commercial CFD package ANSYS FLUENT is used in this thesis work.

FLUENT is capable of analyzing a wide range of fluid flow problems including incompressible and compressible flows, laminar and turbulent flows, viscous and inviscid flows, Newtonian and non-Newtonian flows, single-phase and multi-phase flows, etc. In addition, both steady-state and transient analyses can be performed.

In addition, FLUENT provides solution to heat and mass transfer problems. Conduction and convection can be easily implemented by adding one extra energy equation. Various models are available to simulate more complex phenomena involving radiation. Species transport can be modeled by solving equations governing convection, diffusion and reaction.

3.1.1. Governing equations

FLUENT analyzes fluid flow problems by numerically solving governing equations. For all flows, conservation equations for mass and momentum are solved. For flows involving heat transfer, additional equation for energy conservation is solved. Turbulence models solve additional transport equations for turbulent variables. For flows involving mass transfer, a species conservation equation is solved. Multiphase simulation requires additional equations for each phase.

3.1.1.1. Mass conservation

The equation for mass conservation is described by:
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m
\]  
(3.1.1)

where \( S_m \) is the source term added to the continuous phase from dispersed second phase or user-defined sources.

**3.1.1.2. Momentum conservation**

Momentum conservation equation can be written as follows:

\[
\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g} + \vec{F}
\]  
(3.1.2)

where \( p \) is the static pressure, \( \bar{\tau} \) is the stress tensor, \( \rho \vec{g} \) is the gravitational body force, and \( \vec{F} \) is external forces including user-defined source terms.

The stress tensor is defined as:

\[
\bar{\tau} = \mu \left[ \left( \nabla \vec{v} + \nabla \vec{v}^T \right) - \frac{2}{3} \nabla \cdot \vec{v} I \right]
\]  
(3.1.3)

where \( \mu \) represents the molecular viscosity, \( I \) is the unit tensor.

**3.1.1.3. Energy conservation**

Energy conservation equation in FLUENT is given by:

\[
\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho \vec{v} (\rho E + p)) = \nabla \cdot \left( k_{\text{eff}} \nabla T - \sum_j \bar{J}_j + \left( \bar{\tau}_{\text{eff}} \cdot \vec{v} \right) \right) + S_h
\]  
(3.1.4)

The first three terms on the right-hand side stands for energy transfer due to conduction, species diffusion, and viscous dissipation, respectively, where \( k_{\text{eff}} \) is the effective conductivity (sum of thermal conductivity \( k \) and turbulent conductivity \( k_t \) given by the turbulence model used), and \( \bar{J}_j \) is the diffusion flux of species \( j \).

The total energy \( E \) in Equation 3.1.4 is written by:
\[ E = h - \frac{p}{\rho} + \frac{\nu^2}{2} \quad (3.1.5) \]

where sensible enthalpy \( h \) is defined for ideal gas as:

\[ h = \sum_j Y_j h_j \quad (3.1.6) \]

and for incompressible fluid as:

\[ h = \sum_j Y_j h_j + \frac{p}{\rho} \quad (3.1.7) \]

where \( Y_j \) is the mass fraction of species \( j \) and

\[ h_j = \int_{T_{ref}}^{T} c_{n,j} dT \quad (3.1.8) \]

in which \( T_{ref} \) is 289.15 K.

### 3.1.1.4. Species transport equations

When species transport model is activated, FLUENT solves a convection-diffusion equation for each species to predict their local mass fraction:

\[ \frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \bar{V} Y_i) = -\nabla \cdot \bar{J}_i + R_i + S_i \quad (3.1.9) \]

where the second term on the left hand side represents convective transport, \( \bar{J}_i \) is the diffusion flux of species \( i \) due to concentration and temperature gradient, \( R_i \) is the net generation rate of species \( i \) by chemical reaction, and \( S_i \) is the source term from the dispersed phase and any user-defined source.

### 3.1.2. Finite volume method

Finite volume method (FVM) is a numerical method for discretizing partial differential equations. It is widely used in commercial CFD codes including FLUENT. In FVM, the domain
is divided into a number of control volumes (cells, elements) where the variable of interest is
evaluated at the centroid of the control volume. Volume integral is performed and converts the
divergence term in the partial differential equation (Equation 3.1.10) into a surface integral
(Equation 3.1.11) using divergence theorem. The surface integral is then evaluated as flux at the
surface of each control volume. The flux entering a certain volume is equal to that leaving the
adjacent volumes. Therefore, FVM is inherently conservative by construction.

\[
\frac{\partial u}{\partial t} + \nabla \cdot f(u) = 0 \quad \text{(3.1.10)}
\]

\[
\frac{\partial}{\partial t} \int_V u \, dx + \oint_{\partial V} f_i n_i \, ds = 0 \quad \text{(3.1.11)}
\]

where \( n_i \) represents the unit vector outward normal to \( \partial V \).

### 3.1.3. Discretization scheme

Due to the conversion to surface integral form, face values are required for the
convection and diffusion terms in Equation 3.1.9. However, ANSYS FLUENT stores discrete
values at the cell centroid. Therefore, face values must be interpolated from the cell center. The
diffusion terms are interpolated using central-difference scheme and are always second-order
accurate. The interpolation of the convection terms is accomplished by an upwind scheme.
ANSYS FLUENT offers several choices: first-order upwind, second-order upwind, power law,
and QUICK.

#### 3.1.3.1. First-order upwind

First-order upwind assumes that the cell-center values of any field variable represent a
cell-average value and the face quantities are identical to the cell quantities. Therefore, the face
value \( \phi_f \) is directly replaced by the cell-center value of variable \( \phi \) in the upstream cell. Such
interpolation is first-order accurate.
\phi_j = \phi \quad \text{(3.1.12)}

3.1.3.2. Second-order upwind

Higher-order of accuracy can be achieved at cell faces via a Taylor series expansion of the cell-center solution about the upstream cell centroid. The face value is calculated by the following expression:

\phi_j = \phi + \nabla \phi \cdot \vec{r} \quad \text{(3.1.13)}

\nabla \phi \text{ is the gradient of the quantity in the upstream cell and } \vec{r} \text{ is the displacement vector from the upstream cell centroid to the current cell face centroid.}

3.1.3.3. Central difference

The second-order accurate central difference scheme takes average from both upstream and downstream cells. It computes the face value as follows:

\phi_j = \frac{1}{2}(\phi_U + \nabla \phi_U \cdot \vec{r}_U) + \frac{1}{2}(\phi_D + \nabla \phi_D \cdot \vec{r}_D) \quad \text{(3.1.14)}

This scheme is provides improved accuracy for Large Eddy Simulation but can produce non-physical solutions.

3.1.3.4. QUICK

QUICK scheme is a weighted average of second-order upwind and central difference, which can be give as:

\phi_j = \theta \cdot \phi_{j,CD} + (1-\theta) \cdot \phi_{j,SOU} \quad \text{(3.1.15)}

\theta = 0 \text{ results in a second-order upwind scheme, while } \theta = 1 \text{ yields a central difference interpolation. The implementation in ANSYS FLUENT uses a variable, solution-dependent value of } \theta. \text{ The QUICK scheme is generally more accurate on structured meshes where unique upstream and downstream cells can be identified.}
3.1.4. Buoyancy-driven flows

When the flow is dominated by buoyancy force, e.g., natural convection, it can be modeled in ANSYS FLUENT by various methods that approximate density variation with respect to temperature. The ideal gas law describes the relationship between the density of a gas and temperature at a given pressure. It has satisfactory accuracy for gaseous flows with small pressure change. For liquids, the Boussinesq approximation is frequently used thanks to the relatively fast convergence rate. The model regards density as a constant quantity in all governing equations to be solved, except for the body force term in the momentum equation:

$$(\rho - \rho_0)g \approx -\rho_0\beta(T - T_0)g$$  \hspace{1cm} (3.1.16)

In the above equation, $\rho_0$ is the constant density of the flow, $T_0$ is the operation temperature, and $\beta$ is the thermal expansion coefficient, defined as:

$$\beta = \frac{-1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p$$  \hspace{1cm} (3.1.17)

However, the approximation is valid only when the change in actual density is small, more specifically, when $\beta(T - T_0) \ll 1$. If the criterion cannot be met, the density has to be defined as a polynomial, piecewise-polynomial, and piecewise-linear function of temperature, which increases the complexity of the model dramatically.

3.1.5. Turbulence model

Although turbulence can be modeled by directly solving Navier-Stokes equations (Direct Numerical Simulation, DNS), the application of this approach is severely limited by its extremely high computational cost. A much more practical alternative is to solve Reynolds-Averaged Navier-Stokes (RANS) equations. The basic idea is to decompose velocity into the time-averaged term and the fluctuation term:
\[ u(x, y, z, t) = \overline{u}(x, y, z) + u'(x, y, z, t) \] (3.1.18)

Note that the mean velocity is independent of time and the time average of the fluctuation velocity is zero. RANS equations can be derived by substituting the decomposed form of velocity in the instantaneous Navier-Stokes equations:

\[
\rho u_j \frac{\partial \overline{u}_j}{\partial x_j} = \rho \overline{f}_i + \frac{\partial}{\partial x_j} \left[ -\overline{p} \delta_{ij} + \mu \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \rho \overline{u}_i \overline{u}_j \right] \] (3.1.19)

The right hand side of the equation represents the change of momentum due to the convection of the mean flow. The change is equal to the mean body force, isotropic stress caused by mean pressure field, the viscous stresses, and the stress owing to the fluctuating velocity field, generally referred to as Reynolds stress. This nonlinear term demands additional modeling to achieve closure of the RANS equations. Various techniques have been proposed, ranging from simple one-equation models, such as Spalart-Allmaras, to sophisticated Large Eddy Simulation (LES).

Amongst the wide variety of turbulence models ANSYS FLUENT provides, two-equation models are most commonly used for practical engineering applications. By definition, two additional transport equations are included in two-equation models to represent the effect of turbulence on the mean flow. Usually, the first equation solves for turbulence kinetic energy \( k \) that determines the turbulence intensity. The second variable, on the other hand, varies between different models. In the \( k-\varepsilon \) model, it is the turbulence kinetic energy dissipation rate, \( \varepsilon \); in the \( k-\omega \) model, the variable is specific dissipation rate, \( \omega \). They describe the length-scale and the time-scale of the turbulence, respectively. Both models are widely used as reliable simulation tools in various engineering problems.
In the present study, the Reynolds number is well within the laminar regime, and turbulence is generated solely by thermal perturbation. While $k-\varepsilon$ is generally a high-Reynolds-number model, $k-\omega$ incorporates low-Reynolds-number correction. For that reason, shear-stress transport (SST) $k-\omega$ is chosen to model the low-Reynolds-number thermally turbulent flow. SST $k-\omega$ is a modification based on standard $k-\omega$ model, and thus more accurate and reliable. The equations for turbulence kinetic energy and specific dissipation rate are:

$$\frac{\partial}{\partial\bar{x}_i} (\rho k) + \frac{\partial}{\partial\bar{x}_j} (\rho u_i k) = \frac{\partial}{\partial\bar{x}_j} \left( \Gamma_k \frac{\partial k}{\partial\bar{x}_j} \right) + \overline{G_k} - Y_k + S_k$$  \hspace{1cm} (3.1.20)

$$\frac{\partial}{\partial\bar{x}_i} (\rho \omega) + \frac{\partial}{\partial\bar{x}_j} (\rho u_i \omega) = \frac{\partial}{\partial\bar{x}_j} \left( \Gamma_\omega \frac{\partial \omega}{\partial\bar{x}_j} \right) + \overline{G_\omega} - Y_\omega + D_\omega + S_\omega$$  \hspace{1cm} (3.1.21)

where $\overline{G_k}$ is the generation of turbulence kinetic energy due to mean velocity gradients, $G_\omega$ is the generation of specific dissipation rate; $\Gamma_k$ and $\Gamma_\omega$ represent effective diffusivity of $k$ and $\omega$, respectively; $Y_k$ and $Y_\omega$ are the dissipation of $k$ and $\omega$ due to turbulence; $D_\omega$ accounts for the cross-diffusion term; $S_k$ and $S_\omega$ represent user-defined source terms.

3.1.6. Numerics

Table 3.1 lists the detailed numerics used in the simulation.

<table>
<thead>
<tr>
<th>Code</th>
<th>ANSYS FLUENT v14.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbulence model</td>
<td>Shear-Stress Transport $k-\omega$</td>
</tr>
<tr>
<td>Velocity-Pressure Coupling</td>
<td>SIMPLE</td>
</tr>
<tr>
<td>Gradient</td>
<td>Least Squares Cell Based</td>
</tr>
</tbody>
</table>
### Table 3.1 (cont.)

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Momentum</td>
<td>QUICK</td>
</tr>
<tr>
<td>Pressure</td>
<td>Body Force Weighted</td>
</tr>
<tr>
<td>Turbulent Kinetic Energy</td>
<td>QUICK</td>
</tr>
<tr>
<td>Specific Dissipation Rate</td>
<td>QUICK</td>
</tr>
<tr>
<td>Energy</td>
<td>QUICK</td>
</tr>
</tbody>
</table>

#### 3.2. Geometry

The system consists of a heat exchanger, a tubular reactor, three electric resistance heaters, an insulation box, pumps and other accessories. The heat exchanger is a simple tube-in-shell countercurrent configuration. The cross sectional dimensions are listed in Table 3.2. The length of the heat exchanger is empirically determined to be 0.254 meters (10 inches). Consequently, a simulation is needed to find out the outlet temperatures and heat recovery ratio. Since the primary concern is overall energy balance, the effect of buoyancy is ignored. Thus a 2-D axisymmetric simulation is sufficient.

### Table 3.2 Cross sectional dimensions of the heat exchanger

<table>
<thead>
<tr>
<th></th>
<th>Tube</th>
<th>Shell</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner diameter</td>
<td>0.7036 meter (0.277 inch)</td>
<td>0.021184 meter (0.834 inch)</td>
</tr>
<tr>
<td>Thickness</td>
<td>0.001245 meter (0.049 inch)</td>
<td>0.002108 meter (0.083 inch)</td>
</tr>
</tbody>
</table>

The reactor is comprised of six 1.83-meter (6-foot) straight stainless steel tubes connecting in series. The inner diameter and thickness of the tubes are 0.021184 meter (0.834 inch) and 0.002108 meter (0.083 inch), respectively. The first 0.762 meter (30 inches) of the reactor is heated by three heaters evenly spaced around the tube in a triangle. The space between
the tube and the heaters is filled with sand bath to ensure uniform heating along the circumference. As the remaining portion is exposed to free air, the reactor is enclosed by an insulation box with 2.3368 meters long, 0.1524 meter wide, and 0.8128 meter tall (7’8” × 6’’ × 2’8’’) to maintain the operating temperature (Figure 3.1). Unlike the heat exchanger, more details about velocity and temperature distributions in the reactor are desired. As a result, a 3-D model is necessary due to the absence of axial symmetry. However, some simplification can be made. For instance, only half of the tube is modeled due to the symmetry about the vertical plane passing through the tube axis. In addition, analytical solution can be readily obtained for the fully developed laminar flow far downstream from the heated zone. Therefore, the modeled geometry includes only the first section of the reactor, i.e. first 0.1524 meter (6 inches).

Figure 3.1 Schematic diagram of the reactor geometry (all parts included)
3.3. Mesh

The 2-D heat exchanger model contains 103,200 rectangular elements. The axial length is discretized into 2400 divisions. In radial direction, the inner tube and outer tube consist of 3 layers of mesh each, and the cell size of the hot and cold fluid is 0.000254 meter (0.01 inch) with a growth ratio of 1.25 from the wall (Figure 3.2).

![Figure 3.2 Mesh of the heat exchanger (from the top are: shell, cold fluid, tube, and hot fluid)](image)

The 3-D reactor geometry is comprised of 607,090 structured hexahedral elements. In cross-sections perpendicular to tube axis, there are 40 uniformly spaced cells around the azimuth
and 48 non-uniformly spaced elements across the diameter with higher density near the wall to capture the boundary layer. 4 nodes are created in the tube wall (Figure 3.3). Finer mesh is assigned to the heated zone to resolve the small length scale turbulence features (Figure 3.4).

Figure 3.3 Mesh of the reactor in the cross-section perpendicular to tube axis
3.4. Boundary condition

Specific boundary conditions must be provided to the model to begin with, including inlet velocity and temperature, heat flux through the wall, backflow temperature if any and so forth. Although the system is designed with great flexibility, a set of representative operating conditions is arbitrarily chosen to define the model. Operating temperature, retention time, and reservoir temperature are the independent variables of the model that determine other boundary conditions (Figure 3.5). They are chosen to be 300 °C, 30 minutes, and 25 °C, respectively.
In order to save computational time, the heaters and the insulation box are excluded from the model. Instead, the effects of them are approximated by constant and uniform heat flux and constant free stream temperature convection, respectively. The heat flux value is calculated via energy balance. The ambient temperature within the box is assumed to be maintained at the operating temperature.

In order to model hydrodynamically fully developed flow, a pre-simulation is run with isothermal boundary conditions. The velocity profiles at the outlet are then used as inlet velocity input in actual simulations. Detailed boundary conditions are presented in Table 3.3.
Table 3.3 Boundary conditions of the simulation

<table>
<thead>
<tr>
<th></th>
<th>Velocity</th>
<th>Temperature</th>
<th>Gauge pressure</th>
<th>Heat flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>0.00757 m/s</td>
<td>210 °C</td>
<td>0 Pa</td>
<td>20582 W/m²</td>
</tr>
<tr>
<td>Outlet</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wall</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3.5. Materials

Due to substantially high heat flux, the temperature gradient within the heated zone is expected to exceed 100 °C. Thus, the Boussinesq model is deemed not applicable. The density of water is approximated by a second-order polynomial (Figure 3.6). All other properties are evaluated at average temperature. Water is assumed to remain in liquid phase under the liquefaction condition. Hence the fluid is treated as a single phase, homogeneous domain and no phase change or bubble formation is considered.

![Figure 3.6 Density of water as a function of temperature](image)

\[ y = -0.0059x^2 + 4.4517x + 76.74 \]

\[ R^2 = 0.9958 \]
The property of stainless steel is determined by the default value in ANSYS FLUENT database.
CHAPTER 4
Validation case

The validity of CFD model is assessed by comparison to the results from a frequently cited reference paper (Mori et al. 1966). A model is designed to exactly replicate the actual experiment of Mori. The density of air is approximated as a second-order polynomial of temperature. Other properties are evaluated at average temperature. The geometry is duplicated from Mori’s experimental setup. A horizontal circular brass tube with 14-meter length, 35.6-millimeter inner diameter, and 38-millimeter outer diameter is modeled. First 7 meters of the tube is isothermal and the following 7 meters is uniformly heated. Accordingly, isothermal and constant heat flux boundary conditions are applied, respectively. The heat flux value is calculated from the axial temperature gradient in the paper. In addition, the flow rate is computed by Reynolds number. The mesh contains approximately 1.5 million elements. Detailed model parameters are listed in table. Simulation results are compared with experimental data in the literature (Mori et al. 1966).

Table 4.1 model setup for the validation case

<table>
<thead>
<tr>
<th>Flow</th>
<th>Laminar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity-Pressure Coupling</td>
<td>SIMPLE</td>
</tr>
<tr>
<td>Gradient</td>
<td>Least Squares Cell Based</td>
</tr>
<tr>
<td>Pressure</td>
<td>PRESTO!</td>
</tr>
<tr>
<td>Momentum</td>
<td>QUICK</td>
</tr>
<tr>
<td>Energy</td>
<td>QUICK</td>
</tr>
<tr>
<td>Inlet</td>
<td>Velocity 1.991 m/s</td>
</tr>
<tr>
<td></td>
<td>Temperature 20 °C</td>
</tr>
</tbody>
</table>


Table 4.1 (cont.)

<table>
<thead>
<tr>
<th>Outlet</th>
<th>Gauge pressure</th>
<th>0 Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wall</td>
<td>Heat flux</td>
<td>227 W/m²</td>
</tr>
</tbody>
</table>

Figure 4.1 Wall temperature along the axial direction (Mori et al. 1966)
Figure 4.2 Dimensionless velocity along vertical center-line at 6 m (Mori et al. 1966)

Figure 4.3 Dimensionless temperature along vertical center-line at 6 m (Mori et al. 1966)
A good overall agreement between CFD prediction and experimental data is observed. Figure 4.1 shows the wall temperature variation along in the axial direction from the point where heating begins. After about 1 meter of thermal entry length, fully developed flow is obtained. The theoretical line is given by the assumption that in fully developed flow subject to uniform heat flux, temperature increases linearly along the axis. It is noted that Mori’s data make slightly higher predictions, while the CFD results are in good accordance with theory. The deviation might be caused by the difficulty of perfectly insulating the thermocouple attached to the tube wall from the interference of the heater coil around the tube. Figure 4.2 and Figure 4.3 show the data of velocity and temperature measured along the vertical center-line at z = 6 m. The abscissa shows the position on the center-line relative to the tube radius where -1 is the top and is the bottom. The ordinates are dimensionless velocity and temperature, respectively. Their definitions are given in the Nomenclature. They are non-dimensionalized so that the values remain relatively constant in fully developed flows. Therefore these two parameters are commonly used to describe flow characteristics. Poiseuille flow is the laminar flow through a circular pipe of uniform cross-section. Such flow is well known for the parabolic velocity and temperature profiles in the cross-section. The model successfully captures the deviation of mixed convection flow from Poiseuille flow. In addition the computational forecasts show good quantitative congruence with Mori’s data except minor discrepancy around the boundary layer. In conclusion, the model predicts mixed convection with decent accuracy.
5.1. Heat exchanger

The temperature profile along the center-line in cold and hot fluids is plotted against the axial distance (Figure 5.2). After a short entry length, the temperature difference remains constant, coinciding with the characteristic of countercurrent heat exchangers. The mass flow average temperatures at the cold fluid outlet and the hot fluid outlet are 212.49 °C and 123.19 °C, respectively. We define the energy recovery ratio $\eta$ as the temperature increase of cold fluid divided by the difference between the operating temperature and the reservoir temperature. The ratio under current operating condition is 68.18%, a desirable value for a bench scale system. It is noted that $\eta$ is also affected by some other factors such as flow rate and temperature.

A series of design points with constant reservoir temperature and varying operating temperature were also modeled to investigate the optimal condition in terms of energy efficiency. Figure 5.1 highlighted the exit temperatures of the cold and hot fluids as well as the energy recovery ratio.
Figure 5.1 Outlet temperature and the energy recovery ratio under various operating temperatures
Figure 5.2 Temperature of cold and hot fluids in the heat exchanger along center-lines, respectively

5.2. Velocity and temperature profiles

The temperature distribution of the tube axis is shown in (Figure 5.3). A thermal entry length of about 5 inches precedes a linear increase phase followed by a constant temperature period. Although the inlet temperature is 212.49 °C, identical to cold fluid outlet temperature, the temperature is increased to 250 °C instantaneously due to the reversed flow. As discussed in
literature review, sufficiently high heat flux causes the fluid to flow backward in the upper half of the tube. The hot fluid from the downstream mixes with the cool fluid at the inlet. As a result, the temperature around the inlet is higher than the designated value. After the entry region, the temperature gradient remains constant at 2.03 °C/in until the end of heated zone at z = 30 in. Little heat transfer happens beyond that point as the fluid temperature equals to operating temperature.

Figure 5.3 Centerline temperature and mean temperature in the axial direction

Figure 5.4 illustrates the occurrence of flow reversal within the heated section. Note that the y axis is scaled to twice of its original length for the purpose of display. The vectors are plotted on the grid points in the vertical plane passing through the tube axis. The bulk fluid is moving left to right (positive z direction). It is clear that backflow takes place in the upper half of the tube, generating a secondary circulation along the tube axis.
Figure 5.4 Velocity vectors in the heated zone from 10 in to 20 in (reversed flow in the upper half)

Figure 5.5 Velocity distributions along the vertical center-line at three locations in the heated zone
The velocity distributions along the vertical center-line are measured at $z = 10$ in, $z = 15$ in, and $z = 20$ in (Figure 5.5). The intensity of reversed flow is the greatest near the inlet and slightly decreases as the fluid approaches the end of the heated zone where transition to laminar flow occurs. The velocity profiles are almost identical, indicating fully developed condition.

Streamlines in the cross-section at $z = 15$ in is exhibited in Figure 5.6. Typical mixed convection flow pattern is observed. Fluid moves upward along the tube wall and goes downward in the center. Thus, a vortex symmetric about the vertical center-line is formed.

![Streamlines in the cross-section at z = 15 in showing the secondary vortices due to natural convection](image)

Figure 5.6 Streamlines in the cross-section at $z = 15$ in showing the secondary vortices due to natural convection
Figure 5.7 demonstrates the temperature contour on the plane passing through the tube axis in the heated section. Again, the length in y axis is amplified twice. The isotherms exemplify how the secondary vertex propagates along the tube axis.

![Temperature contour on symmetric plane in the heated zone from 10 in to 20 in](image)

Similarly, temperature distribution measurements are taken at three locations within the heated zone (Figure 5.8). Unlike the validation case, an evident variation around the circumference is noticed. Therefore, wall temperature is evaluated as the average of the top and the bottom values. In spite of its existence, the difference decreases as the fluid gets closer to the end of the heated section. This trend reveals that the secondary flow induced by buoyancy has a manifest effect of mitigating the temperature gradient that would be otherwise constant in a flow under uniform heat flux.
Figure 5.8 Temperature distribution along the vertical center-line at three locations in the heated zone

Figure 5.9 Stratified temperature contours in the cross-section $z = 15$ in
Temperature isotherms are plotted in Figure 5.9 to represent the temperature distribution in cross sections in the heated zone. Due to the coupling between density and temperature, stratification occurs. Fluid of the same temperature stays in the same vertical layer. The phenomenon characterizes the temperature profile of mixed convection flow. In addition, the rather thin boundary is resultant from the high heat flux.

5.3. **Nusselt number**

Nusselt numbers are computed for both cases using the following equation:

\[ Nu = \frac{hD}{k} \]  

(5.1.1)

In the equation, \( D \) is tube diameter, \( k \) is thermal conductivity of the fluid, and \( h \) is heat transfer coefficient given by:

\[ h = \frac{q_s}{(T_w - T_m)} \]  

(5.1.2)

where \( q_s \) represents the surface heat flux, and \( T_w \) and \( T_m \) are wall and mean temperatures respectively.

Figure 5.10 show the variation of \( Nu \) around the circumference, due to that wall temperature varies considerably along the azimuth. The vertical axis ranges from \(-\frac{\pi}{2}\) to \(\frac{\pi}{2}\) with \(-\frac{\pi}{2}\) being the bottom and \(\frac{\pi}{2}\) representing the top. An obvious trend indicates that the lower half of the tube is more efficient in heat transfer than the upper half. This phenomenon can be explained by the fact that both axial velocity and radial velocity are greater in the lower half as shown in Figure 5.5 and Figure 5.6.
In order to calculate the average Nu at each cross section, the mean wall temperature around the periphery is taken and substituted into Equation 5.1.2. Five locations within the fully developed region are measured (Table 5.1). Their mean value is used to represent the Nusselt number of fully developed mixed convection in horizontal tubes. It is concluded that the Nusselt number is markedly increased by buoyancy effect, being about 4.3 times of that of pure forced convection.

Table 5.1 Nusselt numbers of fully developed horizontal mixed convection

<table>
<thead>
<tr>
<th>Z (inch)</th>
<th>Nu</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>16.6608</td>
</tr>
<tr>
<td>12.5</td>
<td>17.3569</td>
</tr>
<tr>
<td>15</td>
<td>18.2773</td>
</tr>
<tr>
<td>17.5</td>
<td>19.5096</td>
</tr>
<tr>
<td>20</td>
<td>21.2184</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td><strong>18.6046</strong></td>
</tr>
</tbody>
</table>
5.4. Effect of tube orientation

Identical model parameters are applied to tubes with vertical orientation. However, due to the alignment between flow direction and buoyancy force, axial symmetry is retained. Therefore, 2-D axisymmetric models are used. It is concluded that in horizontal tubes, natural convection enhances heat transfer by generating secondary vortex. In vertical tubes, however, buoyancy force can either assist or diminish heat transfer depending on the direction of the forced flow. For instance, in upward flows, buoyant motion is in the same direction as the forced motion. Therefore, natural convection strengthens heat transfer. In downward flows, on the contrary, buoyancy is in the opposite direction to the bulk fluid motion. Consequently, natural convection undermines heat transfer.

5.4.1. Velocity and temperature

Figure 5.11 shows the velocity vectors and isotherms for fully developed upward flow. The average velocity is in positive x-direction while the gravity is applying in the negative x-direction. Linear increase in temperature indicates the fully developed condition. A thin layer of thermal boundary layer is identified due to high heat flux. Note that isotherms closely resemble those of ideal plug-flow. The temperature distribution is almost uniform across the diameter except the boundary layer, which is extremely desirable in hydrothermal liquefaction kinetics study.

The flow is concentrated on the near wall region, because buoyant motion greatly outpaces the forced flow. As a result of continuity, the velocity in the tube central area is negligible. Reversed flow with limited speed is observed. A more significant flow reversal is expected if the heat flux is further increased, i.e. stronger natural convection.
Figure 5.11 Velocity and temperature distributions in the fully developed region for upward flow

Similar plots are given in Figure 5.12 for fully developed downward flow. Both forced fluid motion and gravity are in positive x-direction. In contrast to upward flow, significant reversed flow occurs near the wall, whereas the flow in the center is markedly accelerated due to mass conservation constraint. Consequently, the temperature variation across the diameter is magnified.
Figure 5.12 Velocity and temperature distributions in the fully developed region for downward flow

5.4.2. Nusselt number

Five points are measured within the fully developed region and the average value is taken to represent the whole domain. The data are presented in Table 5.2:

Table 5.2 Nusselt numbers of fully developed upward and downward flow

| z = 10 in | 79.26876 | 26.03742 |
| z = 12.5 in | 79.50093 | 25.45723 |
| z = 15 in | 82.20259 | 25.34986 |
| z = 17.5 in | 82.19369 | 25.29093 |
| z = 20 in | 82.06171 | 25.66505 |
| **Average** | **81.04554** | **25.5601** |

It is clear that the Nusselt number of upward flow is significantly larger than that of downward flow. The relationship concurs with the conclusion that upward flow enhances heat transfer while downward flow retards it. However, it is worth mentioning that downward flow, though not as effective as upward flow, improves heat transfer compared to horizontal flow. It is well known that Nusselt number is a function of $Re$ and $Ra$. Although the flow is reversed near
the wall in downward flow, the velocity magnitude is considerably increased thanks to the alignment between gravity and velocity, and so are the local Reynolds number and Nusselt number. In horizontal flow, on the other hand, buoyancy and net flow are orthogonal. Therefore, the augmentation is relatively insignificant. To test the speculation, we conducted a simulation identical to that of downward flow except that gravitational acceleration is set 0.01 to reduce effective Rayleigh number. The Nusselt number is 4.29, lower than that of Poiseuille flow. In conclusion, downward flow impairs heat transfer at low Ra, while enhances it at high Ra.

5.4.3. Inclined tube

Flows in vertical tubes are distinct with those in horizontal pipes, indicating that tube orientation has a significant influence on its hydrodynamic and heat transfer characteristics. Although the analysis has been made for the horizontal case, it is difficult to maintain the tubes perfectly horizontal. Therefore, additional tests are necessary to investigate the scenario where the tubes are a few degrees from the horizon. For simplicity, 5° is assumed a reasonable deviation. All other parameters are identical to previous models. Similarly, upward flow and downward flow must be discussed separately.

Figure 5.13 and Figure 5.14 show the velocity and temperature profiles along the vertical centerline at 15 for the inclined tubes in contrast with the horizontal tubes. The velocity profile for the inclined upward flow is most distinct. The velocity is positive near the wall and diminishes in the core region. It is because the buoyant force near the wall overcomes the reversed flow that is seen in the horizontal flow. Despite the difference in velocity profile, the temperature distribution is similar to that of horizontal tube. On the other hand, the reversed flow in the upper half in preserved in the inclined downward flow. In addition, its magnitude is increased to the buoyant force. As a result of the increased velocity magnitude, heat transfer rate
is also elevated. Consequently, the temperature profile is slightly more uniform than the other two cases.

In summary, the velocity and temperature distribution in the tube is sensitive to its orientation. An inclined angle as small as 5° can cause the profiles to be obviously different than those of the horizontal case. Hence the tubes should be installed as level as possible to avoid expected deviation from the model prediction.

Figure 5.13 Velocity profile along the vertical centerline at 15 in for inclined downward, inclined upward, and horizontal flows
5.5. Residence time distribution

The residence time distribution is obtained for three conditions: constant density, variable density with $g = 0$, and variable density with $g = 9.81 \text{ m/s}^2$. The tracer mass fraction at the outlet is plotted versus time in Figure 5.15. The red vertical line represents the nominal retention time $\tau = 300 \text{ s}$. The figure illustrates that the residence time distribution for all three cases are qualitatively alike. When density is constant, the peak of the cone falls on the nominal residence time, indicating that the mean residence time $t_m$ is equal to $\tau$. When density varies with temperature, the flow is accelerated signified by a considerable forward shift of the cone. The shift is attributed to continuity, i.e. the decrease in density gives rise to velocity. Therefore, the fluid emanates faster than it is expected when the axial temperature gradient is large. It is
surprising that buoyant motion does not have a significant impact on the residence time distribution. The curves of the variable density cases with and without gravity almost completely overlap. It is likely that residence time distribution characterizes the reactor’s macro-mixing and is thus primarily determined by the mean velocity rather than velocity distribution. Values of the parameter pertaining residence time distribution are given in Table 5.3. The mean residence time is shortened by about 60 seconds because of heating. The inconsistency between the nominal residence time and the actual residence time will significantly impede the accurate analysis of the reaction dynamics and mechanism, and must be minimized.

![Figure 5.15 Residence time distribution for 6-feet tube](image)

**Table 5.3 Residence distribution time parameters**

<table>
<thead>
<tr>
<th></th>
<th>Constant ρ</th>
<th>Variable ρ w/o g</th>
<th>Variable ρ w/ g</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_\text{m}(s)$</td>
<td>317</td>
<td>246</td>
<td>250</td>
</tr>
<tr>
<td>$\sigma^2$</td>
<td>58.6</td>
<td>39.6</td>
<td>44.1</td>
</tr>
<tr>
<td>$s^3$</td>
<td>5.96</td>
<td>4.15</td>
<td>4.81</td>
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</table>
Due to the accelerating effect caused by heating, the flow rate of the pump system must be corrected to ensure desired residence time. The key to accurate correction is to account for the variation of velocity with respect to temperature in the heated zone. A simple correction scheme that assumes linear increase of velocity is proposed. First, the total residence time can be decomposed as the sum of residence time in the heated zone and constant temperature zone:

\[ \frac{L_H}{v_H} + \frac{L_C}{v_C} = \tau_{\text{TOT}} \]  

(5.1.3)

The mean velocity in the heated zone is taken as the arithmetic average of the velocities at the inlet and outlet of the heated zone:

\[ \overline{v_H} = \frac{v_{H,\text{in}} + v_{H,\text{out}}}{2} \]  

(5.1.4)

It can be derived from mass conservation that the ratio of the velocities between two cross-sections is the reciprocal of that of the densities which is a known function of temperature:

\[ \frac{v_{H,\text{in}}}{v_{H,\text{out}}} = \frac{\rho(T_{\text{out}})}{\rho(T_{\text{in}})} \]  

(5.1.5)

Finally, since velocity remains constant after the heated zone, the outlet velocity of the heated zone is equal to the velocity of the constant temperature zone:

\[ v_{H,\text{out}} = v_C \]  

(5.1.6)

Inlet velocity \( v_{H,\text{in}} \) can then be solved from Equations 5.1.3 through 5.1.6. The RTD of a new simulation with corrected inlet velocity is compared with the constant density scenario in Figure 5.16. Notice that the distribution falls much closer to the desirable region with the proposed correction. The mean residence time is about 295 seconds, less than 5 seconds apart from the nominal retention time. The correction is effective in predicting the accelerating effect of density change.
Figure 5.16 Residence time distribution with corrected inlet velocity

5.6. Mesh independence study

A mesh with higher grid density is tested under the same model setup to demonstrate that the original grid is sufficiently fine to produce mesh independent results. The refined mesh contains 3,118,730 elements. The grid spacing along the tube axis and within the cross-section perpendicular to the tube axis is both reduced. Dimensionless velocity and temperature profiles are obtained along the vertical center line at z = 15 in and compared with those of the coarse mesh (Figure 5.17 and Figure 5.18). The figures show substantial overlapping, indicating that solution is not improved by further increasing mesh density.
Figure 5.17 Velocity profile at $z = 15$ in for coarse and refined mesh

Figure 5.18 Temperature profile at $z = 15$ in for coarse and refined mesh
CHAPTER 6
Conclusions and recommendations

6.1. Conclusions

A computational fluid dynamics model is established to study the velocity and temperature profiles, heat transfer, and residence time distribution within a continuous tubular hydrothermal liquefaction reactor. The flow regime is best characterized as turbulent combined forced and natural convection in a horizontal circular tube under uniform heat flux. A detailed literature review is conducted to provide a survey of relevant research on such flow field. Water is used as the working medium and its density is approximated as a second-order polynomial function of temperature to account for the buoyancy term in the governing equation.

In addition, the literature reviews analyzed the transition from laminar flow to turbulence for a mixed convective flow. It is concluded that hydrodynamic effect and thermal perturbations are independent of each other. Therefore, the flow regime of the current study is turbulent due to the substantially high heat flux, despite a Reynolds number that is low. Shear stress transport \( k - \omega \) turbulence model is employed given that it includes low-Reynolds-number correction.

The heat exchanger and first segment of the reactor are modeled with 103,200 and 607,090 elements, respectively. The electric resistance heaters surrounding the tube are replaced by constant heat flux boundary condition; the ambient temperature around the reactor is assumed to be uniform and constant. Inlet temperature of the cold fluid in the heat exchanger, operating temperature of the reactor, and retention time are the independent variables of the model. They are arbitrarily chosen as 25 °C, 300 °C, and 30 min to represent a typical HTL reaction. Results are obtained under such conditions:
1. The model is used to simulate a reference case from previous work by Mori et al. (1966). A good concurrence between the CFD predictions and Mori’s experimental data is observed.

2. The heat exchanger is able to recover 68.18% of initial energy input that heats the system to the operating temperature under the current conditions.

3. Both velocity and temperature distributions of mixed convection flow in the modeled reactor were utterly different than Poiseuille flow. In a cross section perpendicular to the tube axis, the fluid rises along the wall. The upward currents from both sides of the wall coincide at the top of the tube and then descend in the central region. The motion creates two vortices symmetric about the vertical center-line. The temperature field is stratified with hotter fluid in the higher layers and cooler fluid in the lower layers. Additionally, temperature varies substantially around the circumference.

4. Marked flow reversal occurs in the upper half of the tube within the heated section. The intensity of the reversed flow decreases as it approaches the end of the heated zone.

5. The secondary flow caused by buoyancy significantly enhances heat transfer. The average Nusselt number in the fully developed region is 18.6. In addition, heat transfer is more efficient in the lower half of the tube.

6. Tube orientation has a consequential effect on heat transfer rate. Upward flow in a vertical tube markedly improves heat transfer, whereas downward flow strengthens heat transfer at high Rayleigh number yet diminishes heat transfer at low $Ra$.

Amongst the three cases, vertical tube with upward flow is the best scenario in terms
of temperature uniformity and heat transfer rate. The temperature contour closely resembles that of ideal plug-flow.

7. The velocity and temperature profiles are sensitive to tube orientation. A 5° inclined angle may lead to a vastly different result.

8. The axial temperature gradient accelerates the effluence of the fluid. The mean residence time is shortened by about 60 seconds. A correction scheme is proposed and successfully reduced the accelerating effect of temperature gradient to less than 5 seconds.

9. Buoyant motion has little to do with the acceleration of effluent.

6.2. Recommendations

This work creates a platform to assess the performance of the new HTL system. Nevertheless, the model is an initial attempt built on various assumptions whose validity has yet to be verified by real experiments. In addition, water is used as a representative medium. However, the properties of water differ a lot from those of the feedstock. Therefore, the model may need further modification when applied to algae solution. In summary, the following recommendations for future research are proposed:

1. The model is validated by another case with different Re and Ra. To better verify the model, experimental data obtained from the actual system is highly preferable.

2. The physical properties of the feedstock including density, specific heat, thermal conductivity, and viscosity are vital to applying the model to predicting real operating conditions.
3. Incorporate the model with the control system of the reactor. For instance, since
   temperature variation alters the effluent time, a correlation needs to be developed to
   help control the pumping system.

4. Test the accuracy of other turbulence models and identify the most suitable one for
   this particular application.
References


## Appendix A

### Physical properties of fluids

Table A.1 Properties of saturated water

<table>
<thead>
<tr>
<th>Temperature ( T, ^\circ \text{C} )</th>
<th>Density ( \rho, \text{kg/m}^3 )</th>
<th>Specific Heat ( C_p, \text{J/(kg⋅K)} )</th>
<th>Thermal Conductivity ( k, \text{W/(m⋅K)} )</th>
<th>Dynamic Viscosity ( \mu, \text{kg/(m⋅s)} )</th>
<th>Prandtl Number ( \text{Pr} )</th>
<th>Volume Expansion Coefficient ( \beta, \text{1/K} )</th>
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<tr>
<td>0.01</td>
<td>999.8</td>
<td>4217</td>
<td>0.561</td>
<td>1.792×10⁻³</td>
<td>13.5</td>
<td>-0.068×10⁻³</td>
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<td>40</td>
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<td>Temperature $T$, °C</td>
<td>Density $\rho$, kg/m$^3$</td>
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