INVESTIGATING METHODS TO IMPROVE THE CO-FIRING OF BIOMASS WITH COAL USING CFD SIMULATIONS

by

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The following individuals certify that they have read, and recommend to the Faculty of Graduate and Postdoctoral Studies for acceptance, the dissertation entitled:

INVESTIGATING METHODS TO IMPROVE THE CO-FIRING OF BIOMASS WITH COAL USING CFD SIMULATIONS

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Abstract

Biomass as a renewable energy source can be burnt with coal in a coal-fired plant to reduce the impact of fossil fuel on the environment. The aim of this research is to investigate methods that can improve the co-firing of biomass with coal. Initially, a CFD model was validated by comparison with experimental data reported in the literature. Three mesh sizes were tested to prove that simulation results are mesh independent. The model was then applied to simulate the co-firing process with a 3:2 biomass-to-coal mixing ratio. Unsophisticated modifications of the furnace geometry near the inlet and the swirl angle were introduced to study their effect on co-firing. CFD simulations were extended to study the influence of particle shrinkage on co-firing due to biomass pelletization. Furthermore, fine coal tailings generated from coal processing (CT), raw biomass (RB), and torrefied biomass (TB) were characterized for subsequent CFD investigation on mono-firing and co-firing of the different fuels. Simulation results show that the modified furnace geometry with gradual expansion and a larger swirl angle leads to uniform temperature distribution (1650-1720 K) in the furnace vs. a more variant temperature profile (950-1500 K) for the original furnace geometry. Besides, an increase in the tangential component of gas velocity near the center from 1 m/s to 3 m/s with the modified furnace geometry results in a longer residence time of the particles and further reduction of unburnt fixed carbon by 55% from coal at the exit. With biomass pelletization, simulation outputs show that the compressed particles with particle density 1000 kg/m³ have slower volatilization rate and surface reaction, as well as a shorter residence time. This in turns causes a higher percentage of unburnt fixed carbon at the exit though NO emission is slightly lower. As for the co-firing of biomass with fine coal tailings, results indicate that CT alone, CT+TB, and CT+RB blended fuel are associated with 13%, 10% and 28% unburnt carbon, respectively. It may be concluded that co-firing coal tailings with torrefied biomass is better for co-firing since CT+TB also has the lowest NO emission among the different fuels.
Lay Summary

To reduce the fossil fuel impact on the environment, renewable energy sources such as biomass can be combusted with coal in a coal-fired plant. This is called co-firing and represents the first step to phase out coal combustion. Solid biomass particles are often densified into pellets to increase its energy density and facilitate its transportation and handling. These pellets when pulverized in a co-firing plant will result in higher density and smaller size particles than before densification. In this research, co-firing was simulated using computational fluid dynamics model. Two modifications on the conventional furnace geometry were simulated and evaluated by this model. Both modifications have shown improvement on combustion efficiency of fuel blend. The model was also used to investigate the influence of particle shrinkage on co-firing due to pelletization. Model was also used to study the possibility of converting waste coal in the form of coal tailings to energy upon co-firing with biomass.
Preface

This PhD dissertation comprises of seven chapters and the appendix. All the literature review, design and conducting experiments, data processing and analysis, CFD modeling and simulations, mesh creation for CFD model, manuscript and thesis preparation have been done by the author Adel Mohammed redha under the co-supervision of Professor Anthony Lau in the Chemical and Biological Engineering Department at the University of British Columbia (UBC) and Professor Maria Holuszko in Mining Engineering (UBC).

Journal article published and manuscripts being prepared for submission are based on the analysis and results presented in Chapters 2, 3, 4, 5 and 6 of this thesis.

Chapters 2 and 4: Adel Mohammed redha, Anthony Lau, Maria Holuszko, Ali Vakil, Shahab Sokhansanj. 2020. CFD Investigation of pelletization effect on co-firing coal with wheat straw. Canadian Journal of Chemical Engineering. In press. CFD modeling and validation as well as the simulations were done by the author. The co-authors have contributed to the scientific contents of the manuscript. Professor Anthony Lau also edited the drafts of the manuscript.


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List of Symbols

A  Frequency constant, \(s^{-1}\)

\(A_p\)  Particle surface area, \(mm^2\)

Bi  Biot number

\(C_p\)  Specific heat capacity, J/kgk

\(C_{sw}\)  Swelling coefficient

\(C_{ub}\)  Unburnt carbon

\(d_H\)  Hydraulic diameter, m

\(d_i\)  Inner diameter, m

\(d_o\)  Outer diameter, m

\(D_o\)  Diffusion rate

\(d_p\)  Particle diameter, mm

\(E\)  Activation energy of devolatilization, J/kgmol

\(E_d\)  Discretization error

\(F\)  Momentum exchange, kg m/s

\(f_{C,t}\)  The carbon content in the ultimate analysis (% DAF basis)

\(F_d\)  Drag force on the particle, N

\(f_{FC}\)  The fixed carbon content in the proximate analysis, (% DAF basis)

\(f_h\)  The fraction of heat of reaction absorbed by the particle during surface reaction

\(G\)  Incident radiation, W/m²

\(g_s\)  Gravity acceleration, m/s²

HHV  Higher heating value, MJ/kg
$H_r$ Heat of reaction, J
$I$ Turbulence intensity
$k$ Turbulent kinetic energy
$K$ Kinetic rate, s$^{-1}$
$K_{ch}$ Kinetic rate of surface reaction, s$^{-1}$
$m_{p}^o$ Particle mass flow rate, kg/s
$m_A$ The mass of ash in biomass particle
$m_{ch,in}$ The mass of fixed carbon at reactor inlet, kg
$m_f$ Mass fraction of combustible gaseous species, kg
$m_o$ Mass fraction of oxygen, kg
$m_p$ Particle mass, kg
$p$ Pressure, N/m$^2$
$R$ Gas constant, J/kg-mol
$r$ Radius, m
$R_{50}$ The rate at which 50% of volatile matter is released, mg/min.
$R_c$ Critical ratio
$Re$ Reynolds number
$R_{max}$ Maximum rate of volatile mass release, mg/min.
$R_o$ Oxidation ratio
$T$ Temperature, K
$t$ Time, s
$T_\infty$ Surrounding gas temperature, K
\( T_{50} \)  
Temperature when 50\% of VM is released, K

\( T_{\text{max}} \)  
Temperature of maximum rate of volatile mass release, K

\( T_p \)  
Particle temperature, K

\( u \)  
x-component velocity, m/s

\( \bar{u} \)  
Mean velocity, m/s

\( \dot{u} \)  
Velocity fluctuation component, m/s

\( u_p \)  
Instantaneous particle velocity, m/s

\( \nu \)  
The \( \gamma \)-components of the local gas velocity, m/s

\( v_F \)  
Stochiometric coefficients for combustible gaseous species, mole

\( v_O \)  
Stochiometric coefficients for oxygen, mole

\( Y \)  
Local mass fraction

\( y_{d} \)  
Accumulative particle mass fraction

\( Y_{i,\text{CFD}} \)  
The average mole fraction predicted by CFD

\( Y_{i,\text{exp}} \)  
Average mole fraction of a gaseous species measured experimentally

\( z_i \)  
Mass fraction of element \( i \)

\( \theta_R \)  
Radiation temperature, K

\( S_i \)  
Source term

\( S_e \)  
The surface area of an equivalent sphere having the same volume as the particle

\( S_a \)  
The actual surface area of the particle, m\(^2\)

\( f \)  
Mixture fraction

\( \bar{d}_p \)  
Mean particle diameter, mm
**Greek Symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>$\phi'$</td>
<td>Fluctuating component</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Rate of dissipation of turbulent kinetic energy</td>
</tr>
<tr>
<td>$\xi$</td>
<td>Vertical relative vorticity</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Gas density, kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_p$</td>
<td>Particle density, kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_{p,1}$</td>
<td>Density before pelletizing, kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_{p,2}$</td>
<td>Density after pelletizing, kg/m$^3$</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>Representative dependent variable</td>
</tr>
<tr>
<td>$\omega$</td>
<td>Angular velocity about z-axis, rad/s</td>
</tr>
<tr>
<td>$\Psi'$</td>
<td>Shape factor</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>Instantaneous property</td>
</tr>
<tr>
<td>$\bar{\varphi}$</td>
<td>Mean value</td>
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**List of Abbreviations**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>BFB</td>
<td>Bubbling Fluidized Bed</td>
</tr>
<tr>
<td>CCOFA</td>
<td>Close-Coupled Over Fire Air</td>
</tr>
<tr>
<td>CFB</td>
<td>Circulating Fluidized Bed</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CHPP</td>
<td>Coal Handling And Processing At The Preparation Plant</td>
</tr>
<tr>
<td>CT</td>
<td>Coal Tailings</td>
</tr>
<tr>
<td>DAF</td>
<td>Dry Ash Free</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>DPM</td>
<td>Discrete Phase Model</td>
</tr>
<tr>
<td>EDC</td>
<td>Eddy Dissipation Concept Model</td>
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<tr>
<td>EDM</td>
<td>Eddy Dissipation Model</td>
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<tr>
<td>ERZ</td>
<td>External Recirculation Zone</td>
</tr>
<tr>
<td>FC</td>
<td>Fixed Carbon Content</td>
</tr>
<tr>
<td>HiTAC</td>
<td>high temperature air combustion,</td>
</tr>
<tr>
<td>IRZ</td>
<td>Internal Recirculation Zone</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
</tr>
<tr>
<td>LOI</td>
<td>Loss On Ignition</td>
</tr>
<tr>
<td>MC</td>
<td>Moisture Content</td>
</tr>
<tr>
<td>OFA</td>
<td>Over-Fire Air</td>
</tr>
<tr>
<td>PDF</td>
<td>Probability Density Function</td>
</tr>
<tr>
<td>PSD</td>
<td>Particle Size Distribution</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds-Averaged Navier-Stokes</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
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<tr>
<td>--------------</td>
<td>-----------------------------------</td>
</tr>
<tr>
<td>RB</td>
<td>Raw Biomass</td>
</tr>
<tr>
<td>RMSE</td>
<td>Root-Mean-Square Error</td>
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<tr>
<td>RNG</td>
<td>Re-Normalized Group</td>
</tr>
<tr>
<td>RR</td>
<td>Recycled Ratios</td>
</tr>
<tr>
<td>RSM</td>
<td>Reynolds Stress Model</td>
</tr>
<tr>
<td>SMC</td>
<td>Spent Mushroom Compost</td>
</tr>
<tr>
<td>SOFA</td>
<td>Separate Over-Fire Air</td>
</tr>
<tr>
<td>TB</td>
<td>Torrefied Biomass</td>
</tr>
<tr>
<td>TGA</td>
<td>Thermogravimetric Analysis</td>
</tr>
<tr>
<td>VM</td>
<td>Volatile Matter</td>
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Dedication

To my Mother Khalida and my Father Fadhel

My wife Jinan and my kids Alzahra, Noorahuda, Mohamed and Ali,

To my brothers, sisters, and friends

To all my Teachers…..

With love
Chapter 1. Introduction

1.1 Background

Coal represents the most abundant fossil energy source available in the world despite the environmental concerns and competitions with other fuels. With increasing concerns of fossil fuel impact on environment, coal has lost some market share in favor of petroleum products and natural gas. However, it continues to be a key source of energy because of the dominant role it has maintained in its core markets [1]. Recently, coal’s role in energy use worldwide has shifted substantially, from a fuel used largely in many sectors of the economy to one that is used primarily for electricity and heat generation and in some key industrial sectors, for instance steel, cement and chemicals production. Today, the combustion of pulverized coal is still widely used throughout the world for power generation and provides about 40% of the global electricity [2, 3]. According to annual energy outlook from energy information administration-USA-2020, electricity generation from coal-fired plants shared 24% of the total fuel types in 2019 and is anticipated to decline to 13% through 2050 [4]. In Canada, coal contributed 9.1% of the total electricity generation in 2017 with 58.9 TWh which is projected to decline to 1.4 TWh (i.e. 0.2% of the total national generation) in 2040. This will lead to more demand on renewable fuel sources to mitigate the environmental impact of fossil fuel and maintain the market demands.

In Canada, since 2005 cumulative installed non-hydro renewable electricity capacity has grown almost 700%, from 2 GW to more than 18 GW in 2017 [5]. Similar target was set by the EU since 2007 for raising the share of renewable energy in the EU to 20% and reducing greenhouse gases by 20% in the year 2020 compared to 1990. Moreover, during the fourth phase of the EU emission trading system (ETS, 2021-2030), the EU is aiming to cut its emissions by at least 40% by 2030, in line with the 2015 Paris Agreement on climate change [6] and intends to achieve a further reduction to 80-90% by 2050 [7]. Recent legally binding climate change obligations according to the Paris Climate Agreement from 2016 [8] sets out how countries should reduce their emissions, adapt to climate impacts, and finance the low-carbon economy over the coming decades [9].

Biomass, as one of renewable fuel sources, has the potential of positive impact on environment by being a CO₂ neutral. Although biomass CO₂ emission is the same as that generated by fossil fuel during combustion, this amount of carbon dioxide is re-absorbed (removed from atmosphere) by growing new plants. Therefore, biomass can be considered a CO₂
neutral fuel as far as it is sustainably harvested and grown [10]. With the growing concern about the environmental impact of fossil fuel on climate change, it is desirable to find alternative or renewable energy sources. One of the alternative techniques used for that purpose is co-firing coal with biomass which has been shown to be the lowest cost method for generating green power and reducing fossil fuel-based CO$_2$ [11, 12]. Conceptually, co-firing originated from coal blends that are commonly used in pulverized fuel-fired power plant. Based on the experience, one type of coal exhibited synergetic effects when co-fired with other type of coal. The rationale is to improve the economic viability by increasing fuel flexibility, improving combustion behavior, mitigating operational problems (e.g. ash deposition), and decreasing gaseous air pollutant emissions [13]. Currently, co-firing may be defined as the process of burning a renewable fuel (e.g. biomass) together with the primary fuel (e.g. coal). Co-firing, among the less expensive alternatives, has recently attracted the interest of electric utilities.

Globally, biomass cofiring has been applied in more than 240 power plants, in which 48%, 24%, 19%, and 9% are equipped with suspension-firing, bubbling fluidized bed (BFB), circulating fluidized bed (CFB), and grate boilers, respectively [14, 15]. As short-term fuel alternative, coal/biomass co-firing in existing coal-fired power plant has been worldwide demonstrated in many installations for a variety of fuels and furnaces [16]. Based on studies in North America and Europe [17], burning biomass with fossil fuel has a positive impact on the environment and the economics of power generation. It has virtually, no sulfur and lower nitrogen content. Co-firing also minimizes biomass waste and the associated problem of waste disposal [9]. However, biomass co-firing has some challenges as well. High capital investment is the major concern in this regard. Moreover, biomass logistics is one of these challenges due to the intrinsic characteristics of biomass, such as scattered harvesting areas, lower energy density than fossil fuels, and seasonality, in addition to the risks related to the technological damages in the existing plant which might be caused by using the additional fuel [18]. In U.S., more than 80 power plants have utilized biomass co-firing and showed a high potential to expand this technology. Canada is also projecting a similar type of growth in biomass co-firing [19].
1.2 Literature Review

Three types of co-firing biomass fuel in coal-fired boilers have been demonstrated on industrial scale in terms of feeding the biomass materials [20]. These are direct, indirect, and parallel co-firing.

1.2.1 Types of Co-firing Biomass

Direct Co-firing

This is the most commonly applied co-firing technique and the least expensive since it does not require a high capital investment for making necessary modifications because, the cost of adapting an existing coal-fired power plant to co-combust biomass is lower than that of building a standalone plant dedicated for combustion of biomass [21]. In the direct co-firing, the biomass and coal are fed and combusted in the same coal boiler but can be pulverised either by the same or separate mills [22]. In this technology, the biomass co-firing share is about 3-5% and may reach to 20% when cyclone boilers are used [23]. Most of co-firing issues appear with increasing biomass mix ratio beyond 5% on mass base, due to the low quality of biomass and/or lack of dedicated infrastructure [24]. However, quantity of shared biomass may also be limited by the capacity of the boiler especially when cyclone boilers are in use. Moreover, the high ash content of some biomass fuels, for instance herbaceous materials, may be a challenge in the coal-boiler since there can be a higher tendency of ash deposition problems such as slagging, fouling and corrosion on the heat transfer surface of the boiler [25]. In most cases, the biomass thermal input in direct co-firing schemes is around 10% due to technical and economical restraints [26, 27].

Indirect co-firing

In this technology the synthetic gas produced by the gasification of solid biomass is co-fired along with fossil fuel such as coal in an existing coal burner. Usually, this is done by installing a separate biomass gasifier in the existing coal-fired unit to convert the solid biomass into syngas which is a low calorific value fuel gas. This fuel gas can be indirectly co-fired either in existing oil- or gas-fired system. Installing a separate biomass gasifier to produce the syngas can make this technology more expensive than direct co-firing. However, capital cost of installing new biomass gasifier for an indirect co-firing system can be regarded as being a pre-processing equipment as in direct co-firing. On the other hand, this type of co-firing has significant degree of fuel flexibility covering many types of biomasses such as sawdust, wood waste, and wood chips with
no pre-drying of the fuel. It can also be adapted with larger quantities of biomass with coal compared to direct co-firing [28, 22].

**Parallel Co-firing**

In this co-firing mode, a biomass boiler runs independently in parallel to the existing coal-fired boiler to produce low pressure and temperature steam. This steam is then utilized to meet the process demand of coal-fired power plant instead of using high-pressure steam from the main coal fired boiler [20]. It can achieve higher efficiency [28] and involves significantly higher capital investment than the afore-mentioned co-firing systems, though it is still less costly as compared to a stand-alone biomass power plant. Parallel and indirect co-firing schemes are more suitable for biomass fuels that contain problematic compounds or when the ash quality is of great importance for subsequent sale, use or disposal separately from coal ash [29]. The economic feasibility of biomass co-firing will mostly depend on the relative cost of coal and biomass available at the plant. Incentives for the mitigation of CO₂ emissions may play a crucial role for economic feasibility of biomass co-firing [30]. Figure 1.1 shows a schematic of the three modes of co-firing.

![Figure 1.1 Schematic of the three co-firing modes.](image)
1.2.2 Reduction of NOx emission

Co-firing biomass with coal has the capability to reduce SOx levels from existing pulverized coal fired power plants [1]. Unlike coal, biomass has low sulfur content; therefore, it is anticipated that co-firing can result in dilution of SO2 emission. However, NOx emission represents one of the problematic issues that have raised environmental concerns about coal and biomass combustion [31]. NOx formation is more complicated than SOx formation and it does not only depend on the available nitrogen mass fraction.

There are three types of NOx formation during fuel combustion - thermal, prompt and fuel NOx. Thermal NOx is mainly associated with atmospheric nitrogen under relatively high temperature of the mixture in a fuel-lean zone during combustion. Prompt NOx can be formed at lower temperature and fuel-rich zones especially if combustion has short residence time [32, 33] and it is relatively small with respect to other two forms of formation. Fuel NOx is formed from nitrogen bound in the solid fuel (fuel-N), and it is usually released as volatile-N and char-N during devolatilization. NOx emission during combustion depends, in part, on the nitrogen bound in parent fuel forming mostly NO, N2O, NH3 and HCN [34, 35]. During devolatilization of coal, HCN is formed as an intermediate product that appears in the fuel-rich eddies in the coal-dominated flame but little or non-detectable concentration of NH3. In contrast, NH3 concentration appears in biomass-dominant flame with little or non-detectable HCN.

For biomass, about 70-90% of fuel nitrogen is originated from volatile matter and released during devolatilization. The remaining nitrogen content of 10-30% is present in the fuel fixed carbon (as char-N). Fixed carbon is the non-volatile carbon remaining in coal or biomass. In some literatures it is also referred to as char. The main form of nitrogen oxide produced during biomass combustion is NO [34, 36]. Some N2O is formed during the fixed carbon oxidation stage (char combustion), but the reported concentrations are very low compared to NO concentration [36]. Besides, NO can be heterogeneously reduced to N2 by fixed carbon [34].

Air staging

Air-staged combustion is considered one of the most efficient conventional technologies for reducing NOx emissions, and it is widely adopted in coal-fired power plants [37]. The general principle of air-staging combustion is to create two distinct zones of combustion inside the furnace. The first zone is fuel rich/oxygen deficient and the second zone is fuel lean/oxygen rich. During air-staging, the released nitrogen intermediates (NH3 and HCN) that are responsible for
NO formation become reduced to N₂ as desired, providing an in-situ thermal de-NOx-ing source [38, 39]. The additional secondary burnout air will help to complete the combustion of unburnt hydrocarbons [40]. Figure 1.2 shows the effect of air-staging on NOₓ formation for a variety of fuels [40]. Both torrefied and untreated biomass have similar NOₓ reduction potential of 82-87%. Co-firing of coal/biomass in a pulverized coal furnace shows that the conversion of fuel-N to NO decreased with increasing percent biomass in the blended fuel [41], which can be explained by the high volatile content of biomass compared to coal.

![Figure 1.1 Impact of air staging on NOx emission for different fuel types](image)

Li et al. [42] further developed a new volumetric combustion technique for up to 100% biomass in coal-fired boiler, based on the concept originally proposed by Blasiak et al. in 2008 [43, 44]. The method is to combine air-staging and internal flue gas recirculation, leading to very intensive mixing and internal recirculation inside the combustion chamber as shown in Figure 1.3. It allows an increase in secondary air up to 30-40% without causing unstable or incomplete combustion.
The rate of NO\textsubscript{x} formation depends on three main parameters namely, temperature, oxygen concentration and residence time [45]. Some burners are designed with over fire air (OFA) system, a NO\textsubscript{x} reduction technique by creating a fuel-rich primary combustion zone through the removal of portion of air in the primary combustion zone to reduce both fuel and thermal NO\textsubscript{x} formation and then the staged air is fed to the secondary combustion zone downstream to complete the combustion and facilitate the full combustion of CO that was produced in the primary zone. This technology has been developed recently to further improve NO\textsubscript{x} reduction from 10 to 50% as in the case of separate over fire air (SOFA) technique with a deep-air-staged with an OFA ratio accedes 25% [46, 47]. SOFA is installed distantly above the burner zone whereby close-coupled over fire air CCOFA is installed immediately above the top burners in a tangential-fired boiler [48, 49].

**Fuel staging**

This technique is also referred to as (reburning) and in some studies has been regarded as combustion modification technology and it is promising strategy for removing NO\textsubscript{x} in combustion systems [50]. It involves injecting a secondary fuel, gaseous, liquid, or solid with high hydrocarbon content downstream of the primary combustion zone to create a secondary fuel-rich zone. Three zones are recognized in this technology. Primary zone, in which about 80% of the fuel heat input is combusted with air access followed by a reburning zone downstream where 20% of the reburning fuel is injected to generate a fuel rich condition so that NO\textsubscript{x} from the primary zone is reduced to N\textsubscript{2} and intermediate nitrogenous species. Lastly, over-fire air is injected to the burnout zone to oxidise the remaining combustible compounds resulted from the reburning zone [51]. This measure aims to benefit from the HCN or NH\textsubscript{3} that is formed as intermediate species during combustion of hydrocarbon fuel so that it reacts with NO that was formed as products of the primary fuel.

Although some new NO will be formed in the reburn zone, the final result is mitigation of NO. The amount of reburning fuel could be 10% to 20 %, on energy basis [52]. Originally, the reburning fuel was natural gas and later it was found that injecting high volatile fuel results in similar behaviour to gaseous fuel and slightly better than coal. Moreover, well ground fuel to produce fine particles and enough residence time enhance the opportunity of lowering the final NO in flue gases [53]. Since, thermal (used for combustion) coals contain 40–50% VM while,
biomass contain up to 80% VM on a DAF basis. Therefore, biomass has the potential to be a very effective reburn fuel when coal is used as the primary fuel [54]. Another measure is called afterburning in which the secondary fuel is injected near the exit of the cyclone in circulating fluidized bed boiler to rise the gas temperature for reduction of N\textsubscript{2}O [55]. NO reduction efficiencies may reach up to 50-60% according to some studies [51, 56].

1.2.3 Fuel mixture

A mix ratio for co-firing, sometimes referred to as co-firing level or co-firing rate, is one of the major challenges in co-firing. It is always restricted by cost and performance of the plant and it varies with different plants [3]. Restriction stems from difficulties to adapt several logistical, economic, and technical factors like quality and availability of biomass used and its supply chain, necessary plant modifications, environmental issues and the quality of by product [57]. For low levels of co-firing (up to 5–8% biomass), wood can be combined with coal prior to pulverization [58]. At medium levels (10–15% biomass), a separate wood preparation and delivery system should be provided with the boiler operation based on the coal characteristics. At moderately high levels (25–50%), a multi-fuel system, such as a fluidized bed, should be used. At high levels (above 50%), a boiler designed specifically for biomass operation should be used exclusively [1]. Although pulverized coal type boilers are more commonly used in co-firing, but co-firing level is limited in this type of the boiler by the particle sizes which can be ground to 10-20 mm whereby coal particles are ground to 75-300 µm and high moisture content of biomass [10, 59]. Research has shown that direct co-firing is about 2% more efficient than the other co-firing technologies in terms of loss on ignition (LOI) that occurs in the biomass gasifiers and boilers [57]. However, the efficiency of direct co-firing plants decreases when biomass co-firing levels increase due to fouling, slagging and associated corrosion that may occur in the boiler in addition to flame stability problems. Another disadvantage of biomass is its relatively low energy density.

Figure 1.3 shows the energy density of fuel types used in this study versus corresponding fuel particle density. Energy density of biomass ranges from 11-27 GJ/m\textsuperscript{3} whereas coal has higher energy density (42-49 GJ/m\textsuperscript{3}). This is because biomass is lighter than coal and its heating value is lower than coal. Consequently, when coal is partially or fully replaced by biomass, a larger
volume needs to be handled by the existing system, i.e., the volume of flue gases will increase with increasing biomass co-firing level.

Figure 1. 3 Fuel energy density versus particle density of fuel types used in this research

1.2.4 Fuel Type

Due to the increasing demand for biomass fuel, and the limited availability of wood resources, efforts have been to extend the span of raw biomass material to include fibrous residues from agriculture and food processing industry such as straws pulps and husks for pelletization [60]. It is difficult to establish a “representative biomass” due to the larger variations in the properties among biomass species when compared to the coal types. A comparison of the properties of biomass and coal is shown in Table 1.1. Biomass has lower fixed carbon content and higher volatile matter content as well as substantially higher elemental oxygen content and lower carbon content. Moreover, biomass has lower nitrogen and ash content, which can vary widely among biomass types, and are directly related to NO\textsubscript{x} emissions, corrosion, and ash deposition. Biomass in general has relatively low or negligible amount of sulfur compared to coal.

These differences will be reflected in the co-firing behavior as the carbon conversion process will slow down due to increasing percentage of biomass in the fuel mix. Fixed carbon oxidation is at the slowest stage during solid fuel conversion and the oxidation rate affects the unburnt carbon in ash which governs the combustion efficiency. Moreover, the high volatile content in biomass leads to earlier ignition while the lower heating value results in a longer and less intense flame compared to coal; hence a longer residence time is required for complete combustion.
Collins et al. [40] studied and compared a variety of fuels and found that the CO level in flue gas was negligible in all cases, as depicted in Figure 1.4 [40]. Fuels with lower NO<sub>x</sub> emissions have higher volatile content even in the case of mono firing. Co-firing biomass with coal produced much less SO<sub>2</sub> due to dilution. However, the extent of reduction in NO<sub>x</sub> is different from SO<sub>2</sub> when co-firing 50% torrefied biomass with coal as NO<sub>x</sub> emission does not only depend on fuel nitrogen content. For instance, NO<sub>x</sub> reduction can result from the higher volatile content of biomass.

![Figure 1.4 CO, NOx and SO2 concentrations in the flue gas at the furnace exit for various fuels [40].](image)

| Properties and composition of the various types of biomass and coal fuel [40] |
|---------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Fuel properties                 | Torrefied forest residue | Torrefied pine | Torrefied Spruce | White wood (untreated) | Lausatian lignite | El Cerrejon hard coal |
| Heating value, (kJ kg<sup>-1</sup>) as received | 19,597 | 20,935 | 20,222 | 18,668 | 21,066 | 27,307 |
| LHV                             | 17,837 | 19,207 | 18,570 | 17,337 | 20,710 | 26,158 |
| Moisture, W                     | 8.00   | 6.83   | 3.35   | 7.90   | 11.30 | 2.74  |
| Ash, A (db)                     | 3.12   | 0.61   | 0.36   | 1.19   | 5.22  | 14.29 |
| Volatiles, V (db)               | 74.53  | 75.49  | 74.35  | 81.21  | 57.33 | 34.43 |
| Fixed carbon, C<sub>f</sub> (db) | 25.47  | 24.51  | 25.65  | 18.79  | 42.70 | 65.62 |
| Ultimate analysis, mass fraction (%)   | C   | H<sub>f</sub> | N | S   | C   | H<sub>f</sub> | N | S   |
| Dry and ash free material (%)    | 54.57 | 4.79 | 0.45 | 0.04 | 55.29 | 6.1 | 0.2 | 0.04 |
|                                  | 54.41 | 6.0  | 0.2  | 0.03 | 50.88 | 6.0  | 0.2  | 0.03 |
|                                  | 50.88 | 6.0  | 0.2  | 0.03 | 50.88 | 6.0  | 0.2  | 0.03 |
|                                  | 66.49 | 5.37 | 0.61 | 0.99 | 66.49 | 5.37 | 0.61 | 0.99 |
|                                  | 79.41 | 5.65 | 1.64 | 0.44 | 79.41 | 5.65 | 1.64 | 0.44 |

The high moisture and ash contents in biomass fuels can cause ignition and combustion problems. The fractional heat contribution by volatile matter in biomass is in the order of 70% compared to 36% for coal. Because of the lower heating values, biomass is accompanied by flame...
stability problems. It is anticipated that blending biomass with higher quality coal will reduce the flame stability problems.

Though biomass materials in general contain less ash fraction than coal, the nature of biomass ash differs from coal ash. Therefore, options of utilizing ash resulting from co-firing is sometimes one of the constraints [24].

1.2.5 Particle size and shape

Pulverized fuel particles have certain shape and size depending on the type of fuel, as well as the method and intensity of grinding. Both particle shape and particle size distribution (PSD) are important factors that can influence drag force, heat conduction across fuel particle, and unburnt carbon which represents the remaining unburnt fixed carbon in the exhaust with ash [3, 12]. Biomass particles are larger than pulverized coal particles when using the same grinding machine to prepare biomass-coal blends. However, pulverized biomass has wider PSD because of the lower grindability of biomass compared to coal [61]. Particle shape and size also influence the combustion efficiency and residence time [62].

Shape factor or aspect ratio [63] is used to describe the asphericity of the fuel particle. It is defined as the ratio of “the surface area of an equivalent sphere having the same volume as the particle” and “the actual surface area of the particle”:

\[
\phi = \frac{S_e}{S_a}
\]

where \( \phi \) is the shape factor, \( S_e \) is the surface area of an equivalent sphere having the same volume of the particle (m\(^2\)), and \( S_a \) is the surface area of the actual particle (m\(^2\)). Particles are assumed to have a spherical shape. According to the study by Rezaei et al. [64], ground wood pellet particles were more spherical than ground wood chip particles, the former having a sphericity of 0.73 as compared to 0.45 for the latter. Asphericity plays a significant role in the overall conversion (time and rate) and its effect becomes greater with increasing particle size and aspect ratio [65].

The solid fuel conversion process consists of four distinct stages. The first stage is inert heating and drying whereby moisture in the fuel is released as water vapor. The heat required for drying is taken from the combustion energy leading to a reduction in the combustion temperature and hence the efficiency. The second stage is devolatilization when the volatile matter starts to be released out of the particles. The third stage is volatile combustion, and the fourth stage is char combustion.
Aspect ratio of particle can affect the rates of volatile yield and char yield. Near-spherical particles are reported to yield slightly lower volatile with respect to other shapes [66]. Particles with large aspect ratio and highly irregular shape will experience significant differences in heating rate at different parts of the particle, so that different combustion stages may coexist within a single particle [67]. According to Lu et al. [66], large temperature gradients can exist in large biomass particles, and the conversion process has been proven to be dominated by heat transfer rather than kinetics since both particle shape and size influence the conversion time.

One of the significant factors that affect the stability and efficiency of a combustion devices is the fluid dynamic analysis [68]. Generally, heat transfer in ducts can be enhanced by swirling flow. Different techniques have been developed and investigated to improve the decaying and non-decaying swirl flow characteristics [68]. Throughout several investigations on swirl combustors, it is found that flame confinement with an intense swirling flow creates two distinguished zones. An external recirculation zone (ERZ) on the top corners and an internal recirculation zone on the centre. A reverse hot flow on the burner centerline impedes the fuel jet axially and induces a rapid mixing and flame stabilisation [69]. Combustion efficiency, stability and pollutant emissions are strongly linked to the significance of the mixing process between the reactants due to the shorter kinetic time scale compared to turbulent timescale [70].

Coghe [69] found that the large IRZ depends on the swirl intensity and the increase in swirl will reduce the temperature gradient throughout the combustion reactions possibly leading to improve the reactant pre-heating and leaning the mixture compared to the inlet condition. Anufriev et al. [71] have carried out a numerical modeling of coal combustion in a vortex furnace and characterized a new design modification by adding a tangential-injection nozzle located at the bottom of the combustion chamber to enhance the swirl intensity at the same time maintaining a more uniform temperature field. S Long [72] et al. have conducted experimental investigations on an application of confined swirl combustors. Multiple Impinging Jets in a Cylindrical Chamber (MIJCC) was investigated which can be related to burner arrangements that have a central fuel jet and co-annular air jet. This arrangement consists of a cylindrical chamber with a conical expansion. The MIJCC is provided with four rotationally symmetric inlet jets distributed around the conical expansion. The effect of fuel jet inclination angle, its azimuthal angle, and aspect ratio of the system on the flow pattern was investigated [73, 74].
**Pelletization**

Since biomass is classified as CO$_2$ neutral fuel by considering its life cycle, it has been attracting attention by energy utilities. Attempts to overcome the poor transport efficiency of raw biomass have resulted in an increasing demand for biomass densification technology such as pelletization [60]. Biomass pelletization is a standard method to produce high-density solid biofuel from biomass by compressing biomass particles into pellet form. It improves the mechanical and physical properties of biomass and facilitates its handling in the supply chain [75, 76]. Pelletizing also reduces the variation in physical properties among the particles [64]. High density of pellets leads to high energy density (i.e. energy content per unit volume of fuel), hence this permits compact storage and improved transport over long distance [77, 78, 79, 80, 81]. Much research has been focused on pellet characteristics, which include the physical and mechanical properties, energy content and transportability which are of high importance before the use of pellets in combustion [81, 82]. In Canada, a study showed that the global demand for pellets production is rapidly increasing and is projected to triple between 2012 and 2020 growing from 16 million to 46 million metric tons per year [83, 84].

The quality of pellets depends on the feedstock and pellet characteristics such as pellet dimensions (length and diameter), pellet density, durability, moisture content, ash content, and other parameters according to different standards for densified fuel. These parameters are important for the design and operation efficiency of a combustion system. High bulk density is associated with lower storage requirement and greater transport capacity [85]. Whereas low bulk density is linked to lower energy density with unfavorable consequences on the transportation costs and storage capacity for pellet producers and the end users [86]. Furthermore, bulk density has a direct link with pellet durability, or mechanical strength; hence it determines whether pellets can be suitably produced or not [82]. The durability of the biomass pellets was found to depend on the physical characteristics of biomass such as particle size [79, 82] and process conditions that include pelletizing temperature and pressure [75].

During pelletizing, compression force decreases the size, and changes the shape of biomass particles; thus, pellet particles become denser after pelletizing [86, 87]. For agricultural and woody biomass, pellets made from smaller particle size (150-300 μm) exhibited higher density and higher yield stress [79]. Using pinewood as the raw material, Rezaei et al [64] investigated experimentally the thermal behavior of a single ground chip particle and a single
ground pellet particle in the range of 0.25~5 mm. The ground pellet particle was found to be 3-4 times denser than the ground chips particle having similar volume [80]. Other experimental studies have been conducted on coal combustion, biomass combustion and co-firing coal with a variety of non-densified fuel that include woody and agricultural biomass [17]. Coal combustion showed smaller flame volume compared to biomass combustion, mainly due to the lower energy content and the greater size and non-uniform shape of the biomass particles.

1.2.6 Biomass Torrefaction

Despite the advantages of utilising biomass as fuel, there are some challenges associated with biomass characteristics in comparison with fossil fuel. Raw biomass co-firing is practically limited to 5–10% due to unfavourable properties of biomass. For instance, biomass has lower density and heating value, higher moisture content, hydrophilicity, fibrous nature and lower grindability, which make biomass more restricted to be used in energy production. To attenuate the negative influences of these disadvantages, much research has been done on biomass pre-treatment methods to upgrade biomass characteristics so that it can be used competitively with coal in co-firing systems or to be burned alone in mono-firing systems [88, 89].

Torrefaction is one of the pre-treatment methods for biomass upgrading. It can be defined as a mild form of pyrolysis which typically takes place between 200–300 °C in the absence of oxygen. The process produces a brown to black uniform solid product, as well as condensable (water, organics, and lipids) and non-condensable gases including CO₂, CO, and CH₄ [88]. Aside from pelletizing, torrefaction is another promising way of producing high quality solid biofuel from raw biomass [90]. The constituents of raw biomass comprise three main components, cellulose, hemicellulose, and lignin in addition to inorganic and other organic components [91, 92]. Cellulose and hemicellulose vary in their thermal decomposition behavior due to their different structures [93, 91]. Hemicellulose thermally decomposes in the range of 220 -315 °C, whereas thermal decomposition of cellulose occurs between 315-400 °C. Lignin will go through more gradual thermal decomposition that takes place between 160 and 900 °C [93, 94].

During torrefaction, biomass can significantly lose moisture and some of the volatiles. The biomass heating value could be significantly improved, depending on the torrefaction process conditions. Typically, more than 70% of the dry matter can be retained as the solid product that contains 90% of the initial energy content, while 30% of the lost dry matter is converted into
condensable and non-condensable gases. Hence, the final product has greater heating value, better grindability, higher hydrophobicity and lower true density. Torrefied biomass can be called “bio-coal” if it has characteristics that closely resemble that of coal [95]. Torrefaction is being investigated through a lot of research to overcome the challenges and to enhance the cost savings in logistic systems. It shows a potential of increasing the energy density by approximately 30%, as torrefied biomass typically contains 70% to 80% of the original solid mass while retaining 80% to 90% of the initial energy content [18, 96]. Therefore, torrefaction can potentially lead to a reduction in the feedstock delivered cost and thus improve the co-firing ratio [97]. Published research indicates a high potential of this pre-treatment method for producing solid biofuel [98, 99].

**Factors that influence the torrefaction of biomass**

When biomass is gradually heated, the main component that starts to decompose is hemicellulose because it is the most reactive polymer of lignocellulosic biomass [100]. It is the organic fraction of biomass that has a lower heating value, lower thermal stability, higher O/C atomic ratio compared to cellulose and lignin that are also affected to some extent depending on the torrefaction temperature and residence time [98]. This selective degradation of hemicellulose would lead to higher carbon and higher energy content in the treated biomass. As a result, the final product of torrefaction process has lower O/C ratio, better grindability, lower moisture and hygroscopicity and less volatile matter content. All these changes make it a more feasible fuel compared to raw biomass [98, 96, 101].

Increasing the torrefaction temperature may result in decline of mass and energy yields [100]. According to torrefaction temperature, the degree of torrefaction can be categorized into mild (200-240 C), medium (240-260 C) and severe (260-300 C). By increasing torrefaction temperature, fixed carbon and ash contents increase. On the other hand, large amount of hemicellulose and part of cellulose decomposes to produce water and light volatile components which results in reduced volatile content of the product compared to raw biomass. The decrease in hydrogen and oxygen contents in the torrefied biomass might be attributed to the release of moisture and the formation of some hydrogen-rich gases during torrefaction. Moreover, studies have shown that increasing torrefaction temperature and residence time improve biomass heating value, energy density and grindability [102, 103].
Heating rate during torrefaction has an influence on the final product composition. More char is produced when the heating rate is slower [102]. Whereas, prolonging the residence time leads to the release of more volatiles so that less solid product or char is produced. Despite the high energy density that results from severe torrefaction, it is not recommended for energy applications because of the high dry matter loss [100] unless the relative amount of the resulting fixed carbon can counteract the dry matter loss. Yet, in terms of transportation, storage and combustion properties, mild torrefaction is not as favorable when compared to severe or medium torrefaction.

1.2.7 Coal tailings

Fine coal tailings are fine-grained wastes produced during the processing of coal and are quite abundant in the coal mining industry. Generally, these wastes are in the form of slurry, and it can be hydraulically disposed at the disposal locations [104]. Coal tailings are generated from fine coal processing streams, which can represent 10-20% or more depending on the processing scenario and the type of coal produced during the Coal Handling and Processing at the Preparation Plant (CHPP) feed [105, 106]. Until recent few decades, fine coals that were difficult to clean using traditional coal processing methods have been rejected during the processing, and large volume of tailings stream were disposed into the environment leading to a loss in energy resources and causing negative environmental impact. As an example, coal preparation plant at Smoky River Coal Ltd, (Grande Cache, Alberta), was producing more than 900 m$^3$/hr tailings that contain less than 3% solids, and about 60% of the coal was discarded in the form of fines [107].

In order to safely dispose such diluted coal tailings, water needs to be removed by thickening and in some instances by mechanical dewatering requiring additional processing units to be included in CHPP [107]. If these additional processing units are not implemented, a huge amount of fine coal is accumulated in the tailing dams which have a hazardous environmental impact on air, soil, and ground water pollution, [108, 109, 110] in addition, to visual impacts on landscape, slag heaps and slag-heap fires, subsidence and general degradation on local biodiversity [111, 112]. However, if these fines are properly recovered or treated, coal waste can be reused in different applications such as building, road making, and so on.

**Sources and availability**
From the utilization point of view, higher rank coals are mainly used for coke production in the steel industry, about 70% of produced coal around the world is used for making coke and close to 40% of the world’s coal production is for electricity generation. The higher-rank coals with high quality are referred to as metallurgical coals, while those used for electricity generation are called thermal or steam coals. The ash content has adverse effect on both the quality and coke production rate. Coke consumption in blast furnace increases by about 4-5% and the furnace productivity decreases by 3-6% for every 1% increase in the ash content of coals [113]. In order for coal to be suitable for coke production, it needs to be in the range of medium to low volatile rank, have low ash content (usually below 10%) and low Sulphur and nitrogen contents as well as the right ratio of organic content in terms of reactive and inert components; also, it needs to possess good thermo-plastic properties.

The purpose of coal preparation is to obtain the right quality product during the processing, while the main objective of cleaning the metallurgical coal is to reduce the ash content (<10%), control the S and if possible, N levels, but very little can be done to control the reactive-to-inert ratio of organic matter. Since run-of-mine coal has usually much higher ash content than required for coke production, cleaning of coal is necessary. Coal processing on industrial scale includes a few circuits (in parallel) for cleaning and each circuit is designed to process a specific size range of coal particles. A combination of gravity separation and froth flotation is used to clean coarse and fine coal respectively, especially for metallurgical coals all size ranges are recovered to capture all valuable coal particles. However, processing is not always efficient especially for very fine coal, hence some fine coal is rejected.

For thermal coals, usually the processing includes only cleaning of coarser fractions, hence very fine coal is automatically rejected as tailings. Tailings from processing of thermal coals usually contain more fines in rejected fraction than in metallurgical coals. For electricity generation all types of coals can be used, low, high or medium rank coals are equally suitable, and cleaning usually is performed to reduce ash and moisture content to adequate levels in order to increase their calorific values in the final product.

Consequently, if the coal tailings are to be reutilized in any form it is paramount to seek eco-innovative solutions with a cost-effective strategy to recover these fine coal tailings for the purpose of energy recovery [114]. Recovery of fine coal from tailings could become a value proposition to overcome the environmental issues. Different approaches were developed and
implemented during the recent decades [115]. Their high ash content and thus low calorific value restrict their applications as energy commodity; hence it is imperative to de-ash coal tailings before re-utilization as energy source. However, removing ash from tailings is more difficult compared to raw coal [116]. Asghari et.al, [111] has conducted different experimental investigations on coal tailings recovery including gravity (jigging, tabling and spiral) and flotation separation techniques to identify the optimum conditions to recover coal by each technique and to evaluate the percentage of coal tailing recovery that can be re-used in steel making industry [111]. Results showed that these methods can recover 90% of value coal particles and reduce ash content to 14%. On the other hand, life cycle analysis by Adiansyah [117], showed that prior selecting a tailing disposal method, it is important to consider the economic analysis along with environmental impact aspects as part of sustainable consideration [118, 117].

**Potential re-use of coal tailings**

Coal tailings have good potential to be reused because, their heating value (depending on the rank of coal) in higher rank coals ranges from 20-30 MJ/kg. It is often disposed in a large settling lagoon close to the colliery as it is the most economical and the most convenient way. Few studies have been focusing on examining coal tailings potential as a fuel (or, as energy source). First successful reported trial was a project by Radolf *et. al.*, [119]. The project was a part of a rehabilitation of a colliery in Australia. Coal tailings briquettes of 5 cm diameter were produced in a capacity of 70,000 ton/year using a double roller press. The produced briquettes were burned in a local coal power station with a mixing ratio about 10%. Adding biomass to coal tailings briquettes can increase the strength of the produced briquettes due to the fibrous nature of biomass. Moreover, it decreases CO₂ emission considering biomass a CO₂ neutral fuel [119]. Finney *et. al.* [120], have investigated energy recovering of spent mushroom compost (SMC) and coal tailings when they are co-fired together in fluidized-bed and packed-bed [120]. Combustion efficiency in a fluidized-bed outperforms the packed-bed while both produced minimal acid gas (NOₓ, SOₓ, and HCl).

The same fuel blend was further investigated by Ryu et.al. [121], to study the characteristics of pellets made of the two waste materials (spent mushroom compost “SMC” and recovered coal tailings). Pellets were manufactured using small compression rig then the pellets quality were assessed according to their density, swelling, tensile strength and durability. Pellets tensile
strength was proportional to the SMC percentage. The SMC pellets were more durable than coal tailing pellets due to the intertwined fibers of SMC [121]. Economic feasibility and cost analysis of pellet production made from the same blend mentioned above showed that the moisture content of both wet materials affected the cost of transportation, drying and energy consumption. The potential targeted market for these pellets were suggested to be the mushroom producers for SMC pellets, sewage sludge incinerators for coal tailings pellets and mixed pellets for power plants [122].

1.2.8 Computational Fluid Dynamics (CFD)

Computational fluid dynamics (CFD) technique provides useful means to simulate a wide spectrum of engineering applications. Among the CFD applications are simulation of fluid flow with the capability of predicting heat and mass transfer, phase changes, multi-phase problems (i.e., solid-liquid-gas interaction), and chemical reactions using different reaction mechanisms [123]. Researchers have been using CFD to simulate and analyze the performance of thermochemical conversion equipment such as fluidized beds, fixed beds, combustion furnaces, firing boilers etc. CFD is proven as a good tool for design optimization and retrofitting. Recent progress in numerical techniques and computing performance has advanced CFD as a widely used approach to provide efficient design solutions in industry [124].

CFD Algorithms

Numerical algorithm of CFD comprises integration of the governing equations of the flow domain after discretizing it into a grid of very small fluid elements then solving these equations as a system of algebraic equations using iterative method. The accuracy of solution depends mainly on mesh design and the definition of the domain geometry whereby more than 50% of the time is spent to maintain these two essential tasks for CFD projects in industry [125].

There are no straightforward guidelines for an accurate converged solution since it is problem dependent. Moreover, the speed to achieve convergence would require considerable experience with the code and can only be maintained by extensive use [125]. Verification of convergence is usually tested by mesh independency study. This is to eliminate errors result from the coarseness of the mesh. It can be assessed by comparing successive refinement of a coarse mesh until there is no significant change in the key results [126]. The solution can be precise (i.e., verified) but not necessarily accurate; hence it should be validated. Validation assessment of CFD results can only be done by comparison with a benchmark experimental result. Hence, CFD does
not replace experimentation rather it is a very powerful additional problem solving and retrofitting tool and can be used to attain deeper understanding of a boundary value problem.

In the simulation of pulverized fuel or co-firing coal with biomass, the flow domain includes continuous and solid phases. Continuous phase i.e., gaseous species are simulated using Eulerian frame of reference. This approach assumes that fluid in the field domain flows through a stationary control volume element in which fluid properties are calculated by a partial differential equation form of Reynolds-Averaged Navier-Stokes (RANS) equations using one of the numerical methods (finite difference, finite elements, or finite volume). RANS is one form of Navier-Stokes equations in a time-averaged version, which describes the turbulence in fluid properties by defining the instantaneous properties in the conservation equations ($\phi$) as mean value plus a fluctuating component.

$$\phi = \overline{\phi} + \phi'$$ (1.2)

Common RANS models assume that an increase in turbulence can be represented by an increase in effective fluid viscosity and the Reynolds stresses are proportional to the mean velocity gradient via the viscosity. Consequently, extra terms appear in Navier-Stokes equations due to the interaction between various turbulent fluctuations. These extra terms can be modeled by turbulence models like re-normalized group (RNG) $k$-$\varepsilon$, $k$-$\omega$, and Reynolds Stress Model (RSM). Large Eddy Simulation (LES) is another approach used to capture the larger eddies by filtering the Navier-Stokes equations to omit the smaller eddies so that the resolved flow is the mean flow plus large eddies then the filtered eddies are solved by RANS. It demands larger storage and volume of calculation due to the sub-grid scale model which solve the unresolved smaller eddies and the solution of the unsteady flow equations [127]. On the other hand, direct numerical simulation (DNS) computes all the turbulent velocity fluctuations at all length and time scales besides the solution of mean flow therefore, this type of calculation is costly and requires more computing resources.

Another approach is known as the two-mixture fraction/probability density function (PDF) model to solve the turbulent-chemistry interaction [125]. In this approach, the individual species transport equations are not solved. Instead, equations for two conserved scalars (mixture fraction of the main fuel stream represented by fixed carbon and mixture fraction of a secondary stream represented by volatiles) and their variance are solved, and individual component concentrations are derived from the predicted mixture fraction distribution. The chemistry is assumed to be fast
enough to achieve equilibrium so that the mixture fraction, $f$, can be written in terms of elemental mass fraction as:

$$f = \frac{Z_j^{ox} - Z_j^{fuel}}{Z_j^{fuel} - Z_j^{ox}}$$

(1.3)

where $Z_j$ is the mass fraction for element $j$, $ox$ and $fuel$ denote the value at the oxidizer stream inlet and the fuel stream inlet, respectively. To improve solution stability, step-by-step procedure can be implemented so that solving of gaseous phase is done first followed by the solution of discrete phase model (DPM) equations then re-calculating the gaseous phase flow field again then re-calculate the discrete phase again until solution is converged.

Ghenai and Janajreh [128] have used the method afore mentioned and determined the properties of the coal/biomass fuel mixture using the weighted average method instead of considering the properties of each fuel stream individually [128]. This may cause some uncertainties in the simulation results. Whereas, in this thesis research, the two streams of biomass and coal can be represented individually with their own properties and interacting with each other as two different fuels.

**CFD simulation of coal and biomass conversion**

Several CFD studies have been conducted on simulation of both coal and biomass to understand some influencing parameters on coal and biomass conversion. Backreedy et.al. [129], have conducted a CFD modeling study with experimental validation to examine burnout of larger particles of pinewood blended with bituminous fine coal from UK by a limited mix ratio of 3% (mass basis). Gaseous flow turbulence model used in that study was (RNG) of $k$-$\varepsilon$ turbulent model to account for swirl flow.

Biomass particles smaller than 200µm showed a fast rate of combustion compared to larger particles depending on size and shape and they maintained their irregular shape during combustion unlike coal particles which are usually soften and become more spherical. Combustion rate of larger biomass particles was found faster when they are flatter. The final flame was dominated by coal rather than biomass kinetics [129]. Ma et.al [67], have used the same model combined with model of NO$_x$ formation and potassium release to calculate both the potassium in the gas flow and the remaining potassium in the biomass ash to develop the advanced ash deposition models for the combustion system [67].

Yin et.al. [130] presented a CFD modeling study of co-firing wheat straw with coal in a 150kW swirl-stabilized dual-feed burner flow reactor. Whereby, coal and biomass are fed
independently via different injectors. Multiple simulations have been performed, using three meshes, two global reaction mechanisms for homogeneous combustion, two turbulent combustion models, and two models for fuel particle conversion.

Two sub-models were used by Yin et.al. [130]. The first sub-model is for small biomass particles where the particle temperature was assumed to experience no temperature gradient across particle diameter (i.e. Bi \ll 0.1). The second sub-model predicts the temperature distribution across the bigger biomass particles that were discretized into number of concentric shells. For each shell, the one-dimensional mass, energy, and species balance equations for gas and solid are solved. Results showed that the user defined 1-D particle model has not made a big difference compared with the default PDM laws in the conversion of biomass particles in this reactor. Gas phase combustion was modeled using two different mechanisms: Westbrook and Dryer (WD) two-step mechanism [130] and the Jones and Lindstedt (JL) four-step mechanism [130]. The WD 2-step mechanism is derived for the oxidation of hydrocarbon fuels in flames and consists of two reactions with CO as the intermediate species, in which the last step is oxidation of CO to CO$_2$. In the (JL) mechanism, the two volatiles are considered as a mixture of real species ($C_3H_8$, CH$_4$, H$_2$, HCN, NH$_3$, CO, CO$_2$ and SO$_2$). The turbulence-chemistry interaction was modeled by Eddy Dissipation Concept (EDC). This model represents an extension of the Eddy Dissipation model (EDM). It provides an empirical expression for the mean reaction rate assuming that the chemical reaction takes place in the regions of small turbulent structures called “the finite scale” where the dissipation of turbulence energy occurs. This is done by turbulent mixing in the Kolmogorov structures where fluid motion is dissipated to thermal energy due to viscous forces. Species are assumed to react in that fine structure over a specific time scale. Reactions undergone over the time scale are governed by Arrhenius rate. The source term in the conservation equation for the mean species is dependent on the length fraction of the fine scale, the time scale, and the fine-scale species mass fraction after the reaction for that time scale [131].

Gubba et.al. [2] have conducted a CFD simulation on a 300 MWe tangentially fired pulverised coal furnace with two biomass loading (6% and 12%). In this model coal particles were assumed to be spherical while biomass particles were assumed to be non-spherical. The heat transfer across the particle is modeled using one dimensional (spherical or cylindrical coordinate) of energy equation [2, 67]. Heat transfer inside the particle is governed by conduction and particle surface boundary condition is governed by convection and radiation. 78.5% of biomass fuel-N is
released as volatile-N from which 10% is converted to HCN. The rest (i.e., 21.5%) is assumed char-N and is converted totally into NO. Increasing biomass loading from 6% to 12% showed reduction in NO$_x$ emission. Moreover, for big particles internal heat transfer within biomass particle is important for more accurate results.

Bhuiyan et.al. [132] have performed CFD investigation of co-combustion coal and biomass under air and oxy-fuel conditions (recycled ratios RR, O$_2$/CO$_2$ of 68 and 75%) in a small furnace with 20 and 40% biomass loading on mass basis. Particle size of two fuels ranges from 75 µm to 300 µm and biomass has larger particles than coal. Turbulent flow is modeled by considering $k$-$\varepsilon$ model coupled with eddy break up model. The three-step mechanism was used with devolatilization modeling and two-step mechanism for fixed carbon combustion was applied. Species concentration and unburnt carbon in ash was predicted in air and the two cases of oxy fuel burning.

Further CFD investigation was conducted by the previous authors to examine oxy-fuel of (25, 30, and 35%) and compare it to reference air-fuel case maintain a 30 kW in a swirl-stabilized furnace [133]. Pure coal and pure biomass combustion were studied by investigating flame temperature, burnout, and NO$_x$ emission. Higher flame temperature was observed and higher burnout yield in oxy-fuel cases in addition to lower CO concentration downstream compared to air fired cases. Moreover, cofiring 20% of straw with coal does not significantly change the temperature profile compared to 100% coal firing. Jo et.al. [48] have conducted a CFD simulation of flow rate distribution of CCOFA and SOFA for NO$_x$ reduction in the standard 500 MWe tangential-fired boiler. Increasing SOFA ratio to 15% and 20% was for different stochiometric ratio had a significant improvement on NO$_x$ formation, unburnt carbon remaining with fly ash, and furnace exit gas temperature [48].

1.3 Problem Statement and Research Objectives
Co-firing biomass with coal has more positive impact on the environment as compared to coal combustion [11, 12]. It reduces the emissions that are pertinent to fossil fuels while minimizing the problem of waste biomass disposal. Despite the advantages of co-firing as an alternative to fossil fuel combustion, there are still some shortcomings associated with co-firing biomass in an existing coal-fired power plant [18].
One major challenge with co-firing coal and biomass is the restriction on the percentage of biomass in the blended fuel (i.e., the co-firing level) [24, 26]. It varies according to the type of plant and has direct effect on the plant performance. The restrictions can be attributed to logistical, economic, and technical factors. The efficiency of direct co-firing plant decreases with an increase in the co-firing level due to the differences in particle size and shape between coal and biomass, problems with the flame stability, and the relatively low energy density of biomass [27]. Some research work has been done to study the high percentage co-firing by air staging [37] reaching a 100% switch to biomass combustion. However, at high levels of co-firing (i.e., percentage of biomass more than 50%), the boiler should be designed exclusively for biomass operation which is associated with high capital risk [1].

Unlike coal, biomass has different particle size distribution (PSD) and relatively non-uniform particle shape aside from the differences in fixed carbon, volatile matter, oxygen, nitrogen, sulfur, and ash contents. Another major problem is the larger variations in the biomass feedstock properties versus coal. Biomass densification by pelletizing is an example of enhancing the transport efficiency and increasing the energy density of biomass. It reduces the variation in the physical properties among biomass particles and permits compact storage and rational transport over long distance [64]. Although much research has been published about pellet characteristics, including the physical and mechanical properties, energy content and transportability that are of high importance before the use of pellets for power production by combustion, few studies have addressed the effect of particles densification on the combustion process. Raw biomass can also be upgraded by torrefaction, a mild pyrolysis process in the absence of oxygen. Literature review indicates that torrefied biomass is a suitable secondary fuel that can be co-fired with coal.

Unfavorable impact of coal on the environment is not restricted to the emission of air pollutants from coal-fired power plants. Coal tailings are generated from fine coal processing operation. Cumulatively, with a large amount of coal tailings stream being disposed into the environment, it will have negative impact on the eco-system in addition to the loss in energy resources. Yet, these coal waste can be recovered or treated in various ways [114]. To-date, few studies have been done to investigate the feasibility of re-utilizing coal tailings as an alternative fuel for co-firing with biomass.
CFD modeling and simulation has provided an effective way to gain a good understanding of many boundary value problems before experimentation. Therefore, CFD can also be used to simulate, study, and retrofit the thermochemical conversion equipment and to understand the influencing parameters on coal and biomass co-firing [2, 48, 128, 132]. This will contribute to reducing the cost of retrofitting by predicting the potential implication of applying certain change on the original plant before the practical implementation of this change.

**Research Objectives**

Co-firing biomass with coal can be seen as a promising short-term alternative to mitigate environmental impact due to fossil fuel utilization. CFD modeling can be applied to address the shortcomings associated with biomass/coal co-firing and the uncertainties about the improvement in the combustion efficiency using raw or torrefied biomass for co-firing with coal. It can also be an effective tool to examine suggested modifications on furnace geometry and design.

The main goal of the thesis research is to adapt and evaluate a CFD model that can predict both the mono-firing and co-firing biomass and coal in a dual-feed furnace and use this model to help improve the combustion efficiency by making unsophisticated furnace geometry changes and study the effect of operating and boundary conditions on the combustion and emissions.

The specific objectives of this research are:

1. To investigate the effect of unsophisticated furnace geometry and design modifications on the combustion efficiency of biomass and coal at a high co-firing level.
2. To study the impact of biomass densification on the co-firing efficiency and NOx emission.
3. To compare the combustion efficiency of raw biomass vs. torrefied biomass as the fuel; and
4. To assess the technical feasibility of reutilizing metallurgical coal tailings and co-firing it with raw and torrefied biomass.

The structure of the thesis, which is based on the research objectives, is outlined below. Chapter 2 presents the CFD model used in this study with a detailed explanation of the equations involved, followed by model validation. In Chapter 3, possible modifications on the furnace geometry were suggested and CFD simulation was used to investigate its impact on the combustion efficiency. The objective of Chapter 4 is to investigate the influence of the change in biomass particle density.
due to pelletizing on combustion when biomass is co-fired with coal. Chapter 5 describes the experiments that were conducted to obtain the fuel properties required for running the CFD simulations in the next chapter. Chapter 6 elaborates on the CFD simulation of mono-firing and co-firing metallurgical coal tailings with biomass to evaluate the possibility of converting waste coal to energy. Finally, Chapter 7 summarizes the key results and findings; also, recommendations for future studies are suggested.
Chapter 2. CFD Modeling and Validation for Co-firing Biomass and Coal

2.1 Introduction

This chapter contains detailed description of the mathematical model that is used to describe the boundary value problem under study and the computational fluid dynamics (CFD) models that were implemented in the simulations. It also includes description of mesh construction used to adapt the furnace geometries of this work. The CFD model solution is tested for the mesh independence to verify the proper mesh size and quality that can be used in simulations. CFD modeling results will be compared with data published in the literature for model evaluation in section 2.4.

Damstedt [134] conducted experiments on a 150-kW swirl-stabilized down-fired reactor, and biomass was co-fired with coal using a dual feed fuel injector (details of this reactor was described in [134]). General description of the particle and gas sampling and data collection is placed in section 2.5 of the thesis. For co-firing, two fuel-streams are fed from the top center of the reactor - a central stream of fuel is injected through a circular tube that is surrounded by an annulus tube for the second fuel stream. The two fuel streams are surrounded by secondary air flowing in an annulus funnel with swirl flow. The furnace is vertically oriented, with a height of 250 cm and a cylindrical cross section 75 cm in diameter.

Cofiring mix ratio (biomass-to-coal 67:33) was used for the baseline simulation because of two main reasons. Firstly, this ratio was used in the experimental work by Damstedt [134] that is selected as a benchmark to evaluate the CFD model. Secondly, this ratio represents a high level of co-firing (greater than 50 wt% biomass [26]); so the challenges associated with high-level co-firing can be studied as one of the thesis research objectives.

The CFD model presented in section 2.2 was tested for mesh independence. Then, it was used to simulate the co-firing and conversion of wheat straw and a type of bituminous coal in the 150-kW swirl-stabilized down-fired reactor. Simulation results were compared to the experimental data reported by Damstedt [134] (using the same fuels) for validation purposes. The boundary and operating conditions are also the same.
2.2 CFD Model

In this research, combustion of coal and biomass particles was simulated individually using CFD technique. The simulation is applied on a laboratory scale furnace [134]. In the computational model, the gaseous phase is solved by means of time-averaged conservation equation for steady turbulent flow. Radiation heat transfer is modeled by the discrete ordinate model once every 10 iterations in the solution process. The dispersed phase is simulated by solving equations of motion, heat transfer and momentum in a Lagrangian frame of reference. For every 50 iterations
in the solution process, this is updated with the gaseous phase results. CFD simulation was conducted using ANSYS FLUENT software (CMC Microsystems, Kingston, ON). Simulation results were compared with experimental results reported in the literature for validation [134].

Combustion of suspended biomass particles can be modeled using different approaches [125], some of which have been mentioned in Chapter 1 (Section 1.8.2). It resembles the modeling of coal particles with some differences due to the variances in properties, size, shape and constituents between biomass and coal particles. Therefore, combustion of biomass is further complicated [135]. The model consists of four sub-models for the various processes and mechanisms involved,

1) Navier-Stokes set of equations for solving the continuous gaseous flow;
2) Predicting the moisture, devolatilization and homogenous reaction of coal and biomass;
3) Solving the heterogeneous surface reaction of fixed carbon; and
4) Conservation equations of solid particles flow to solve for the discrete phase.

All of the sub-models are simultaneously solved by iterative technique to obtain convergence of solution. A detailed description of the models is presented below.

2.2.1 Continuous flow model

In this model, momentum equation of gaseous flow in the reactor is solved using the realizable k-ε turbulence model to capture the high rate of turbulence in the flow domain especially near the reactor entrance [136, 58, 131]. Interaction between chemistry and turbulence is modeled by implementing the finite rate/eddy dissipation model. In this model, both the Arrhenius kinetics equation and the eddy dissipation rate are calculated then the net reaction rate is taken as the smaller of these two rates. In general, the eddy dissipation rate is slower than the Arrhenius kinetics rate; thus, once the flame is ignited the reactions are limited by mixing. The turbulence dispersion of particles is simulated by applying the stochastic random walk method to the instantaneous perturbations of velocity and the effect on the particle trajectories.

**Gas phase** - The momentum equation for the gas phase takes the following form,

\[
\frac{\partial}{\partial t}(\bar{\rho}\bar{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\bar{u}_j\bar{u}_i) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(\bar{\tau}_{ij} - \bar{R}_{ij})
\]  

(2.1)

where \(\bar{u}_i\) refers to Favre-averaged of velocity vector and \(\bar{p}\) is the pressure field. The viscous and Reynolds stresses arising from the Favre-averaging of the momentum equations are:
\[\tau_{ij} = \mu \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right) \] (2.1A)

\[\bar{R}_{ij} = -\bar{\rho} \bar{u}_i' \bar{u}_j'' + \mu_t \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \left( \frac{2}{3} \rho k + \mu_t \frac{\partial \tilde{u}_k}{\partial x_k} \right) \delta_{ij} \] (2.1B)

where \(\mu_t\) is the turbulent eddy viscosity and \(k\) is the turbulent kinetic energy. The Reynolds stresses are closed using the realizable k-\(\varepsilon\) turbulence model to capture the high rate of turbulence in the flow domain especially near the reactor entrance [58, 135, 137]. Turbulent kinetic energy and its rate of dissipation are given by Eq 2.2 and Eq 2.2A, respectively.

\[\frac{\partial}{\partial t} (\bar{\rho} k) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j k) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{P_{Re}} \right) \frac{\partial \tilde{u}_i}{\partial x_j} \right] + \left( -\rho u'' u'' \right) \frac{\partial \tilde{u}_i}{\partial x_i} - \bar{\rho} \varepsilon \] (2.2)

\[\frac{\partial}{\partial t} (\bar{\rho} \varepsilon) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j \varepsilon) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{P_{Re}} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_1 \frac{k}{\varepsilon} \left( -\rho u'' u'' \right) \frac{\partial \tilde{u}_i}{\partial x_i} - C_2 \frac{\varepsilon^2}{k} \] (2.2A)

where \(\mu_t = C_\mu \bar{\rho} \frac{k^2}{\varepsilon}\) is eddy viscosity ; \(C_\mu = 0.09, C_1 = 1.44, C_2 = 1.92\)

In the realisable k-\(\varepsilon\) turbulence model, the Reynolds stress and eddy viscosity equations are combined to form the normal Reynolds stress for incompressible strained mean flow as:

\[\overline{u^2} = \frac{2}{3} k - 2 \left( C_\mu \frac{k^2}{\varepsilon} \right) \times \frac{\partial \bar{u}}{\partial x} \] (2.3)

where, \(\overline{u^2}\) is the normal Reynolds stress (realizable form); \(C_\mu\) is a constant (0.09); \(k\) is the turbulent kinetic energy; \(\varepsilon\) is the turbulence dissipation rate. Therefore, the realizable model is valid when \(\overline{u^2} > 0\) , i.e. \(\frac{k}{\varepsilon} \times \frac{\partial \bar{u}}{\partial x} < 3.704\).

Validations by several studies have shown the preference of realisable k-\(\varepsilon\) turbulence model compared with the standard k-\(\varepsilon\) turbulence model in capturing the turbulence [138].

The initial values of \(k\) and \(\varepsilon\) are calculated based on \(I_T\), the turbulent intensity at the inlet boundary conditions. \(I_T\) is calculated using the following correlation [139, 131],

\[I_T = \frac{\bar{u}}{\bar{u}} = 0.16/Re^{0.125} \] (2.4)

where \(Re\) is Reynolds number based on the hydraulic diameter \(D_H\), \(\bar{u}\) is the mean gas velocity, \(\bar{u}\) is the fluctuation component beyond the mean gas velocity. For circular tubes, \(D_H\) is the tube diameter. For annular tube, \(D_H\) is the difference between the outer diameter and the inner diameter.
i.e. \((D_0 - D_1)\). Details of time averaged turbulent kinetic energy and rate of turbulent kinetic energy dissipation equations are mentioned in Appendix A.

2.2.2 Devolatilization model

Conversion of coal, or biomass, consists of four stages - heating, evaporation, devolatilization and char combustion that occur either sequentially or simultaneously [135]. Models in this research assume sequential conversion stages for coal and biomass. It is also assumed that temperature gradient across the particle radius is negligible because of the small size of fuel particles [140]. Combustion of gaseous species of the volatile matter is modeled by two-step global reaction mechanism [141]. This mechanism comprises of two reactions with CO as the intermediate species. Virtual hydrocarbon with chemical formula \(\text{CH}_x\text{O}_y\text{N}_z\text{S}_{xx}\) represents the volatiles. The values of \(x, y, z\) and \(xx\) are calculated based on proximate analysis and ultimate analysis of the fuel (Table 2.1). Sample calculations can be found in Appendix B.

Table 2. Fuel properties and mass flow rates [130, 135, 134]

<table>
<thead>
<tr>
<th>Coal Properties</th>
<th>Ultimate Analysis % (DAF)</th>
<th>Wheat Straw Properties</th>
<th>Ultimate Analysis % (DAF)</th>
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<tbody>
<tr>
<td>Proximate analysis %</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fixed Carbon</td>
<td>50.4</td>
<td>C</td>
<td>81.2</td>
</tr>
<tr>
<td>Volatile</td>
<td>39.8</td>
<td>H</td>
<td>5.5</td>
</tr>
<tr>
<td>Ash</td>
<td>7.7</td>
<td>O</td>
<td>11.0</td>
</tr>
<tr>
<td>Moisture</td>
<td>2.1</td>
<td>N</td>
<td>1.7</td>
</tr>
<tr>
<td>High Heating Value (MJ/kg)</td>
<td>30.7</td>
<td>S</td>
<td>0.6</td>
</tr>
<tr>
<td>Volatile chemical composition</td>
<td>(\text{CH}<em>{2.58}O</em>{0.32}N_{0.0574}S_{0.0088})</td>
<td>Volatile chemical composition</td>
<td>(\text{CH}<em>{2.14}O</em>{0.98}N_{0.0154})</td>
</tr>
<tr>
<td>Particle density (kg/m³)</td>
<td>1400</td>
<td>Particle density (kg/m³)</td>
<td>600</td>
</tr>
<tr>
<td>Annular fuel (Coal) mass flow rate (g/s)</td>
<td>2.1</td>
<td>Central fuel (Straw) mass flow rate (g/s)</td>
<td>4.2</td>
</tr>
<tr>
<td>Annular air mass flow rate (g/s)</td>
<td>3.3</td>
<td>Central air mass flow rate (g/s)</td>
<td>2.5</td>
</tr>
<tr>
<td>Annular Secondary air mass flow rate (g/s)</td>
<td>44.4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The gas phase global reactions of biomass fuel stream are:

\[
\text{CH}_{2.14}O_{0.98}N_{0.0154} + 0.54O_2 \rightarrow \text{CO} + 1.07H_2O + 0.0077N_2
\]

\[
\text{CO} + 0.5O_2 \rightarrow \text{CO}_2
\]

Whereas the coal stream volatile reaction is:

\[
\text{CH}_{2.58}O_{0.32}N_{0.0574}S_{0.0088} + 0.99O_2 \rightarrow \text{CO} + 1.29H_2O + 0.0287N_2 + 0.0088SO_2
\]
The rate of particle mass loss during devolatilization can be predicted by the following single rate model:

\[ -\frac{dm_p}{dt} = K \left[ m_p - (1 - f_{v,i})(1 - f_{m,i})m_{p,i} \right] \quad (2.5) \]

\[ K = A e^{-E/(RT)} \quad (2.5A) \]

where \( f_{v,i} \) is initial volatile mass fraction in the particle, \( f_{m,i} \) is initial moisture fraction in the particle, \( m_p \) is the current particle mass, \( m_{p,i} \) is initial particle mass (kg), \( K \) is the devolatilization rate (s\(^{-1}\)), \( A \) is the frequency constant (s\(^{-1}\)), \( E \) is the activation energy of devolatilization (J/kgmol), \( R \) is gas constant (J/kgmol.K) and \( T \) is temperature (K). The activation energy and frequency constant of volatilization in the Arrhenius equation for biomass and coal are listed in Table 2.2.

### Table 2.2 Kinetic data of devolatilization used in the simulations [130, 136].

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Frequency constant ( A ) (s(^{-1}))</th>
<th>Activation energy ( E ) (J/kgmol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal</td>
<td>( 3.12 \times 10^5 )</td>
<td>( 4.7 \times 10^7 )</td>
</tr>
<tr>
<td>Straw</td>
<td>( 1.56 \times 10^{10} )</td>
<td>( 1.38 \times 10^8 )</td>
</tr>
</tbody>
</table>

Devolatilization depends on the amount of the volatiles remaining in the particle, that is, the term \( [m_p - (1 - f_{v,i})(1 - f_{m,i})m_{p,i}] \) in Equation (2.5). Coal particle diameter during devolatilization is predicted by introducing swelling coefficient, \( C_{sw} \), into following equation:

\[ \frac{d_{p}}{d_{p,i}} = 1 + (C_{sw} - 1) \frac{(1 - f_{m,i})m_{p,i} - m_p}{f_{v,i}(1 - f_{m,i})m_{p,i}} \; ; \quad (2.6) \]

#### 2.2.3 Surface reaction model

This model assumes the beginning of char combustion when the volatile component of the fuel particle is completely evolved. At this point, the combustible fraction of the remaining fuel particle mass (fixed carbon) starts with surface reaction. Char combustion model that describes the particle surface reaction in this research is the kinetic rate/diffusion-limited model. The surface reaction rate in this model is determined by the dominance of the kinetic rate vs. the diffusion rate during combustion (Equation 2.7) [142, 139]. The diffusion rate \( D_o \), Equation (2.7A)
and the kinetic rate of surface reaction $K_{ch}$, Equation (2.7B) are weighted to determine a char combustion rate as described by Equation (2.7):

$$\frac{dm_p}{dt} = -A_p p_{ox} \frac{D_o K_{ch}}{D_o + K_{ch}}$$  \hspace{1cm} (2.7)$$

$$D_o = C_1 \left[ \frac{T_p - T_\infty}{2} \right]^{0.75}$$  \hspace{1cm} (2.7A)$$

$$K_{ch} = A e^{-E/(RT)}$$  \hspace{1cm} (2.7B)$$

where $A_p$ is the surface area of the particle ($\pi d_p^2$), $p_{ox}$ is the partial pressure of oxidant in the gas surrounding the combustion particle; $K_{ch}$ is the kinetic rate of char combustion; so that the frequency constant of kinetics-limited rate $A = 0.002$; the activation energy of the kinetics-limited rate $= 9.7 \times 10^7$ J/kgmol, $C_1 = 5 \times 10^{-12}$ \cite{131}, \cite{130}; $T_p$ is the particle temperature assuming no significant temperature gradient across the particle; $T_\infty$ is the temperature of the surrounding gas.

The char surface reaction is generally considered to produce CO which rapidly oxidizes to CO$_2$ in the gas phase i.e., the two step-reaction is:

$$C(s) + 0.5O_2 \rightarrow CO$$

$$CO + 0.5O_2 \rightarrow CO_2$$

Therefore, the chemical surface reaction of particle fixed carbon is simplified as follows:

$$C(s) + O_2 \rightarrow CO_2$$

Based on that, the fraction of heat of reaction in equation 2.11 that is released during surface reaction is considered 1.0 if the reaction product is CO because the surface reaction in that case takes place at the particle surface whereas this fraction will be 0.3 if the product of reaction is CO$_2$, since CO$_2$ is produced away from the particle surface \cite{143}.

2.2.4 Discrete phase model

For the solid phase particles to be predicted along with the gas phase, Eulerian – Lagrangian frame of reference can be applied, so that gas phase flow is simulated in the Eulerian frame of reference whereas the trajectory of solid phase particle is modeled in the Lagrangian frame of reference. The equation of particle motion is presented in the form of:
\[
\frac{du_p}{dt} = F_d(u - u_p) + g_x \frac{(\rho_p - \rho)}{\rho_p} + F_x ;
\]  

(2.8)

where \( x \) represents any of the three Cartesian coordinates. The instantaneous particle velocity, \( u_p \), is defined as:

\[
u_p = \frac{dx}{dt}
\]

(2.8A)

The drag force on the particle, \( F_d \), is:

\[
F_d = \frac{18\mu \, C_D Re'}{\rho_p d_p \, 24} ;
\]

(2.9)

The relative Reynolds number, \( Re' \), is expressed as:

\[
Re' = \frac{\rho d_p |u_p - u|}{\mu}
\]

(2.9A)

The drag coefficient \( C_D \) is calculated based on spherical drag law given by

\[
C_d = \frac{C_1}{Re} + \frac{C_2}{Re} + C_3
\]

(2.9B)

where \( C_1, C_2 \) and \( C_3 \) are constant depending on \( Re' \) and given by Morsi and Alexander [130, 144]

\( \mu, C_D, \rho, \rho_p, d_p, u \) and \( u_p \) are the dynamic viscosity, drag coefficient, gas density, particle density, gaseous and particle velocity. The momentum transfer between the continuous phase and the discrete phase is computed by examining the change in momentum of a particle as it passes through each control volume. Thus, the momentum exchange, \( F \), can be described by the following equation:

\[
F = \sum \dot{m}_p d_u_p = \sum \left[ F_d(u - u_p) + g_x \frac{(\rho_p - \rho)}{\rho_p} + F_x \right] \dot{m}_p \Delta t
\]

(2.10)

The change in particle temperature \( T_p \) during the combustion process is given by Equation (2.11):

\[
\dot{m}_p C_p \frac{dT_p}{dt} = h\dot{A}_p (T_\infty - T_p) - a \frac{d\dot{m}_p}{dt} + A_p \varepsilon_p \sigma (\theta_R^4 - T_p)
\]

(2.11)
where $a = h_{fg}$ during the evaporation stage and $a = f_h H_r$ during the char combustion stage. $A_p$ is the particle surface area, $C_p$ is the specific heat at constant pressure, $h_{fg}$ is the latent heat of evaporation, $f_h$ is the fraction of heat of reaction absorbed by the particles during surface reaction, and $H_r$ is the heat of reaction released during surface reaction. The recommended value for $f_h$ is 1.0 and 0.3 if CO and CO$_2$ are the char combustion products, respectively.

The heat transfer coefficient $h$ is commonly given by the Ranz and Marshall correlation as follows:

$$Nu = \frac{h d_p}{K_\infty} = 2 + 0.6 Re_d \frac{1}{2} Pr(\frac{1}{2})$$

where $Nu$ is the Nusselt number, $K_\infty$ is the gas phase thermal conductivity, and $Pr$ is the Prandtl number.

$$\theta_R = \left( \frac{G}{4 \sigma} \right)^{\frac{1}{4}}$$

where, $(G = \int_{\omega=4\pi} l \cdot d\omega)$ is the incident radiation (W/m$^2$), (l) refers to radiation intensity and $\omega$ is solid angle.

The Discrete Ordinates (DO) model is used for radiation heat transfer. It approximates the solution of radiative transfer equation by discretizing the complete solid angle of $4\pi$ to several small solid angles. In each small solid angle radiation intensity is assumed constant and the differential form of the radiative transfer equation is solved numerically. The more the number of finite solid angles the more accurate solution is obtained and more computationally expensive is the solution [145]. The DO model solves the radiative transfer equation in the direction $\vec{s}$ and position $\vec{r}$ for the spectral intensity $I_\lambda(\vec{r}, \vec{s})$ of an absorbing, emitting, and scattering medium. The governing equation for spectral intensity takes the following form:

$$\nabla \cdot ( I(\vec{r}, \vec{s}) \vec{s} ) + (a_\lambda + \sigma_\lambda) I_\lambda(\vec{r}, \vec{s})$$

$$= a_\lambda n^2 I_{b\lambda} + \frac{\sigma_\lambda}{4\pi} \int_0^{4\pi} I_\lambda(\vec{r}, \vec{s}') \Phi(\vec{s}, \vec{s}') d\Omega'$$

(2.12)
where, $\lambda$ is the wavelength, $a_\lambda$ is the spectral absorption coefficient, $I_{b\lambda}$ is the black body intensity, $n$ is the refracting index, $\sigma_s$ the scattering coefficient, $s'$ is the scattering direction vector, $\Omega'$ is the solid angle, $\Phi$ is the phase function. The discrete model transforms the radiative equation into a transport equation for radiation intensity in spatial coordinates. As with the transport equations for fluid flow and energy, an identical solution method, such as the finite volume scheme with a conservative variant of discrete ordinates, can be used to solve the radiative heat transfer equation [131].

The momentum transfer from the continuous phase to discrete phase is calculated by examining the change in momentum of a particle as it passes through each control volume. Same thing happens with mass and heat.

2.2.5 Three-Dimensional flame volume prediction

Determination of high temperature air combustion (HiTAC) flame volume is useful in the design of furnace [146]. Flame lengths are usually estimated by predicting the contour surface where stochiometric ratio is satisfied for fuel and oxidizer. It, therefore, represents the locations at which volatiles and oxygen are mixed in a stoichiometric ratio [147]. Flame volume can be predicted by calculating the oxidation ratio $R_o$ as in equation (2.13) where $m_o$ and $m_f$ are the mass fractions of oxygen and combustible gaseous species, respectively; $s$ is calculated as in equation (2.13A) where $\nu_o$ and $\nu_f$ are stoichiometric coefficients for oxygen and combustible species (moles) and $MW$ is their molecular weight (kg/mole).

$$R_o = \frac{m_o}{m_o + \sum_i s_i m_{f,i}}$$  \hspace{1cm} (2.13)

$$s = \frac{\nu_o MW_o}{\nu_f MW_f}$$ \hspace{1cm} (2.13A)

Equation (2.13) can also be written as

$$R_o = \frac{1}{1 + \sum_i s_i \frac{m_{f,i}}{m_o}}$$  \hspace{1cm} (2.14)

In pulverized fuel, the flame is enveloped by the critical ratio ($R_o = R_c$) which is assumed to have a value of 0.99. This value limits the lean flammability and indicates the outside borders
of the flame [147, 37, 146]. Hence, \( R_o \) will map the flame volume so that it lies in the range \( 0 \leq R_o \leq 0.99 \).

### 2.2.6 Unburnt carbon

The evolution and burnout of the volatiles can be monitored by observing the ratio \( \frac{CO}{CO+CO_2} \) along the height of the furnace. The level of loss on ignition (LOI) throughout the furnace will be evaluated by calculating the percent unburnt carbon, \( C_{ub} \) (in \%), at the exit of the furnace using the following equations:

\[
m_{ch} = \sum_{i=1}^{n} m_A \frac{f_{ch,i}}{(1 - f_{ch,i})} \tag{2.15}
\]

\[
C_{ub} = \frac{(m_{ch}/m_{ch,in}) \times f_{FC}}{f_{C,t}} \times 100 \tag{2.16}
\]

where \( m_{ch} \) is the remaining fixed carbon in biomass particle at the exit (kg), \( f_{ch,i} \) is the final mass fraction of fixed carbon in biomass particle \( i \), \( m_A \) is the mass of ash in biomass particle (kg), \( n \) is the total number of particles, \( m_{ch,in} \) is the mass of fixed carbon at reactor inlet (kg), \( f_{C,t} \) is the carbon content in the ultimate analysis (% DAF basis), \( f_{FC} \) is the fixed carbon content in the proximate analysis (% DAF basis).

### 2.2.7 NO\(_x\) formation

In this research it is assumed that fuel-N is partitioned into 70% volatile-N and 30% char-N [131, 148]. Char-N is released into the gas phase at a rate that is proportional to the carbon burnout rate. Since the chemistry of char-N conversion is complex, the simulation assumes a fixed fraction of char-N being directly converted to NO with the rest of N converted to N\(_2\) [149, 150]. Most of biomass volatile-N will be converted to NH\(_3\) while the dominant part of coal volatile-N will be released as HCN [151, 152]. These two intermediate products assist in reducing the nitric oxide (NO) produced from thermal-N to N\(_2\). Transport equations 2.17, 2.18 and 2.19 are solved for NO, NH\(_3\) and HCN.

\[
\frac{\partial}{\partial t} (\rho Y_{NO}) + \nabla \cdot (\rho \vec{v} Y_{NO}) = \nabla \cdot (\rho D \nabla Y_{NO}) + S_{NO} \tag{2.17}
\]

\[
\frac{\partial}{\partial t} (\rho Y_{NH_3}) + \nabla \cdot (\rho \vec{v} Y_{NH_3}) = \nabla \cdot (\rho D Y_{NH_3}) + S_{NH_3} \tag{2.18}
\]

\[
\frac{\partial}{\partial t} (\rho Y_{HCN}) + \nabla \cdot (\rho \vec{v} Y_{HCN}) = \nabla \cdot (\rho D Y_{HCN}) + S_{HCN} \tag{2.19}
\]
where \( Y_i \) is the mass fraction of the species (HCN, NH\(_3\), and NO); \( \rho \) is the gas density; \( v \) is the gas velocity; \( D \) is the effective diffusivity coefficient, and \( S_i \) is the source term which can be determined based on the NO\(_x\) formation mechanism.

Source terms are scalar additional functions appear in conservation equations. It can be a mass source or energy source. In gas-solid phase flow, particles interact with gaseous phase producing source terms, could be positive (source), or negative (sink) [143]. For instance, the product of the surface reaction represents a positive source in the gas phase when solving the transport equation for these species. Similarly, surface reaction consumes/produces energy by the heat of reaction. This energy will be added to the energy conservation energy as a source term [131].

Fuel nitrogen partitioning for NH\(_3\) and HCN as intermediate species is used when burning solid fuel like coal or biomass at high temperatures. The general reaction pathways are described in the following scheme.

\[
\begin{align*}
S_{NO} &= S_{1,NO} + S_{2,NO} \\
S_{NH_3} &= S_{p,NH_3} + S_{1,NH_3} + S_{2,NH_3} \\
S_{HCN} &= S_{p,HCN} + S_{1,HCN} + S_{2,HCN}
\end{align*}
\]
where $S_{1,NO}$ and $S_{2,NO}$ are the production and consumption rate of NO in Oxidation and reduction mentioned above, $S_{p,NH_3}$ is the rate of NH$_3$ production, $S_{1,NH_3}$ and $S_{2,NH_3}$ are the mass consumption rate of NH$_3$ in oxidation and reduction respectively (as shown in the schematic diagram above), $S_{p,HCN}$ is the rate of HCN production, $S_{1,HCN}$ and $S_{2,HCN}$ are the mass consumption rate of HCN in oxidation and reduction respectively (as shown in the schematic diagram above).

### 2.3 Meshing

The flow domain of the furnace in this work is discretized into small elements to create a three-dimensional mesh to be examined for mesh independency of the solution. One of the big challenges of setting up a CFD simulation is the mesh generation. It can be a significant source of error if it is not created with proper element sizes and shapes. Among the error sources are elements of high skewness, high aspect ratio, large jump in volume or face area between the adjacent cells. In this work, grids are generated primarily by two meshing tools. The first mesh is generated by ANSYS Fluent after the 3-dimensional geometry of the furnace is drawn inside fluent design modular. The second tool was ANSYS ICEM CFD 17.2 [153] by which, multi-block structured, or unstructured mesh can be created. Then the mesh can be imported into ANSYS Fluent solver.

The first tool was not successful for approaching convergence. Therefore, ICEM CFD was used to create three multi-blocks structured meshes: first mesh with 319,000 cells, a finer mesh with 550,000 cells and a refined mesh of 927,000 cells. Each mesh covers the whole furnace flow field. Figure 2.2 illustrates the first mesh according to the original furnace geometry. The latter three meshes were designed to have denser grids in the core zone and at the inlet of the furnace where more turbulent flow and changes in properties are expected. The first step of meshing is to create the geometry of flow domain inside ICEM by its geometry topology package. One block is then created to envelope the whole geometry which is subsequently divided into a multi-block structure before creating an O-grid mesh from each block individually. This gives the opportunity to control the mesh size (refining or coarsening) at each block separately. Hence, it will help to build a mesh with homogenous hexahedral elements for each block as fine as needed in the flow field.
Figure 2. 2 X-Y section of the 3-D mesh, original furnace geometry

2.3.1 Mesh independence

The verification of mesh independence was performed by comparison between the coarse and fine meshes. The 3-D multi-block structured meshes with 319,000, 550,000 and 927,000 cells are examined for mesh independency of the solution results.

The dimensionless wall distance, $y+$, which depends on the distance of the first node from the wall and the wall shear stress is useful for estimating the first layer thickness of the meshes and simulating the near wall treatment. In this research, the wall function model was implemented to capture the near-wall boundary layer. The first node distance was evaluated to match the $y+$ value that is suitable for the flow conditions and the $k$-$\varepsilon$ model for predicting the flow. The second order upwind was used for all the equations. The SIMPLE algorithm was used for the pressure-velocity coupling. The convergence criteria of continuity equation, momentum equation and turbulence and species transport are based on references [128, 130, 131]. These references are cited in the revised thesis in Chapter 2 section 2.3.1.

The three-dimensional multi-block structured meshes with 319,000, 550,000 and 927,000 cells were examined for mesh independency of the solution results. These meshes will be referred
as mesh 1, mesh 2 and mesh 3, respectively. Since CFD solution is a numerical approximation of the exact solution, then finer the mesh the closer to the exact solution. The discretization error that is attributed to the difference between the numerical and exact solutions can be quantified by a systematic refinement of the spatial and the temporal meshes. Thus, it can give an indication about the mesh independency of the results on mesh refinement. In this study, the discretization error was estimated for all three meshes following the guidelines of Roache [125]. Two levels of refined meshes were represented for comparison. Based on the Roache guidelines, the two refinement levels maintained the same refinement ratio (1.71 in our case).

The discretization error of the selected property, oxygen mass fraction, on the first level mesh is described as $E_d = \frac{U_2 - U_1}{1 - R_r}$. The refined mesh discretization error is defined as $E_d = R_r^p \frac{U_2 - U_1}{1 - R_r^p}$, where $U_1$, and $U_2$ are the values of $O_2$ mole fraction from mesh 1 and mesh 2, respectively; $R_r$ is the refinement ratio $\frac{h_2}{h_1}$; $h_1$ is the number of cells in the first mesh, $h_2$ is number of cells in the refined mesh; $p$ is the observed order of truncation rate decay, which is defined as $$p = \ln \frac{U_3 - U_2}{U_2 - U_1} / \ln R_r$$

In Figure 2.3a the oxygen mole fraction along the central line of the reactor is plotted against the reactor height using the two meshes mentioned above for comparison. The plots are almost aligned to each other; they become a bit more influenced by mesh resolution as the radial distance increases. Figure 2.3b shows the discretization error of results from figure 2.3a based on Roache guidelines. Similar behavior is observed for the oxygen mole fraction along radial distance of 7.5 cm and 22.5 cm from the centerline of the reactor, Figures 2.3b and 2.3c. The first mesh with 319,000 cells is considered in this study for its shorter time of convergence.
2.4 Fuel properties

Wheat straw particles enter the furnace in ten sets of particle diameter that range from 50 μm to 1000 μm. The mass fraction of the particles in terms of particle diameter is described by Rosin Rammlar distribution function with spread index of 3.2 and average particle diameter of 451 μm (Eqn. 4.1). The particle density of wheat straw is 600 kg/m³. It contains about 16% of fixed carbon and 84% of volatile matter, (dry ash free) basis, and the HHV (higher heating value) of wheat straw is 18 MJ/kg. It has relatively high oxygen content (43.7%) compared to coal (11.0%). The molecular weight of fuel particle is 24 kg/kg mol. Based on proximate and ultimate analyses (Chapter 5), a virtual volatile matter of wheat straw is assumed to have the chemical composition \( CH_{2.14}O_{0.98}N_{0.0154} \) and molecular weight 30 kg/kg-mol.

Coal particles are smaller than wheat straw and are fed into the furnace in ten sets of diameters that range from a minimum diameter of 25 μm to a maximum diameter of 250 μm. It is
also described by Rosin Rammlar distribution (Equation 2.20) with a spread index of 4.1 and average particle diameter of 110 μm (Figure 2.4). The particle density is 1400 kg/m³. It comprises of 56% fixed carbon and 44% volatile mater (daf), and its HHV is 30.7 MJ/kg [134]. Based on these proximate and ultimate analyses, the virtual volatile matter of coal can be represented as \( \text{CH}_{2.58}\text{O}_{0.32}\text{N}_{0.0574}\text{S}_{0.0088} \) and molecular weight 21 kg/kg-mol.

\[
Y_d = \frac{1}{\varepsilon^{(d_p/\bar{d}_p)^n}} 
\]

(2.20)

where \( d_p \) is the particle diameter (mm); \( \bar{d}_p \) is the mean particle diameter (mm); \( n \) is the spread factor and \( Y_d \) is the mass fraction of accumulative particles having diameters bigger than \( d_p \).

Figure 2.4 shows a comparison of particle size distribution between coal and wheat straw as used in the validation of CFD results.

**Figure 2.4** Rosin Rammler particle size distribution of wheat straw and coal

### 2.5 Evaluation of CFD simulation results

The data being used for model evaluation was obtained from the experimental work conducted by Damstedt [134] on the co-firing of coal and wheat straw (biomass-to-coal ratio of 67:33) in a dual feed burner. Separate measurement probes were used for gas sampling and particle sampling to cover the entire flow field (axially and radially) in order to explore the flame structure and the fuel nitrogen chemistry. The gas sampling system includes measurement probe, particle filter,
sampling line, pump, an FTIR based gas cell analyser, desiccant, flow meter and a gas analyser. The gas sampling probe was a hollow, water-cooled jacket adaptable to different equipment tips. The probe center is an electrically heated, temperature controlled (at 180°C), stainless steel tube.

Damstedt [134] was aware that the recirculation zone is an aerodynamic flame holding mechanism, and hence placing a probe into the recirculation zone will disrupt the flow pattern, and potentially the flame structure. Several considerations were taken to establish a steady, repeatable, and accurate sampling system for the quantitative measurements of the major species O₂, CO₂, CO, and H₂O. The sample line must be leak-proof and prevent water from condensing anywhere along the sampling train. The gas sample is quickly quenched to a temperature below 800°C whereas the line components are maintained at 180°C to prevent sample gas reacting and to eliminate any possibility of water condensation. Measurements were replicated at several specified axial locations to quantify the potential variation in the data.

Subsequently, data collected by Damstedt [134] revealed a small aberration only in the first section of the reactor, where O₂ increased somewhat as the combustion of the fuel progresses, suggesting possible impact of the intrusive measurement probe. However, the probe impacts were found to be minimal in other parts of the reactor where the probe passes completely through the recirculation zone. Hence, he used the non-disrupted data for further data analysis.

The first evaluation perimeter will be the average concentration or flux of species as a function of axial position of the reactor since the species concentration should vary with increasing the axial position. Axial averages are obtained by integrating the species mole flux across the longitudinal axis of the reactor, Damstedt [134] which is expressed in Equation (2.21):

\[
Y_i(x) = \frac{\int_{-R}^{R} \frac{p}{\mathcal{R}T(r, x)} \cdot y_i(r, x) \cdot \frac{v(r, x)}{MW(r, x)} \pi r dr}{\int_{-R}^{R} \frac{p}{\mathcal{R}T(r, x)} \cdot \frac{v(r, x)}{MW(r, x)} \pi r dr} \tag{2.21}
\]

where \(Y_i(x)\) is the average mole fraction of species, \(y_i(r, x)\) is the local mole fraction of species at specific radius \(r\) and distance \(x\) along the reactor longitudinal axis, \(v(r, x)\) is the average local gaseous velocity at specific radius \(r\) and distance \(x\) along the reactor longitudinal axis, \(R\) is the radius of the reactor and \(\mathcal{R}\) is the universal ideal gas constant. This function represents the molar
flow rate of a species through a plan at certain $x$ location if the ratio of temperature to velocity is assumed constant. The numerator represents the molar flow rate of species $i$ through a circular cross-sectional area of $A_i (= 2\pi rdr)$ and the denominator is the total molar flow. Assuming the change in pressure $P$ and molecular weight $MW$ are insignificant along the radial coordinate of the reactor through the same plane and reducing the constants from both numerator and denominator, Equation (2.21) can be written as:

$$Y_i(x) = \frac{\int_{-R}^{R} y_i(r, x) \frac{v(r, x)}{T(r, x)} rdr}{\int_{-R}^{R} \frac{v(r, x)}{T(r, x)} rdr}$$

(2.22)

Although, significant temperature gradients exist throughout the reactor, a rapid increase in temperature has no effect on the average radial velocity at a given axial location. By assuming that the ratio of average axial velocity to the average temperature is independent of radial position, Equation (2.22) is reduced to:

$$Y_i(x) = \frac{\int_{-R}^{R} y_i(r, x) rdr}{\int_{-R}^{R} rdr} = \frac{\int_{-R}^{R} y_i(r, x) rdr}{R^2} ;$$

(2.23)

$$\{ x: 0 \leq x \leq H \}; \ H = \text{reactor height} = 2.5m$$

Species that are considered for validation purposes are oxygen, carbon dioxide, carbon monoxide and water vapor. The average mole fractions were calculated using Equation (2.34). In the experimental work, [134] measuring probes and sampling points were distributed longitudinally along the reactor at different locations, $x$; for the radial direction, a horizontal plane was discretized into three segments, with the outer radii being (7.5, 22.5, and 37.5 cm) [134]. As a matter of consistency, the same segment size was used in calculating the average mole fractions from the CFD results.

The root-mean-square error (RMSE) which represents the standard deviation of residuals between the experimental and simulation values can be calculated according to Equation (2.24).

$$RMSE = \sqrt{\frac{\sum (Y_{i,exp} - Y_{i,CFD})^2}{N - 2}}$$

(2.24)
Where $Y_{i,\text{exp}}$ is the average mole fraction of a gaseous species, $Y_{i,\text{CFD}}$ is the average mole fraction predicted by CFD, and $N$ is the number of data points.

Figure 2.5(a) demonstrates that both the experimental and CFD simulation results exhibit the same general trends. The calculated value of RMSE for average oxygen mole fraction is 0.034. A rapid decrease in oxygen concentration occurs at the entrance of the reactor followed by a gradual decrease in oxygen concentration with an increase in the axial (longitudinal) distance. Interestingly, while Damstedt [137] described the presence of small aberration where oxygen concentration starts to increase during the combustion process, this does not occur in our CFD results. Aberration was expected in experimental results because of the interaction between the measurement probe and the flow in this zone. Therefore, it disappeared in the CFD simulation results.

The average CO$_2$ mole fraction is presented in Figure 2.5(b), and the calculated value of RMSE is 0.01. Figure 2.5(c) shows that the concentration of CO is an order of magnitude lower when compared to O$_2$ and CO$_2$ concentrations since it is an intermediate and minor species produced via the combustion of volatile matter. CO attains a maximum value around 75 cm from the reactor inlet. The range of $x$-axis (240 cm) as determined according to the experimental results does not cover the entire reactor height (300 cm) of the furnace; hence, trace amount of CO is seen at the end of the curve. For water vapor, as particle is heated up near the reactor inlet, moisture within the particles starts to evaporate into the gaseous phase and leaves the particle. Similar trend between the CFD and experimental results is shown in Figure 2.5(d) with an RMSE of 0.0275, indicating that CFD simulation can be applied to predict the species concentrations throughout the reactor from inlet to outlet with an acceptable error.
Sensitivity analysis was conducted to study the effect of particle sphericity on the mole fractions of the various gas species. Sphericity is quantified by the shape factor, which is defined as “the ratio between the surface area of a spherical particle to that of an actual particle having the same volume”. The values of shape factors used for this sensitivity analysis are (1.0, 0.9, and 0.8). Figure 2.5 also shows the results that include the sensitivity analysis. A lower shape factor
means larger surface area of the particle. The variation in particle surface area can be linked to the rates of moisture and volatiles release, and heat transfer between the particle and the surrounding gas. It can also affect the surface reaction rate due to the exposure of particle surface to the oxidizer.

Figure 2.6 shows the average mole fractions of the gas species that are calculated based on equation 2.21 and equation 2.23, and both sets of simulation results are compared with the experimental data [134] in order to evaluate the impact of these assumptions on the results. Differences can be seen between the two sets of results, especially in the region of high temperature gradients (near the entrance of the reactor) where it is expected that the assumptions mentioned above are not completely valid. For oxygen mole fraction, the calculated values of RMSE are 0.026 (Eqn. 2.21) vs. 0.034 (Eqn. 2.23).

Figure 2.6 Impact of the assumptions made to simplify equation 2.21 for calculating the average mole fraction of O2, CO2, CO and H2O versus reactor axial distance.
2.6 Conclusions

The 3-dimensional meshes of (319,000), (550,000) and (927,000) hexahedral cells were tested for mesh-independency of the CFD solution for the steady 3-dimensional swirl flow. The mesh was verified for obtaining a mesh independent CFD solution. Discretization error was calculated and mesh independency test was performed according to the Roache guidelines. The model was validated by comparing the CFD simulation results and the experimental data presented in the literature. Both the experimental and CFD predicted results were found to exhibit the same general trends in terms of the average concentrations of gaseous species (O2, CO, CO2 and H2O). RMSE was used for the evaluation of validity.

Contribution of the current CFD Model of three-dimensional, two-phase, reacting flow simulation can be summarized as follows:

1. The current CFD model is able to perform 3-D, two-phase, reacting flow simulations.

2. The 3-D swirl flow simulation is capable of capturing the particle trajectories as compared to 2-D axisymmetric simulation. It enables the study of the interaction of the continuous flow aerodynamics with particle trajectories and tracking the particle conversion during combustion.

3. The Favre-averaged Navier-Stokes equations are solved instead of the Reynold’s averaged equations in order to account for the density change in a compressible flow. The gas experiences a large change in density (from 0.20 to ~1.23 kg/m3) since the flow is a reacting and compressible flow.

4. Modification near the furnace entrance is introduced and results reveal improvement in fuel burnout.
Chapter 3. Effect of Furnace Geometry Modification on Co-firing

3.1 Introduction

One of the issues of co-firing coal with biomass is the loss on ignition (LOI) that is usually associated with a high percentage of biomass in the mixed fuel. The problem is mainly due to the differences in the properties between biomass and coal. Various techniques have been implemented to avoid such undesirable consequences accompanied with co-firing and some of them are mentioned in the literature review (chapter 1) of this research. In this chapter, CFD simulation is used to investigate the effect of two possible furnace geometry modifications on the combustion efficiency.

3.2 Furnace geometry modification

The furnace that was used in the model validation (chapter 2) is used here as the baseline case. For comparison with the furnace geometry modifications. In the baseline case, the burner quarl has a diffusing angle of about 30°, ending with a diameter of 20 cm, then a sudden enlargement to the furnace inner diameter of 75 cm. This sudden expansion can enhance the creation of an external recirculation zone (ERZ) in the upper part of the furnace (Figure 2.1, chapter 2).

Simulation involves a high percentage of biomass in the mixing ratio (67 wt% wheat straw, 33 wt% coal), which can have a greater potential for serious problem during co-firing. The fuel properties are as mentioned in Table 1.2 (chapter 1). One fuel stream (wheat straw) is injected with primary air into the furnace through the central circular pipe, and the other fuel stream (coal) is injected with primary air through the annulus pipe.

Experimental results [134] show that a bulk of secondary air ends up recirculating in the upper corners of the furnace that forms the ERZ. No combustion is taking place and the fuel particles are not dispersed in this zone, thus creating a conical barrier between the ERZ and the internal recirculation zone. The secondary swirl flow is supposed to increase the tangential velocity component, which in turn would promote flow mixing and lengthen the fuel particles trajectories to enhance heat transfer and combustion in the furnace [69-74]. It also increases particle residence time as in cyclone burner [23].

ERZ contains an intense vortex flow that is fed by the fluid flow momentum. Therefore, it is postulated that making the conical expansion at the furnace entrance can eliminate this zone from the furnace geometry and allow the flow aerodynamics to gradually expand to the furnace tube and improve the mixing rate of the gaseous and discrete phase flow. The modification from
sudden expansion to gradual enlargement is accomplished by introducing a circular diffuser at the quarl exit. This diffuser has an angle of 47.7° and length of 25 cm to displace the volume occupied by the ERZ.

The baseline swirl angle of 45° corresponds to a swirl number (S) of 0.6, and this angle is 11.5° less than the swirl angle of 56.5° (corresponding S = 1.0). To further investigate the effect of swirl intensity on the flow characteristics, the swirl angle was increased from 45° to 68° (S = 1.65), which is 11.5° greater than 56.5°.

Figure 3.1 shows a comparison between the furnace with the baseline and the modified geometry (outer configuration). The quarl dimensions, boundary and operating conditions, fuel and all other parameters are the same for both furnaces. Meshing of the flow domain is done by ANSYS ICEM CFD v17.2 to facilitate the simulations. The mesh created for the modified furnace is around 327,000 hexahedral cells. Finer cells were created near the core and entrance of the furnace, taking the high rate of variation in the flow properties and the expected turbulence into consideration.
Figure 3.1 Mesh of the baseline furnace and modified furnace geometry

The next factor being considered for implementing the geometry modification is the swirl angle of secondary air. For the modified furnace with gradual enlargement, the swirl angle is increased from $45^\circ$ to $68^\circ$ as a further geometry modification. This will increase the tangential velocity component of secondary air with respect to axial velocity component while maintaining the same flow rate of secondary air. Figure 3.2 demonstrates the difference between the furnaces with two swirl angles in terms of the secondary air velocity vectors at the inlet of the quarl.

![Figure 3.2 velocity vector (m/s) of secondary air at the inlet of the quarl](image)

Table 3.1 shows the three cases of CFD simulations. The baseline case (case 1) has the original geometry with sudden enlargement of the burner quarl to the furnace entrance and a swirl angle of $45^\circ$. Case 2 has the modified geometry with gradual enlargement cross-section and a swirl angle of $45^\circ$. Case 3 is pertinent to modified geometry with a gradual enlargement and a swirl angle of $68^\circ$.

<table>
<thead>
<tr>
<th>Case</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sudden enlargement, Swirl angle $45^\circ$</td>
</tr>
<tr>
<td>2</td>
<td>Gradual enlargement, Swirl angle $45^\circ$</td>
</tr>
<tr>
<td>3</td>
<td>Gradual enlargement, Swirl angle $68^\circ$</td>
</tr>
</tbody>
</table>

### 3.3 Results
The percentage of unburnt carbon that remains in the ash during cofiring was used as the main criterion for assessing the improvement in the combustion efficiency. The effect of increasing
the swirl angle of secondary air on the flow aerodynamics and to what extent this can be connected to the combustion efficiency will also be discussed.

Figure 3.3 shows the temperature profiles through X-Y plane for the three cases. The maximum gas temperature in case 2 and case 3 (2127 and 2143 K) are about 10% higher than that of case 1 (1960 K). However, temperature distribution in the two furnaces with geometry modifications is less variant compared to the furnace without modification. The high temperature zone in the upper part of the baseline case furnace becomes spreading out and translating upward in case 2; and it becomes circumferential and more limited in case 3. This can be a good indication of a higher level of recirculation gaseous flow in the latter two cases.

![Figure 3.3 Temperature profile of gaseous flow for cases 1, 2 and 3](image_url)
The vertical relative vorticity, $\xi$, normal to the X-Y plane and throughout the furnace was calculated using Equation 3.1 to evaluate the recirculation intensity,

$$\xi = \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) k = -2\omega$$

(3.1)

where, $v$ and $u$ are the $x$- and $y$-components of the local gas velocity (m/s), respectively and $\omega$ is the angular velocity about z-axis (rad/s). Because of the high values of vorticity throughout the X-Y plane and in order to view the variant of $\xi$ more clearly, $\log |\xi|$ is represented in the X-Y plane instead of $\xi$, so that when $-4348 < \xi < 4213$; $\lim_{\xi \to 0} \log |\xi| = -\infty$.

Figure 3.4 shows the contours of vorticity normal to X-Y plane for the three cases. Internal recirculation zone (IRZ) remains whereas, the external recirculation zone (ERZ) is eliminated in the modified furnace configuration. The flow in IRZ of case 2 is expanded to a wider angle than in case 1, and the relative vorticity becomes higher near the diffuser wall as shown in case 3. The tangential and radial velocity components are larger compared to the axial velocity component. The vorticity has multi circulations centers (Figure 3.5) that leads to high mixing rate in that region and consequently more efficient combustion [154].

Figure 3. 4 Relative Vorticity normal to X-Y plane for case 1, 2 and 3
Figure 3.5b shows the development of the tangential component of gas velocity near the center through the three cases. The tangential velocity component in case 1 is smaller than the other two cases. The maximum tangential velocity component beyond the diffuser in the combined modification is about 3 m/s, whilst it is about 2 m/s when only the gradual enlargement is implemented; however, it is about 1 m/s in the same region with the sudden expansion arrangement. This indicates the better mixing rate of which was induced by the new
modifications. It also shows that flow aerodynamics is an essential factor in improving co-firing in terms of increasing the particle residence time and combustion efficiency at high biomass mixing ratio.

For case 1, this can be explained by the tendency of large particles to flow near the center and not being influenced by the swirl flow. In case 2 where the gradual expansion is implemented, the tangential velocity component increases so that bigger particles from the core zone of the furnace can be drifted by the swirl flow. And for case 3 where gradual expansion is applied and swirl angle is increased to 68°, the tangential velocity near the center further increases and makes it easier to induce the bigger particles from the core zone of the furnace to the circumferential zone, thus leading to increased residence time of these particles.

Figure 3. 6b Gas tangential velocity contours at 150 cm from the furnace inlet.

Most of the devolatilization occurs in the IRZ. Even though biomass and coal become mixed fuel after injection into the furnace due to the high rate of turbulence in the flow, the ANSYS Fluent software can distinguish between the volatile mass fraction of each fuel and visualize them individually. Figure 3.7 shows the volatile mass fraction of biomass fuel stream
for three cases. Volatile mass fraction in the furnace with gradual expansion extends to a shorter distance and the IRZ is stretched horizontally toward the furnace walls. In the modified furnace with a larger swirl angle (68°) the volatilization zone is even shorter and closer to the quarl intake. Despite coal having less volatile matter compared to biomass, similar trend can be seen in Figure 3.8 which presents the volatile mass fraction of coal. This means, the devolatilization process takes place in a smaller space in the furnace with gradual expansion and this space gets even smaller by increasing the swirl angle. This will provide a better opportunity for char combustion to take place closer to the furnace entrance, and hence having more space to complete the burnout with the existence of multi-recirculation zones.

Figure 3.7 Volatile mass fraction of biomass in the three cases
In Figure 3.8, the oxidation mixture ratio ($R_o$), Equation 2.14, is shown for the three cases. In the furnace with sudden enlargement (baseline case), the biomass flame length extended to 150 cm, and the flame radius reaches a peak of 30 cm at 40 cm from the inlet. The flame length becomes 101 cm in the furnace with gradual enlargement, and the maximum flame radius is 32 cm at 38 cm from the inlet. Moreover, the central part of the flame is lifted-off about 18 cm compared to only 3 cm in the baseline case. In case 3, the flame length decreases to 80 cm, with maximum flame radius of 26 cm at distance of 32 cm from the inlet, but the central flame lift-off is 9 cm.
Figure 3.9 Comparison of biomass flame length for the three cases

Unburnt fixed carbon with the ash was calculated for biomass and coal using Equations (2.15 and 2.16). Despite the high biomass percentage (67 wt%) in all three cases, it is interesting to note that the biomass in cases 2 and 3 is completely burned out. Whereas the unburnt biomass fixed carbon at the exit of the furnace in case 1 is about 20%. By comparison, coal burnout is also improved as indicated in Figure 3.10. Unburnt fixed carbon in the ash is reduced to 13% in the gradual enlargement furnace and it is further reduced to 5.8% by increasing the swirl angle in case 3.
3.4 Conclusions
In this chapter, CFD simulation is performed to study the effect of furnace geometry modification on the combustion efficiency of co-firing coal with a high percentage of biomass (wheat straw) in the mixed fuel. The study involves two possible furnace geometry modifications. Firstly, the sudden enlargement section between the furnace and the quarl in a typical furnace is replaced by gradual enlargement with a conical diffuser (angle 47.7°) to eliminate the ERZ and reduce the losses due to the eddies. The results show that with the new configuration, wheat straw is completely burned out with no LOI. There is also good improvement on the burnout of coal. The unburnt fixed carbon coal in ash at the exit of the furnace was reduced by 33% of the baseline case. The predicted average gas temperature was higher and less variant throughout the furnace compared to the baseline case. The level of circulation inside the IRZ was higher in the furnace with modified geometry. Flame length was horizontally stretched and vertically compressed upward.

Secondly, the swirl angle of secondary air flow is increased from 45° to 68° for the modified furnace with gradual enlargement. This was to enhance the swirl component by promoting tangential air velocity component that can potentially drift out some big fuel particles.
from the central part of the furnace to the circumferential zone. Results show that the maximum temperature of the gaseous flow is higher than the previous (sudden enlargement) modification and it has less variant than the baseline case. Moreover, the biomass has burned out completely without any LOI, and the unburnt fixed carbon from coal at the exit was further reduced by 55% as compared to the previous modification.
Chapter 4. Effect of Pelletizing on Co-firing

4.1 Introduction

This chapter presents study of the effect of biomass densification on biomass co-firing with coal. The 3-D CFD model that has been validated was used to simulate the co-firing of coal and wheat straw. The effect of pelletization on biomass particle combustion was investigated by considering shrinkage in particle size due to compression during pelletizing. A baseline case (case1) and two other cases are analyzed in this study. Comparison is made between these three cases (Table 4.1) to investigate the effect of pelletizing on particles combustion. Simulation case 1 represents the uncompressed wheat straw particles with a particle density of 600 kg/m$^3$ [130, 135]. The two simulation cases of densified particles have particle density 800 kg/m$^3$ and 1000 kg/m$^3$, respectively. Fuel properties, boundary and operating conditions will be same as those explained in chapter 2. Flame length, particles trajectories, unburnt fixed carbon in ash and NO$_x$ emissions will be investigated through the CFD simulation results.

Table 4.1 Three cases of study for the effect of pelletization

<table>
<thead>
<tr>
<th>#</th>
<th>Simulation case</th>
<th>Particle density, kg/m$^3$</th>
<th>Average particle diameter, μm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>baseline</td>
<td>600</td>
<td>451</td>
</tr>
<tr>
<td>2</td>
<td>compressed particles</td>
<td>800</td>
<td>410</td>
</tr>
<tr>
<td>3</td>
<td>compressed particles</td>
<td>1000</td>
<td>380</td>
</tr>
</tbody>
</table>

Particles are assumed to have a spherical shape and their diameters are calculated by Equation (4.1). The values 800 and 1000 kg/m$^3$ were adapted from [155] but assumed to be 10% greater to allow for the difference between pellet density and particle density due to the presence of voids. Particle diameter that would also change due to pelletizing is calculated as:

$$d_2 = d_1 \left(\frac{\rho_{p,1}}{\rho_{p,2}}\right)^{1/3}$$

(4.1)

where $\rho_{p,1}$ is the density before pelletizing kg/m$^3$, $\rho_{p,2}$ is the density after pelletizing kg/m$^3$. $d_1$ is the diameter of uncompressed particle (i.e., particles without pelletizing), $d_2$ is the diameter of compressed particle. Figure 4.1 shows Rosin Rammler particle size distribution of the fuels used in this study.
In this section, a general overview of flow characteristics will be presented followed by the discussion of the three cases. Gaseous temperature profile will be presented throughout the reactor besides the velocity vectors of gaseous flow to evaluate the flow pattern. Then, volatile matter and oxygen mass fraction will be discussed to evaluate the evolution of volatiles along the reactor, and unburnt carbon is presented to show the influence of pelletizing. Finally, nitric oxide emission will also be discussed.

4.2.1 Temperature distribution and flow characteristics

For the gaseous phase, temperature profile inside the furnace describes the flame envelop of the combusted fuel. The high temperature zone is associated with a high rate of combustion, and this is expected in regions that are relatively rich in oxygen and where the volatile matter is released especially, with biomass which has high percent of volatiles. Gas aerodynamics is also of discernable importance since it can affect the residence time of combustion and facilitates the predictability of fuel particles’ trajectory behavior. In a pulverized fuel furnace, certain aerodynamic behavior can help enhance flame stability by increasing the mixing rate of fuel and air, and this is what usually happens in the internal recirculation zones [156].

Figure 4.2a shows the 3-D temperature distribution of the gaseous phase throughout the reactor for the baseline case (case 1) with uncompressed biomass particles. Since the temperature
profile depicts axisymmetric with respect to the centerline of the reactor, all subsequent plots associated with the results of flow properties and species profiles will be represented on the X-Y plane of symmetry along the reactor.

Figure 4.2b shows the simulated velocity vectors near the inlet of the reactor, along with a sketch of the common flame feature shown in Figure 4.2c, based on experimental work [134]. Two recirculation zones are seen in the top part of the reactor. Firstly, an internal recirculation zone (IRZ) appears around the centerline of the reactor. Most of the particles with particle diameters from 50 to 800 μm are influenced by the flow within this zone that extends their residence time. Bigger particles with particle diameters from 894 to 1000 μm, are not involved in this circulation zone. Secondly, an external recirculation zone (ERZ) exists in the top corner of the reactor. In there, no fuel particles are available due to the secondary swirl flow of air which acts as a barrier between fuel-air mixture and the external recirculation zone.

![Temperature distribution of gaseous phase throughout the reactor for case 1 (baseline case)](image)

a) Temperature distribution of gaseous phase throughout the reactor for case 1 (baseline case)
Contours of temperature distribution and mass fraction of species of simulation cases 1, 2 and 3 on the X-Y plane of the reactor are illustrated in Figure 4.3. Evidently, the highest temperature within the reactor is about the same (1960 K) in all three cases. The temperature profile extends a bit farther axially in case 3 vs. cases 1 and 2. In case 1, temperature at the centerline reaches a maximum of 1464K at a distance $x = 96$ cm while it reaches almost the same temperature (1463K at $x = 106$ cm in case 2) and (1453K at $x = 136$ cm in case 3). This can be attributed to the delay of devolatilization in case 3 vs. case 2, and similarly for case 2 vs. case 1, as depicted in the mass fraction contours of volatile matter, Figure 4.4 The biomass volatiles are evolved around the center of the reactor. Subsequently, the mass fraction of the volatiles vanishes at 1.33 m from the entrance of the reactor (case 1) whereas it extends to 1.77 m and 1.90 m (case 2) and (case 3), respectively of this chapter.

The same trend is shown in oxygen mass fraction contours in Figure 4.5, which represents the oxygen concentration on the same plane throughout the reactor for the three cases. There is a delay in devolatilization in the compressed biomass particles compared to the uncompressed particles. Subsequently, this will lead to the retardation of char combustion since it is assumed that char combustion starts after volatilization is completed.
Figure 4. 3 Profiles of gaseous temperature through the X-Y plane of symmetry: (a) Case 1: particle density 600 kg/m³, (b) Case 2: particle density 800 kg/m³, (c) Case 3: particle density 1000 kg/m³)

Figure 4. 4 Profiles of wheat straw volatiles mass fraction through the X-Y plane of symmetry: (a) Case 1: particle density 600 kg/m³, (b) Case 2: particle density 800 kg/m³, (c) Case 3: particle density 1000 kg/m³)
Figure 4.5 Profiles of Oxygen mass fraction through the X-Y plane of symmetry: (a) Case 1: particle density 600 kg/m³, (b) Case 2: particle density 800 kg/m³, (c) Case 3: particle density 1000 kg/m³

The denser particles are assumed to have smaller volume, yet they have the same amount of volatile matter. Table 4.2 shows that the distance at which the volatiles are totally released is directly proportional to particle density and inversely proportional to the particle surface area. The longer distance required may also be due to the particle aerodynamics and its impact on the residence time. For the same particle in all three cases, the particle temperature vs. particle residence time is also shown in Table 4.2. The largest particle of the discrete phase stream is supposed to be flowing close to the centerline of the reactor most of the time. The particle residence time of 9.6 s is the longest (case 1), followed by 7.1 s (case 2) and 5.6 s (case 3).

Table 4.2 Length of devolatilization zone, particle surface area and residence time of the largest particle size in case 1, 2 and 3

<table>
<thead>
<tr>
<th>Particle density (kg/m³)</th>
<th>Particle diameter (µm)</th>
<th>Particle surface area (mm²)</th>
<th>X_{vol=0%} (m)</th>
<th>Residence time (s)</th>
<th>Particle T_{max} (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>600</td>
<td>1000</td>
<td>3.1</td>
<td>1.33</td>
<td>9.6</td>
<td>1011</td>
</tr>
<tr>
<td>800</td>
<td>909</td>
<td>2.6</td>
<td>1.77</td>
<td>7.1</td>
<td>975</td>
</tr>
<tr>
<td>1000</td>
<td>843</td>
<td>2.2</td>
<td>1.9</td>
<td>5.6</td>
<td>963</td>
</tr>
</tbody>
</table>
Figure 4.6 shows the burnout of volatile by representing the ratio \([\text{CO}/(\text{CO} + \text{CO}_2)]\) along the centerline of the reactor. Since the homogenous reaction of volatile is modeled by two-step global reaction mechanism in which CO is an intermediate product, therefore this ratio refers to volatile matter burnout. However, this figure also indicates that volatile matter burnout is completed faster for lower particle density while it takes longer for higher particle density.

![Figure 4.6 CO/(CO+CO2) ratio along the reactor centerline for case 1, 2 and 3](image)

4.2.2 Unburnt Carbon

Volatile matter content in biomass exceeds the contents of fixed carbon and other species. However, the heating value of the volatiles is lower compared to fixed carbon. This is one of the reasons that make the heating value of biomass lower than that of coal [134]. The burning of fixed carbon plays a significant role in biomass combustion. To evaluate and compare the completeness of biomass burnout in the three cases of this research, the unburnt carbon needs to be calculated.

The percentage of unburnt carbon in the biomass particles at the reactor exit is calculated using Equation (2.16) for the three cases of particle density (600, 800, and 1000 kg/m³). As shown in Table 4, the unburnt carbon in the baseline case (case 1, 600 kg/m³) and case 2 (800 kg/m³) are 18.6% and 20%, respectively. For case 3 (1000 kg/m³) the unburnt carbon is 26%; hence 7.4% more of biomass fixed carbon is not burnt out vs. the baseline case and 6% more of fixed carbon is unburnt vs. case 2.
Table 4.3 Percentage of unburnt carbon

<table>
<thead>
<tr>
<th>Particle density (kg/m$^3$)</th>
<th>Unburnt carbon %</th>
</tr>
</thead>
<tbody>
<tr>
<td>600</td>
<td>18.6</td>
</tr>
<tr>
<td>800</td>
<td>20</td>
</tr>
<tr>
<td>1000</td>
<td>26</td>
</tr>
</tbody>
</table>

Figure 4.7 shows the variations of biomass particle residence time with particle diameter for case 1. Ten particle diameters are represented in this figure, starting from minimum diameter of 50 μm to maximum diameter of 1000 μm. The average residence time is longer for bigger particles except for the two largest particle diameters ($d_p = 894$ and 1000 μm) in the biomass fuel stream. This would most likely be due to the late response of the largest particles to the swirl flow. As these particles break through the core of the reactor for about 1.5 m from the reactor inlet (Figure 4.8) they do not drift into the recirculation zone before being induced by the swirl flow, resulting in a shorter residence time. Large particles that constitute a significant part of biomass fixed carbon is expected to have more influence on the percentage of unburnt carbon in the biomass particles. Furthermore, due to the shrinkage of biomass particles after pelletization, the compressed particles will have a smaller surface area and a slower rate of surface reaction (as described by Equation 2.7) than the uncompressed particles. Therefore, compressed biomass particles have an increase in the percentage of unburnt carbon (Table 4.3).

In the simulations, 10 different particle bins or diameters were used to represent the Rosin-Rammler distribution. One simulation was also conducted with 20 particle bins. A comparison of the tracks of biomass particles with diameter (894-1000 μm) is shown in Figure 4.8, which depicts the conversion stage of the biomass particles. The number of particle tracks is 4810 and 9620 for 10 and 20 bins, respectively. Simulation results in terms of the maximum gas temperature have negligible differences (about 0.3%) between 10 and 20 bins, suggesting that the results are independent of the number of tracks,
4.2.3 NOx Formation

In this research it is assumed that fuel-N is partitioned into 70% volatile-N and 30% char-N [131, 157]. Char-N is released into the gas phase at a rate that is proportional to the carbon burnout rate. Since the chemistry of char-N conversion is complex, the simulation assumes a fixed fraction of char-N being directly converted to NO with the rest of N converted to N$_2$ [157, 158]. Most of biomass volatile-N will be converted to NH$_3$ while the dominant part of coal volatile-N will be released as HCN [151, 152]. These two intermediate products assist in reducing the nitric oxide (NO) produced from thermal-N to N$_2$. 

Figure 4.7 Average biomass particle residence time vs. particle diameter

Figure 4.8 Tracks of biomass particles of diameter 894-1000 µm traced by the conversion laws
Figure 4.9 plots the mass fraction and concentration of NO at the reactor exit against the radial distance across the exit area for the three particle densities. The NO mass fractions and concentrations associated with case 1 and case 2 show little difference. But for case 3, both the mass fraction and concentration of NO are lower than that in cases 1 and 2. This can be attributed to the higher concentration of NH$_3$ at the exit for case 3.

Figure 4.9 Nitric oxide mass fraction and concentration across the exit surface area of the reactor. Comparison between three cases of particle densities 600, 800 and 1000 kg/m$^3$. 

(a) Nitric Oxide mass fraction

(b) Nitric oxide concentration
The role of NH$_3$ in reducing the mass fraction of NO in the zone where it evolves can be seen in Figure 4.10. The mass fraction of NH$_3$ increases with the axial distance in the volatilization zone, as it is associated with the volatile-N of biomass during the devolatilization process. NO mass fraction attains its minimum value at the location where NH$_3$ mass fraction reaches the maximum. Complete burnout is usually associated with high temperature, which might create a suitable environment for higher NO$_x$ emissions and vice versa.

![Graph](image)

Figure 4. 10 NH$_3$, NO and biomass volatile mass fraction vs. reactor axial distance (particle density 600 kg/m$^3$)

The contours of NO and NH$_3$ throughout the X-Y plane of the reactor as displayed in Figures 4.11 and 4.12 indicate that they are in opposite trends. As seen in Figure 4.12, NO formation is extended farther through the axial (x) direction in case 2 as compared to the baseline case. Some fluctuations in the concentrations of volatile matter, NH$_3$, and NO as well as the gaseous temperature begin to occur. The fluctuating behavior becomes more obvious in case 3. Such intermittency in concentration is expected in lazy dynamic flow [137, 134]. The region of intermittency is characterized by lower volatile matter concentration and higher combustion rate, which is accompanied by higher gas temperature and vice versa.
Figure 4. Contours of NH3 mass fraction through the X-Y plane of symmetry (a) Case 1: particle density 600 kg/m$^3$, (b) Case 2: particle density 800 kg/m$^3$, (c) Case 3: particle density 1000 kg/m$^3$
4.3 Conclusion

In this chapter, the effect of pelletizing biomass is introduced by considering particle shrinkage due to compression during the process of pelletization. Three cases of wheat straw particle densities are studied. The baseline case is for uncompressed particles having a particle density of 600 kg/m$^3$ and average diameter 451 µm. The two cases of densified particles have particle density of 800 kg/m$^3$ and 1000 kg/m$^3$, and average diameter of 410 µm and 380 µm, respectively.

Temperature difference between the three cases is insignificant. However, when compared to the baseline case, compressed particles due to pelletization would experience slower volatilization and surface reaction rates. This leads to a greater percentage of unburnt carbon for compressed particles vs. uncompressed particles. Larger wheat straw particles ($d_p > 894$ µm) have different aerodynamic interaction compared to smaller particles in terms of residence time and particle trajectory. They penetrate axially through the center of the reactor unaffected by swirl preferential flow until they become lighter by completely losing their moisture and volatile contents, leaving only fixed carbon and ash when they start to drift into the swirl flow.
CFD results show that the formation of NO during combustion is shifted downstream as the particle density increases and particle size decreases. NH$_3$ as the intermediate product from biomass volatile-N has contributed to the reduction in NO emission during the volatilization process. Compressed particles would exhibit lower NO emission at the exit than uncompressed particles.
Chapter 5. Fuel preparation and characterization

5.1 Introduction
This chapter covers the preparation and characterization of fuels, and the results were used as inputs to the CFD simulations for mono-firing and co-firing in Chapter 6. Two major types of fuel are involved. The first type of fuel is waste biomass (Douglas fir wood chips), and it was prepared in two forms: 1) raw untreated biomass (RB), and 2) torrefied biomass (TB). The second type of fuel is metallurgical coal tailings (CT) from flotation, which is usually blended with other fine coal rejects at the processing plant and is disposed and classified as mining waste [5]. The fuels RB, TB and CT can be used for mono-firing, whereas the two blended fuels (RB + CT) and (TB + CT) can be used for co-firing in a power plant.

5.2 Fuel preparation
Wood chips having average particle size of 30-50 mm were collected from the wood biomass handling terminals of Fibreco Export Inc. (North Vancouver, BC). After collection, the wood chips were immediately sealed in plastic bags and stored in a cold room at 4ºC. Metallurgical coal tailings originated from the bench-scale flotation tests of the medium volatile coal from British Columbia coalfield.

5.2.1 Grinding of wood chips
Both the raw biomass and torrefied biomass (wood chips) were ground using a 1.5 kW knife mill (Model SM100, Retsch Inc. Newton, PA) with a 2 mm round-hole screen (Appendix C, Figure C.1).

5.2.2 Torrefaction of biomass
Torrefied biomass was produced by thermally treating the wood chips in a lab-scale torrefaction unit in the laboratory of Chemical and Biological Engineering Department. The torrefaction process has been described in Chapter 1 and the technical description of the experimental unit can be found in [159].

A single layer of the biomass sample (200 g) was placed in a 350 mm diameter tray, which is suspended in the center of the torrefaction chamber (dimensions: 650 mm x 480 mm x 410 mm). The treatment of wood chips involves several steps. It started with heating at a constant rate of 10 ºC/min to a maximum temperature of 260º C in an inert environment that contains nitrogen gas, and this temperature was kept constant for 20 min. Thereafter, the sample was rapidly quenched under nitrogen flow to prevent further reaction and cooled down to ambient
temperature. The sample weight was monitored during the torrefaction process, and its mass loss was calculated using a computer program linked to the unit for data acquisition. Finally, the torrefied wood chips were ground to produce the final fuel particles.

![Figure 5.1 Prepared fuel: a) Flotation coal tailings, b) torrefied biomass, c) raw biomass](image)

5.3. Fuel characterization

5.3.1 Physical and thermal properties

The physical and thermal properties include density, calorific value, moisture content, ash content, volatile matter content, fixed carbon content, and elemental (C H N O S) contents. Measurements for the raw biomass and torrefied biomass samples were conducted in the laboratory of the Department of Chemistry at UBC. Samples of coal tailings were sent to Bartley Coal & Minerals Testing Division of GWIL Industries (Calgary, AB) for ultimate analysis.

Particle density of the fuel samples (RB, TB, CT) was measured by using a pycnometer (Model MVP-6DC, Quantachrome Instruments) (Appendix B). The sample was loaded into a calibrated sample chamber of known volume. Analysis gas (N₂) was then introduced to the chamber allowing the gas molecules to rapidly fill its void volume that includes the very tiny pores of the sample. The measurements were repeated seven times. The volume of the sample solid phase is the difference between the volume of the empty chamber and this new void volume, and it is calculated by Equation (3.1),

\[
V_{\text{sample}} = V_{\text{cell}} - V_{\text{ref}} \cdot \left[ \frac{P_1}{P_2} - 1 \right]
\]  

(5.1)

where \(V_{\text{sample}}\) is the sample solid volume, \(V_{\text{cell}}\) is the total volume of sample chamber, \(V_{\text{ref}}\) is the reference volume, \(P_1\) is the initial pressure, and \(P_2\) is the final pressure.

Calorific value (higher heating value HHV) was measured by a bomb calorimeter (Model Parr 6100). The device consists of a combustion vessel in which the fuel powder is placed and
attached to the heating wire. The vessel is submerged into an insulated bucket filled with 2 L distilled water (Appendix C, Figure C.2). The device was calibrated using a pellet (1.0 g) with known HHV. The water temperature was measured before and after combustion to determine the amount of heat released to the water during the combustion process. The combustion vessel was charged with oxygen at 20 atm pressure to ensure complete combustion of the sample. Measurements were repeated five times for each fuel tested.

5.3.1.1 Proximate analysis

Proximate analysis was performed for RB, TB, and CT. It involves four parameters - moisture content, volatile matter content, fixed carbon content, and ash content. Moisture content and volatile matter content were evaluated from the outcomes of Thermogravimetric analysis (TGA) - mass loss and DTG (derivative thermogravimetric) curves.

Ash content was determined following the ASTM Standard Method Number E1755-01 and ASTM D3174-17 for biomass and coal tailings, respectively. Muffle furnace was used for that and samples were heated to 575 ºC and 950 ºC for biomass and coal tailings, respectively, under a heating rate program controlled at 20ºC/min until the samples are completely burned out. Then the samples were kept inside the furnace for 6 hours to cool down. The residue left after combustion represents the ash content of the samples. Each measurement was replicated three times. Fixed carbon content is calculated by subtracting the previously determined moisture, volatile matter, and ash from the initial weight of the sample.

5.3.1.2 Ultimate Analysis

Ultimate analysis involves the determination of elemental contents, ash content, and moisture content. In addition, moisture content of the fuel was measured using a moisture analyzer (A&D Model MF 50), via measuring the weight loss of the sample while it is exposed to a uniform heat source at 105 ºC to evaporate the moisture until a constant mass of the sample is achieved. Triplicate measurements were made, and each measurement involves 10 g of the fuel sample. Moisture content measured by this method was used to determine the HHV of the fuels.

5.3.2 Thermogravimetric analysis

The main purposes of conducting thermogravimetric analysis are to evaluate each sample via proximate analysis and to study their thermal behavior during pyrolysis. Fuel particles of coal flotation tailings (CT), raw untreated biomass (RB), and torrefied biomass (TB) were tested by a
thermogravimetric analyzer (PerkinElmer Model TGA 4000) in the laboratory of the Mining Engineering Department at UBC (Appendix C - Figures C.3 and C.4).

Aside from RB, TB, and CT, two blended fuels were involved in the TGA tests. They have various proportions of biomass and coal flotation tailings - (20, 40, 60 and 80%, of RB with CT) and (20, 40, 60, and 80 of TB with CT). Each sample test was replicated three times; hence the total number of samples was 33. The TGA apparatus measures and records the biomass weight loss with respect to temperature and time. The mass of sample ranged from 25 mg in the case of untreated biomass samples to 114 mg in the case of coal tailings samples. All samples were loaded into a two-piece carousel of the apparatus.

For each test, initially nitrogen was used as the inert purging gas at a rate of 20 ml/min. Then, the heating program was implemented. It started by holding the furnace temperature at 35 ºC for 2 min, then further raising the temperature to 110 ºC with 10 ºC/min heating rate. Temperature was held at 110 ºC for 30 min to allow evaporation of free moisture and to release some loosely bound water. Thereafter, temperature was increased to 260 ºC with a heating rate of 10 ºC/min. Again, this temperature was held for 30 min, during which hemicellulose is expected to decompose and yield some volatiles as the non-condensable gases. This stage also represents a mild torrefaction process whereby the volatiles with low molecular weights would begin to evolve. Finally, the samples were heated to 900 ºC at a rate of 20 ºC/min, and this temperature was held for 10 min to complete the devolatilization stage. The furnace was automatically cooled down at the end of the test to prepare for the next sample test. Pyris software (from PerkinElmer) was used to analyze and plot the data obtained from these tests.

5.4 Results

5.4.1 Physical and thermal properties

Table 5.1 shows the average densities of RB, TB, and CT. The density of coal flotation tailings is 12% greater than the type of coal that is used in the simulations for model validation (Chapter 2). There is no significant difference between the densities of raw biomass and torrefied biomass. The average values of HHV of RB, TB and CT are also shown in Table 3.1. Coal flotation tailings have the highest HHV of 31.1 MJ/kg, whereas HHV of torrefied biomass at 22 MJ/kg is 12% greater than that of raw biomass at 19.7 MJ/kg.
Table 5.1 Fuel particle density, moisture content and calorific value of RB, TB, and CT

<table>
<thead>
<tr>
<th>Fuel sample</th>
<th>Fuel density g/cm³</th>
<th>Moisture content %</th>
<th>Higher heating value (MJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RB</td>
<td>1.28</td>
<td>12</td>
<td>19.7</td>
</tr>
<tr>
<td>TB</td>
<td>1.24</td>
<td>7</td>
<td>22.0</td>
</tr>
<tr>
<td>CT</td>
<td>1.57</td>
<td>4</td>
<td>31.1</td>
</tr>
</tbody>
</table>

5.4.2 Thermogravimetric analysis

Figure 5.2 shows the derivative thermogravimetric (DTG) curves of RB, TB, and CT respectively, which represent the percentage mass loss of the sample based on initial mass at certain heating program. These curves were generated from the TGA processed results (Appendix C, Figure C.5) that are the immediate outputs from the TGA tests by the Pyris software program.

As depicted in Figure 5.3, the slight weight decrease at the beginning of the process elucidates the drying stage in which moisture is released. The first peak in the DTG curve of each fuel represents this stage. The weight loss of RB was observed to be the greatest, followed by TB then CT due to the low moisture content in coal flotation tailings and torrefied biomass versus raw biomass. The maximum reactivity temperature at which the maximum rate of sample mass loss occurs is identified as the lowest point in the DTG curves. This temperature for RB and TB is relatively close to each other at 375-380 °C. Prior to this stage, another peak in the biomass DTG curves was noticed at the beginning of the devolatilization stage when the temperature was held at 260 °C, indicating that the volatiles were released and going through a mild torrefaction process. Here, the DTG curve shows that the torrefied biomass had a lower rate of weight loss than raw biomass because the former has already lost some of the volatiles during torrefaction. Thereafter, sample weight started to drop again around 280 °C for both types of biomass.

Between 300-400 °C, significant weight loss was observed as a result of the thermal decomposition of the hemicellulose, cellulose, and lignin components. Hemicellulose is the most reactive of the three constituents, thermally degrading over the temperature range 220–315 °C. Cellulose degrades between 315-400 °C. Lignin, which is the most chemically complex component, gradually breaks down over a wide temperature range between 160 and 900 °C [160].
RB and TB demonstrate similar trends with respect to temperature during the pyrolysis process. Though the torrefied biomass has less volatiles and less moisture as compared to raw biomass [161]. After the drying stage is completed, the weight loss of CT was much less than RB and TB because of the high reactivity of biomass vs. the coal tailings [162] though the coal tailings demonstrated a higher maximum reactivity temperature at 515 °C.

Figure 5. 2 DTG curves of the fuels for mono firing (RB, TB, and CT)
Figure 5.3 Comparison of TGA weight loss for RB, TB, and CT

The DTG curves for RB-CT blends and TB-CT blends for a range of mixing ratios are illustrated in Figures 5.4 and 5.5, respectively. In these two plots, at least two distinguishable
regions of devolatilization can be seen. A high shoulder is exhibited in the first region where the maximum rate of weight loss takes place, followed by a smaller shoulder that is developed as the percentage of coal tailings in the blended fuel increased. For the RB-CT blends, this second shoulder in the DTG curves becomes more recognizable when the percentage of raw biomass in the blend is 40\% or lower due to increased contribution of lignin from coal tailings. As for the TB-CT blends, the second shoulder becomes obvious when the percentage of torrefied biomass in the blend is 20\% or lower. On the other hand, the second region is pulled up gradually with reducing biomass blend ratio. This region is likely ascribed to the cellulosic content of the blend that is found in biomass. It elucidates a drop of reactivity of the blend due to adding more coal tailing to biomass.

Furthermore, in Figures 5.4 and 5.5, there is no significant difference between the maximum temperature associated with the first peak of the DTG curve for both the RB-CT and TB-CT blends. Nevertheless, there was some effect on the maximum weight loss that can be attributed to the blended fuel’s reactivity. The shoulder of the peak becomes less sharp, indicating a retardation of the reaction as more coal tailings are mixed with biomass. Whereas the second shoulder in the DTG curve is building up by adding more coal tailings to form a second temperature peak around 510 °C. This may be interpreted as a type of non-synergetic relationship between biomass and coal tailings, and in particular, the raw biomass.
Figure 5. 4 DTG curves – fuels for co-firing with various RB: CT percent mixing ratios (100:0, 80:20, 60:40, 40:60, 20:80 and 0:100)
Figure 5. DTG curves – fuel blends with various TB: CT percent mixing ratios (100:0, 80:20, 60:40, 40:60, 20:80 and 0:100)
5.4.3 Proximate analysis

Figure 5.6 shows the proximate analysis parameters of coal flotation tailings (CT), raw biomass (RB) and torrefied biomass (TB). Coal flotation tailings has a fixed carbon (FC) content of 63.3% and volatile matter content of 21.7% (as received).

RB had the highest volatile matter (VM) content among the three fuel samples; TB had 7% less VM content due to torrefaction but 44% more fixed carbon content. Ash content in CT is the highest as expected while it is minimal in both RB and TB. Proximate analysis of RB-CT mixtures is depicted in Figure 5.7. Adding coal tailings to biomass reduces the VM content, but the blend gains more fixed carbon that would raise its calorific value. Figure 5.8 shows the proximate analysis of TB-CT mixtures. Similar behavior is demonstrated for these blends when the coal tailings percentage is increased. For instance, adding 20% of coal tailings to the torrefied biomass reduces the VM content by 14% while enriching the fixed carbon content by 55%. This will also lead to improved calorific value of the fuel mixture.

Figure 5.6 Comparative proximate analysis of RB, TB, and CT from TGA results

<table>
<thead>
<tr>
<th>Table 5.2 Proximate analysis of raw biomass, torrefied biomass, and coal tailings</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fuel Type</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>RB</td>
</tr>
<tr>
<td>TB</td>
</tr>
<tr>
<td>CT</td>
</tr>
</tbody>
</table>
5.4.4 Ultimate Analysis

Table 5.3 shows the results of ultimate analysis of the three fuels CT, RB, and TB. The carbon content of coal tailings exceeds that of raw biomass and torrefied biomass by 65% and 50%, respectively. However, RB and TB have 2.7 and 2.5 times more oxygen content, respectively, as compared to CT.

Table 5.3 Ultimate analysis of the fuels for mono-firing (RB, TB, and CT)

<table>
<thead>
<tr>
<th>Fuel Type</th>
<th>Elemental contents, % db</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>C</td>
</tr>
<tr>
<td>RB</td>
<td>46.5</td>
</tr>
<tr>
<td>TB</td>
<td>51.2</td>
</tr>
<tr>
<td>CT</td>
<td>76.7</td>
</tr>
</tbody>
</table>

Figure 5. 7 Proximate analysis of RB-CT blends from TGA results.

Figure 5. 8 Proximate analysis of TB-CT blends from TGA results.
Beyond ultimate analysis, the Van Krevelen diagram of the individual fuels and blended fuels is presented in Figure 5.9. The H/C and O/C ratios were calculated for the RB-CT and TB-CT blends based on the CHO contents to get an idea about their potential behavior during combustion. The RB-CT blends illustrate the transition of the fuel characteristics from that of biomass towards that of the coal tailings as the biomass fraction (percentage) in the blend increases. The transition appears to occur faster at low biomass fractions, and it gets slower when approaching 100% coal tailings.

In Figure 5.10, the rate at which 50% of volatile matter is released ($R_{50}$) is plotted against the percentage of biomass in the blended fuel. The temperature ($T_{50}$) that corresponds to $R_{50}$ is also shown. At lower biomass percentages, $T_{50}$ is high for both the RB and TB cases, but $R_{50}$ is slower at the same time, implying the dominance of coal flotation tailings in the mixed fuel. At biomass percentages greater than 80% in the blend, $R_{50}$ starts to drop because the loss of volatile matter becomes faster, and this indicates the dominance of biomass in the mixed fuel. Figure 5.11 shows the maximum temperature ($T_{\text{max}}$) for all four fuel blends and the corresponding maximum volatile matter release rate ($R_{\text{max}}$). Changes in $T_{\text{max}}$ with biomass percentage are small, but $R_{\text{max}}$ has pronounced increases with increasing biomass percentage until biomass constitutes 80% in the blend.

![Van Krevelen diagram of the fuels used in the CFD simulations of mono-firing and co-firing in Chapter 6](image)

Figure 5.9 Van Krevelen diagram of the fuels used in the CFD simulations of mono-firing and co-firing in Chapter 6
In this Chapter, coal flotation tailings and biomass were prepared and characterized for performing a CFD simulation of mono-firing and co-firing. Two forms of biomass were prepared, untreated and torrefied biomass. The physical and thermal properties include heating value, particle density, moisture content, ash content, volatile matter content, fixed carbon content, and elemental (C H N O S) contents. Thermogravimetric analyses of coal flotation tailings, untreated
biomass and torrefied biomass was conducted with additional coal tailings and biomass blends for a range of mixing ratios.

Coal flotation tailings had the highest ash content among the other fuels with the higher heating value at the same time. Untreated biomass had the highest volatile matter, yet it is of the lowest heating value among other fuel types. Torrefied biomass had a percentage of weight loss of 3.5% due to the light torrefaction process. The resulted heating value of torrefied biomass was 12% higher than the parent fuel.

In fuel blends, at biomass percentages greater than 80%, R50 starts to drop because the loss of volatile matter becomes faster, and this indicates the dominance of biomass in the mixed fuel. Whereas T50 was decreasing with higher TB% and RB% in the blend. Moreover, T50 of RB mixture is higher than TB mixture because of the higher content of volatiles in RB which takes more time to evolve. Maximum rate of (VM) release is increasing with increasing the biomass share in the blend. Adding coal tailings to biomass reduces the VM content and increases the ash content, but the blend gains more fixed carbon that would raise its calorific value. Rapid change in the rate of volatilization happens when adding small amount of biomass to coal tailings but increasing biomass percentage in the blended fuel does not change the rate significantly at high biomass percentage.
Chapter 6. Mono-firing and Co-firing of Biomass with Metallurgical Coal tailings

6.1 Introduction
In this chapter, CFD simulation is applied to predict and analyze the combustion performance of mono-firing and co-firing of biomass and coal tailings, which involves five scenarios. Scenarios 1, 2, and 3 are pertinent to the mono-firing of coal tailings, raw (untreated) biomass, and torrefied biomass, respectively. Scenarios 4 and 5 are pertinent to the co-firing of coal tailings with raw biomass, and coal tailings with torrefied biomass, respectively.

6.2 CFD simulations for mono-firing
Damstedt experimental furnace unit [134] was again used in the simulations. Biomass was co-fired with coal using a dual feed fuel injector. For co-firing, two fuel-streams are fed from the top center of the reactor - a central stream of fuel is injected through a circular tube that is surrounded by an annulus tube for the second fuel stream. The two fuel streams are surrounded by secondary air flowing in an annulus funnel with swirl flow. The furnace is vertically oriented, with a height of 250 cm and a cylindrical cross section 75 cm in diameter. Furnace wall temperature is kept constant at 800 K.

For mono-firing, fuel particles are injected from the central tube, 30 mm in diameter, at a specified mass flow rate. Particles are airborne through the central tube by primary air at a specified mass flow rate. The secondary air is fed through the outer annular tube at a specified mass flow rate. At the inlet, the secondary air velocity makes an angle of 45° with the X-axis. This will initiate a swirl velocity component in the secondary flow.

The minimum, average and maximum particle sizes for each fuel are shown in Table 6.1. Other fuel characteristics required as inputs to the simulation are taken from Chapter 3 and used in the simulations. Table 6-2 shows the boundary and operating conditions for the three scenarios of mono-firing. Fuel injection rate was calculated based on the input power and the measured higher heating value (HHV) of the fuel. Table 6-3 shows the boundary conditions of the two co-firing scenarios.
Table 6. 1 Fuel particle size for the three mono-firing scenarios

<table>
<thead>
<tr>
<th>Fuel type</th>
<th>Particle size, μm</th>
<th>Spread factor</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Minimum</td>
<td>Average</td>
</tr>
<tr>
<td>CT</td>
<td>25</td>
<td>110</td>
</tr>
<tr>
<td>RB</td>
<td>50</td>
<td>540</td>
</tr>
<tr>
<td>TB</td>
<td>30</td>
<td>293</td>
</tr>
</tbody>
</table>

Table 6. 2 Boundary and operating conditions for the three scenarios of mono-firing

<table>
<thead>
<tr>
<th>Fuel type</th>
<th>HHV (kJ/kg)</th>
<th>Particle density (kg/m³)</th>
<th>Primary air flow (kg/hr)</th>
<th>Secondary air flow (kg/hr)</th>
<th>Fuel mass flow (kg/hr)</th>
<th>Fuel/Air equivalence ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>CT</td>
<td>31132</td>
<td>1570</td>
<td>12.4</td>
<td>180.6</td>
<td>16.2</td>
<td>0.8</td>
</tr>
<tr>
<td>RB</td>
<td>19681</td>
<td>1280</td>
<td>8.6</td>
<td>138</td>
<td>25.6</td>
<td>0.97</td>
</tr>
<tr>
<td>TB</td>
<td>21979</td>
<td>1240</td>
<td>8.5</td>
<td>136</td>
<td>22.9</td>
<td>0.97</td>
</tr>
</tbody>
</table>

Table 6. 3 Air and fuel mass flow rates for the two co-firing scenarios

<table>
<thead>
<tr>
<th>Fuel type</th>
<th>Biomass stream (kg/hr)</th>
<th>Coal stream (kg/hr)</th>
<th>Central air (kg/hr)</th>
<th>Annular air (kg/hr)</th>
<th>Secondary air (kg/hr)</th>
<th>Total air (kg/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>80CT +20TB</td>
<td>3.4</td>
<td>13.8</td>
<td>1.3</td>
<td>8.7</td>
<td>147.0</td>
<td>156.9</td>
</tr>
<tr>
<td>80CT+20RB</td>
<td>3.5</td>
<td>14.0</td>
<td>1.2</td>
<td>8.8</td>
<td>147.4</td>
<td>157.5</td>
</tr>
<tr>
<td>33CT+67RB</td>
<td>14.4</td>
<td>7.1</td>
<td>4.8</td>
<td>4.5</td>
<td>142.5</td>
<td>151.8</td>
</tr>
</tbody>
</table>

Volatile matter combustion is modeled by two-step mechanism which describes the oxidation of hydrocarbon in gas phase [130]. For mono-firing, the volatile matter in each fuel can be represented by a virtual species in the form of $CH_aO_bN_cS_d$, where (a, b, c, d) are derived based on ultimate and proximate analyses of the fuel. For the three types of fuel - coal tailings (CT), raw biomass (RB), and torrefied biomass (TB), the gas phase combustion can be described by two chemical reactions with CO as an intermediate species,

**CT:**

$CH_{21.929}O_{5.7884}N_{0.524}S_{0.0764} + 3.12629 O_2 \rightarrow CO + 10.9645 H_2O + 0.00262N_2 + 0.03821SO_2$

$CO + 0.5 O_2 \rightarrow CO_2$
Volatile matter of biomass is 3.37 times greater than that found in coal tailings (daf); in contrast, coal tailings contain 5.36 times more fixed carbon than biomass (daf).

**RB:**

\[
CH_{2.35478}O_{1.076898}N_{0.009606} + 0.550246 \text{ } O_2 \rightarrow CO + 1.17739 \text{ } H_2O + 0.003548 \text{ } N_2
\]

The volatile matter fraction in torrefied biomass is only 7% less than raw biomass (daf), whereas the fixed carbon fraction in torrefied biomass is 1.44 times greater than that in raw biomass (daf).

**TB:**

\[
CH_{2.310186}O_{1.024303}N_{0.006463} + 0.565395 \text{ } O_2 \rightarrow CO + 1.155093 \text{ } H_2O + 0.003232 \text{ } N_2
\]

The volatile reaction mechanism of the co-fired coal tailings and biomass is same as that for mono-firing, with the same corresponding virtual volatile matter composition. Besides, the same particle size distribution (Table 6.1) that was used in the mono-firing cases is used in coal tailing/biomass co-firing.

**6.3 Simulation results for mono-firing**

The simulated combustion performance will be evaluated through the gaseous temperature profiles and velocity vectors, species concentration (volatile matter, oxygen, and carbon monoxide), chemical flame length, and unburnt carbon of fuel particles at the furnace exit. NO\textsubscript{x} concentration at the exit is also presented for the co-firing scenarios.

**6.3.1 Volatile matter combustion**

Figure 6.1 (a, b, c) illustrates the gaseous temperature profile in a vertical X-Y plane that passes through the centerline of the furnace for the three scenarios of mono-firing – CT, RB, and TB combustion.

For coal tailings combustion, high temperature is observed near the furnace inlet and internal recirculation zone with a maximum value of 2329 K. Temperature rise is due in part to oxidation of the devolatilized gas. Figure 6.2 (a, b, c) shows the mass fraction of CO, O\textsubscript{2} and volatile matter in the central X-Y plane of the furnace that is 75 cm from the furnace inlet. CO is produced in that zone as an intermediate product in the first step of volatilization reaction mechanism and it shows its maximum concentration in the exact region with maximum
temperature. Therefore, oxygen is almost fully consumed in that region. Gas temperature is higher in the outer peripheral zone of the furnace (1200 K) but decreases from the flame envelope towards the central zone (950 K). As volatile matter is released from the fuel particles, it starts burning and is driven radially by swirl flow to the peripheral zone where combustion is completed.

In the case of raw biomass combustion, the temperature is higher in the regions with high chemical reactivity of the volatiles and reaches a maximum of 1052 K. Figure 6.3 shows that volatile mass fraction is concentrated in the core zone and it extends to 1.14 m from the furnace inlet. CO vanishes completely at this distance, and this will delay char combustion since it starts after the volatile is released [135]. This distance is longer than that in coal tailings as raw biomass has greater volatile mass fraction compared to coal tailings. The volatile matter is largely consumed in the peripheral zone where high temperature zone appears.

As for torrefied biomass combustion, the maximum temperature is 2170 K. Higher gaseous temperature is seen near the flame boundary where both step 1 and step 2 reaction rates are high. Volatile matter released from the torrefied biomass vanishes at 0.775 m (Figure 6.4), which is 0.365 m closer to the furnace inlet compared to raw biomass burning. This is in line with the differences in volatile mass fraction between the two scenarios, as shown in Figure 6.4.
Figure 6. 1 Gaseous temperature profiles on X-Y central plane of the furnace a) CT, b) TB, c) RB

Figure 6. 2 Species mass fraction and gaseous velocity magnitude vectors through X-Y central plane of the furnace, CT
Figure 6.3 Species mass fraction and gaseous velocity magnitude vectors through X-Y central plane of the furnace, RB (left) and TB (right)
Figure 6.4 Comparison between volatiles mass fraction at centerline of the furnace for RB, TB and CT mono-firing

### 6.3.2 Chemical flame length

Figure 6.5 (a,b,c) depicts the chemical flame based on the oxidation mixture ratio, $R_o$ (Equation (2.14)) of fuel combustion. Flame boarders are identified by the critical flame radius ($R_c = 0.99 R_o$) [30, 29], which separates the fuel-rich zone (inside the flame) and the oxygen-rich zone (outside the flame). Coal tailing flame front is at 0.44 m with a lift-off from the furnace inlet about 0.07 m. Thus, the total flame length is about 0.37 m with maximum flame diameter, $R_{max}$, of 0.21 m. The oxidation mixture ratio of raw biomass combustion gives rise to a wider and longer flame than coal tailings. Due to the higher volatile matter content of raw biomass than coal tailings, the fuel-rich zone forms most of the flame envelope for raw biomass burning, with a flame length of about 1.25 m from the furnace inlet and maximum flame radius is about 0.35 m from the center of the furnace. By comparison, the flame front of torrefied biomass lies at 0.8 m from the furnace inlet, and this is intermediate between coal tailings and raw biomass. Its flame maximum diameter is same as that of raw biomass. Again, torrefied biomass has lower volatile matter content; hence, heterogeneous reaction of biomass fixed carbon starts earlier and there is a smaller flame volume. Therefore, char particles can have longer residence time inside the furnace, potentially resulting in less unburnt carbon.
6.3.3 Unburnt carbon

Coal tailing (CT) particles were grouped into a set of 10 particle diameters (25, 44.5, 64, 84, 108, 122, 142, 161, 180, and 200 µm). Based on the simulation results, the particles have an average residence time of 7.3 s. Figure 6.6 shows that 13.3% of the total carbon and 13.7% of the fixed carbon contained in the particles remains unburned, respectively. The burned-out particles exit the furnace as incombustible ash content. However, the unburned fixed carbon at the exit is carried with the three larger size particles (161, 180 and 200 µm) which comprise 73% of the initial (input) amount of fixed carbon in the coal tailings.

Particle sizes of the raw biomass (RB) are grouped as (50, 104, 159, 213, 268, 322, 377, 431, 486 and 540 µm). The particles have an average residence time that is almost the same as that of the coal tailings. The smaller particles (50-268 µm) that comprise 14% of the fixed carbon in the fuel are completely burned out. The larger particles (322-540 µm) leave the furnace with percent unburned fixed carbon of 45.6% in the particles (Figure 6.6). It shall be noted that unlike coal tailings, fixed carbon constitutes a relatively small part of the combustible material (about 15% of the total fuel DAF) in the raw biomass, though the heating value of fixed carbon is greater than that of volatile matter. Thus, taking the complete combustion of volatile matter into consideration, only 13.6% of the total carbon contained in the particles remains unburned (Figure 6.6). Although the percent unburned carbon in coal tailings is very close to that of raw biomass,
coal tailings exhibit more efficient combustion as the higher volatile matter content of raw biomass leads to a delay in the ignition of fixed carbon especially for the larger size particles.

Similar to the previous two scenarios, particle sizes of torrefied biomass (TB) are sorted as (30, 59, 88, 118, 147, 205, 235, 264 and 293 µm). The average residence time of the partially burned particles is longer at 13.5 s while the average residence time of all particles is also longer at 10.7 s. Smaller particles (diameters less than 147 µm) that comprise only 3% of the torrefied biomass’ fixed carbon are completely combusted. The bigger particles are partially burnt, leaving the furnace with percent unburned fixed carbon of 29.2% (Figure 6.6). Considering the carbon content of torrefied biomass, the percent unburned carbon of 11.4% is the lowest among the three types of fuel (coal tailings, raw biomass, torrefied biomass). On average, the torrefied biomass particles have spent longer residence time inside the furnace, resulting in more efficient combustion of fixed carbon compared to raw biomass.

Figure 6.6 also demonstrates that loss on ignition (LOI) is lower in torrefied biomass compared to raw biomass and LOI is the lowest compared with coal tailings. This can be attributed to the higher percentage of unburned fixed carbon along with ash in the particles that exit the furnace for the raw biomass scenario. Volatile matter has a lower calorific value than fixed carbon, but the combustion of fixed carbon is slower than volatile matter. Hence, the percentage of volatiles and fixed carbon in the fuel could also be indicative of LOI aside from the unburned carbon content.

![Figure 6.6 Carbon burnout graph includes unburnt fixed carbon and unburnt carbon comparisons for mono-firing cases](image-url)
6.4 Co-firing coal tailings with biomass

Two scenarios are presented for co-firing coal tailings with biomass (untreated and torrefied). In each scenario, two fuel streams are injected separately. The biomass fuel stream is injected to the furnace through the central pipe with primary air flow. Particles of the coal tailings stream enters the furnace through the annular pipe surrounding the central pipe with its primary air flow rate. Secondary air flow is fed from the outer annular pipe of the quarl. Primary air velocity of the two fuel streams are assumed normal to the inlet surface area. The secondary air velocity is assumed to have swirl angle of 45°. For the co-firing of coal tailings with raw biomass, coal tailings take up 80% and 86.4% of the mixed fuel on weight basis and energy basis, respectively. For the co-firing of coal tailings with torrefied biomass, coal tailings take up 80% and 85% of the mixed fuel on weight basis and energy basis, respectively.

6.5 Simulation results for co-firing

6.5.1 Volatile combustion and gaseous properties

The two co-firing scenarios are evaluated through the comparison between different properties and species concentration. Figure 6.7 shows the temperature profile through x-y central plane in the two cases. Temperature of (CT+RB) case is slightly lower than (CT+TB) case. Compared to mono firing cases 1,2 and 3 in table 6.1, the maximum temperature is lower than coal tailing case and higher than biomass cases.

Figure 6.7 Temperature profile of Co-firing coal tailings with biomass
Figure 6.8 shows the mole fraction ratio of (CO/(CO+CO₂)) at the center line of the furnace for the first 1m from the furnace intake for the two co-firing scenarios. In both cases, the CO is completely combusted at the beginning of the furnace at around 40 cm from furnace inlet.

Figure 6.8 CO/(CO+CO₂) ratio of two fuel blends, (CT+RB and CT+TB)

Figure 6.9 shows the volatile mass fraction in the two cases. The two mixture have the same fraction of coal tailing therefore, the difference will be directly attributed to the volatile mass fraction in raw biomass and torrefied biomass. In (CT+TB) case, the rate of volatile release is slower than (CT+RB) case and extends further although (CT+RB) case evolves more volatile matter.

Figure 6.9 Volatile mass fraction of the fuel blend along the centerline and at radius of 25cm and 75 cm
6.5.2 Unburnt carbon

Figure 6.10 illustrates the comparison of unburned fixed carbon and unburned carbon in the six cases previously mentioned in Table 6-1. It shows that the percent unburned fixed carbon in coal tailings (CT) is less than that in torrefied biomass (TB), which in turn is less than that in raw biomass (RB). When 20 wt% RB is co-fired with 80 wt% CT, the percent unburned fixed carbon is increased from 13.7% (CT alone) to 34% (80CT+20RB) though it is still less than the percent unburned fixed carbon (45.6%) of RB mono firing. By comparison, co-firing 20 wt% TB with 80 wt% CT results does not lead to a significant change in the percent unburned fixed carbon (i.e. 13.7% vs. 13%). This is in line with the fact that the particle sizes of torrefied biomass is comparable to coal tailings though the former’s particle density is lower. In addition, the mass fraction of fixed carbon in torrefied biomass (approx. 20% DAF) is less than that of the coal tailings (approx. 75% DAF).

An additional simulation run was conducted using 67:33 biomass-to-coal tailings ratio. Results (temperature profile, unburnt carbon, and NOx emission) are compared to the simulation run using a 20:80 biomass-to-coal tailings ratio.

6.5.3 Flame length

Through CFD simulation, it is possible to predict the 3-dimensional chemical flame of coal tailings and biomass fuel individually and study them seperately, though this is likley not achievable in practice since the flames are overlapped on each other. The length and width of the chemical flame for biomass is comparable to that of coal tailings although the former has higher volatile matter content than the latter, and the blended fuel is only 20% share of biomass versus 80% share of coal tailings. Coal tailings flame is noticed to be slightly lifted off the furnace inlet compared to that of biomass; this is expected because the devolatiltization of coal tailings starts later than biomass as previously shown in Chapter 5.
Unburnt fixed carbon remaining with ash compared to unburnt carbon of the fuel in the six cases

**6.5.4 NO\textsubscript{x} formation**

Table 6.4 shows the mass fraction of NO at the center of furnace exit for all five scenarios of CFD simulations.

For mono-firing, coal tailings have the highest mass fraction of NO followed by raw biomass, and torrefied biomass has the lowest NO mass fraction. Partitions of HCN and NH\textsubscript{3} intermediate species for biomass NO\textsubscript{x} formation are at 20% and 80%, respectively, whereas for coal tailings, HCN and NH\textsubscript{3} partition are at 70% and 30%, respectively.

For the co-firing scenarios of coal tailings and biomass, Table 6.4 shows that the NO is lower compared to the mono-firing scenarios of both raw biomass and torrefied biomass. Figure 6.11 depicts that in co-firing coal tailings and raw biomass, the intermediate species NH\textsubscript{3} and HCN have higher concentrations but lower NO concentration. The results support the effect of these species in reducing NO formation. It is also noticed that the NO concentration continues to decrease even after NH\textsubscript{3} is consumed due to the existence of HCN during the fixed carbon burnout of coal tailings. The same trends are found for co-firing coal tailings and torrefied biomass.
Table 6.4 No mass fraction at furnace exit center

<table>
<thead>
<tr>
<th>Scenario</th>
<th>NO mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mono-firing</td>
<td></td>
</tr>
<tr>
<td>RB</td>
<td>$5.35 \times 10^{-4}$</td>
</tr>
<tr>
<td>TB</td>
<td>$1.28 \times 10^{-4}$</td>
</tr>
<tr>
<td>CT</td>
<td>$8.26 \times 10^{-4}$</td>
</tr>
<tr>
<td>Co-firing</td>
<td></td>
</tr>
<tr>
<td>80CT+20RB</td>
<td>$4.33 \times 10^{-4}$</td>
</tr>
<tr>
<td>33CT+67RB</td>
<td>$3.59 \times 10^{-4}$</td>
</tr>
<tr>
<td>80CT +20TB</td>
<td>$3.50 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Figure 6. 11 NO, NH$_3$ and HCN mass fraction of co-firing coal tailings with raw biomass

### 6.6 Conclusions

This chapter simulates the combustion of coal tailings and biomass in a lab-scale furnace (presented in the literature, Ref [134]) in order to predict the combustion behavior and possibility of converting waste coal in the form of coal tailings to fuel. About 86% of fixed carbon in coal tailings is burned out during mono-firing, whereas this percentage is 70% and 55% in torrefied and raw biomass, respectively. Coal tailings particles that have a diameter smaller than 161µm are completely burned out, while larger particles are partially burned. Torrefied biomass and raw biomass particles with diameter larger than 147µm and 322µm are incompletely combusted, respectively. Coal tailings’ flame length is shorter than torrefied biomass, which in turn is shorter than raw biomass. This has required longer residence time for raw biomass char particles (which contains only FC and ash) to complete burnout as combustion starts right after devolatilization ends. Maximum gas temperature throughout the furnace and flue gas temperature at the exit in coal combustion are both higher than those associated with biomass combustion.
Torrefied biomass particles require a longer residence time inside the furnace and have a greater tendency to burnout. This is in part due to their small size, which allows the particles to be involved in the swirl flow. In mono-firing, coal tailings scenario has the highest NO formation, followed by raw biomass, then torrefied biomass. In the co-firing two scenarios, coal tailings with raw biomass (CT+RB) has experienced higher NO at the exit than coal tailings with torrefied biomass (CT+TB). The contribution of the intermediate species NH₃ and HCN is evident in reducing NO emission.
Chapter 7. Overall Conclusions and Recommendations

7.1 Overall conclusions

In this thesis, the combustion of solid biomass particles and coal particles was simulated using computational fluid dynamics models to investigate the key parameters influencing the combustion of biomass and coal. Based on the objectives of this research thesis, the key results and findings can be summarized below.

1- One of the big challenges in co-firing biomass with coal, especially when direct co-firing is involved, is the restrictions on the percentage biomass in the blended fuel (i.e. co-firing level). For co-firing level greater than 50%, the furnace should be designed for adopting biomass combustion which can be costly to implement. To overcome this challenge, furnace geometry modifications can be introduced to the co-firing system. In this thesis, two types of unsophisticated geometry modifications were simulated, using wheat straw and coal as the blended fuel to improve the co-firing combustion performance.

   The first modification is by replacing the sudden expansion in conventional furnace geometry near the furnace inlet with a gradual expansion having an angle of 47.7º and 25 cm length. This conical diffuser has fully removed the external recirculation zone (ERZ). The new configuration saved the flow energy that was wasted in eddies and circulations in the (ERZ) and facilitated developing higher swirl flow. Based on the CFD simulation results, this new modification leads to a complete combustion of biomass fixed carbon and has reduced the unburnt fixed carbon of coal by 33% compared to the old geometry. Circulation inside the internal recirculation zone (IRZ) is higher in the modified furnace. The flame length is horizontally stretched and vertically compressed upward.

   The second modification is by increasing the swirl angle of the secondary air from 45º to 68º. CFD results show that the combination of the two modifications (i.e., the gradual expansion + the larger swirl angle) has further reduced the unburnt fixed carbon in coal by 55%.

2- Biomass pelletizing has been one of the efficient choices of biomass densifications to overcome some transport challenges and improve the mechanical and physical properties of biomass in addition to facilitating it’s handling in the supply chain. In this research, the
influence of particle shrinkage, due to biomass densification, on biomass combustion was investigated in co-firing furnace using wheat straw and coal. Investigation was done by CFD modeling. A baseline case (particle density of 600 kg/m$^3$ with no particle shrinkage) and two cases of densification (particle densities 800 kg/m$^3$ and 1000 kg/m$^3$) were considered in this investigation. CFD results showed that densified particles have experienced slower volatilization and surface reaction leading to a higher unburnt fixed carbon in biomass particles at the exit of the furnace.

The larger wheat straw particles ($d_p > 894 \ \mu m$) are unaffected by the swirl flow and penetrating axially through the center of the furnace until the FC combustion stage starts and particles become lighter. On the other hand, NO formation during combustion of the densified particles is less than that during none-densified particles.

3- Coal tailings and biomass were prepared and characterized. Experimental results were used in the CFD simulations for mono-firing and co-firing. Torrefied biomass was produced using a light torrefaction process (weight loss at 3% dry basis) on raw biomass. Based on the results of thermogravimetric analysis (TGA), the fuel blend characteristics was dominated by biomass at high co-firing level (80% biomass).

4- CFD results show that about 86% of fixed carbon in coal tailings is burned out during mono-firing, whereas this percentage is 70% and 55% in torrefied and raw biomass, respectively. Coal tailings particles with diameter greater than 161 $\mu m$ are partially burned out; and for torrefied biomass and raw biomass, the threshold particle diameter is 147$\mu m$ and 322$\mu m$, respectively. Coal tailings flame is relatively short compared to biomass flame length. Maximum gas temperature throughout the furnace and flue gas temperature at the exit in coal combustion are both higher than that associated with biomass.

    Torrefied biomass particles require a longer residence time inside the furnace and have greater tendency to burnout. This is in part due to their small size compared to raw biomass and lower density compared to coal tailings. This enables the torrefied biomass particles to merge into the swirl flow more readily than biomass and coal tailings particles.
5- NOx emission results show that, for densified particles the formation of NO during combustion is shifted downstream as the particle density increases and particle size decreases. NH$_3$ as the intermediate product from biomass volatile-N has contributed to the reduction in NO emission during the volatilization process. Compressed particles would exhibit lower NO emission at the exit than uncompressed particles.

In mono-firing, coal tailings have the highest NO formation, followed by raw biomass, then torrefied biomass. Whereas the co-firing of coal tailings with torrefied biomass leads to lower the NO emission as compared to co-firing coal tailings with raw biomass. The results suggest that co-firing coal tailings with torrefied biomass is a better option due to its lower NO emission and lower percent unburnt carbon.

7.2 Recommendations for future work
A validated CFD simulation is an efficient tool for virtual investigation and retrofitting prior to the actual experimental work. Experiments on the combustion of biomass and coal have a lot of safety and cost concerns. CFD simulations can represent the first choice, if possible, before the real experiments are conducted. Practically, many challenges are associated with biomass and coal combustion, handling, drying, and so on. CFD can also be part of the solution to meet these challenges though it cannot be a replacement of experimentation.

Based on the results of this research, the following suggestions are recommended for further studies:

1- CFD simulation
   a. Consider implementing a new techniques of biomass fuel staging based on particle size when injecting fuel particles into the furnace.

   b. The current CFD model cannot capture particulates matter including PM$_{10}$ and PM$_{2.5}$ which can pose a significant air pollution problem that has impacts on human health and the environment if not adequately treated. Future work shall extend the model to predict and investigate the formation of particulates matter during the co-firing of biomass and coal.
2- Perform a comprehensive investigation of the pelletization process by using a CFD model that takes the effects of factors such as particle shape, particle collision, and coincident conversion stages into consideration.
   a. Introduce the effect of biomass particle shape to address its impact on simulation results.
   b. Study the effect of conical diffuser angle at the furnace entrance on the combustion efficiency and NOx emission.

3- Conduct experimental evaluation of coal tailings combustion and co-firing with biomass to further study the feasibility of utilizing metallurgical coal tailings as fuel.

4- Experimental study of the effect of gradual expansion on the augmentation of heat transfer by enhancing the swirling flow by investigating the effect of conical diffuser angle on the furnace entrance.
References


Appendices

Appendix A – Mathematical Model and Essential Governing Equations

The time averaged gas phase equations for steady, turbulent flow is:
\[
\frac{\partial}{\partial x_j} (\rho u_i \phi) = - \frac{\partial}{\partial x_i} \left( \Gamma_0 \frac{\partial \phi}{\partial x_i} \right) + S_m
\]

1- Continuity Equation:
\[
\frac{\partial \rho u_i}{\partial x_i} = S_m
\]

2- Momentum Equation:
\[
\frac{\partial (\rho u_i u_j)}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{\partial (t_{ij} + \tau_{ij})}{\partial x_j} + F
\]

\( t_{ij} \) is the viscous stress tensor = \( \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \);

\( \tau_{ij} \) is the average Reynolds stress tensor = \( \mu_t \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \) \( \frac{2}{3} \left( \rho k \delta_{ij} \right) \)

The average turbulent kinetic energy is \( k = \frac{1}{2} \bar{u}_i \bar{u}_j \)

The turbulent eddy viscosity is \( \mu_t = C_\mu \frac{\rho k^2}{\bar{u}_j} \); \( C_\mu = 0.09 \)

\( \bar{\varepsilon} \) is the average dissipation rate of turbulent kinetic energy = \( \bar{\varepsilon} \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} \)

3- Turbulent Kinetic Energy Equation:
\[
\frac{\partial (\rho u_i \bar{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu + \mu_t}{\sigma_k} \frac{\partial \bar{k}}{\partial x_j} \right) + G_k - \bar{\rho} \bar{\varepsilon}
\]

Where, \( \sigma_k = 1; G_k \) is the production of the turbulent kinetic energy defined as:
\[
G_k = \mu_t \left[ \left( \frac{\partial u_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_j} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right] \left[ \mu_t \frac{\partial \bar{u}_j}{\partial x_k} + \bar{\rho} \right]
\]
4- Dissipation of Kinetic Energy Equation:

\[
\frac{\partial \rho \varepsilon u_j}{\partial x_j} = C_{\varepsilon 1} \frac{\varepsilon}{k} G_k + \frac{\partial}{\partial x_j} \left[ (\mu + \frac{\mu_t}{\sigma_\varepsilon}) \frac{\partial \varepsilon}{\partial x_j} \right] - C_{\varepsilon 2} \bar{\varepsilon}^2
\]

where; \(C_{\varepsilon 1} = 1.44, C_{\varepsilon 2} = 1.92\sigma_\varepsilon = 1.3\)

5- Turbulent Intensity (T.I): It is the ratio between the RMS of the turbulent velocity (velocity fluctuation) and the average velocity at the same location.

\[
u = \bar{u} + \hat{u} \quad ; \quad T.I \ (\%) = \frac{\hat{u}}{\bar{u}} \times 100
\]

For \(k-\varepsilon\) model, T.I can be calculated using the following correlation:

\[
T.I = \frac{\hat{u}}{\bar{u}} = \frac{0.16}{Re_{HD}^{0.125}}
\]

HD is the hydraulic diameter, HD = D for circular tubes; HD = D_o - D_i for annular tube

6- Energy Equation:

\[
\frac{\partial \left( \rho \bar{E} + \overline{P} \right) u_j}{\partial x_j} = \frac{\partial}{\partial x} \left[ \left( k_{eff} \right) \frac{\partial \bar{T}}{\partial x_j} - \Sigma h_j J_j + (\tau_{eff} u_j) \right] + S_h
\]

7- Volatile mass balance equation:

\[
- \frac{dm_p}{dt} = k \left[ m_p - \left( 1 - f_{v,i} \right) \left( 1 - f_{m,i} \right) m_{p,i} \right]
\]

where: \(f_{v,i}\) is initial volatile mass fraction;

\(f_{m,i}\): initial moisture fraction in the particle

\(f_{v,i}\): initial volatile fraction in the particle

\(m_{p,i}\): initial particle mass

\(m_p\): current particle mass (kg)

\(k\): devolatilization rate (\(s^{-1}\)) = \(A e^{-E/(RT)}\)

Where: \(A\) is the frequency constant; \(E\) is the activation energy of devolatilization.

Assuming single rate model devolatilization depending on the amount of volatile remaining in the particle i.e. \[m_p - \left( 1 - f_{v,i} \right) \left( 1 - f_{m,i} \right) m_{p,i}].\]
8- Equation of particle motion:

\[
\frac{du_p}{dt} = F_d(u - u_p) + g_x \frac{(\rho_p - \rho)}{\rho_p} + F_x \; ; x \text{ is any of the three cartesian coordinates}
\]

\[
u_p = \frac{dx}{dt}
\]

\[F_d = \text{drag force} = \frac{18\mu C_D Re}{\rho_p d_p^2 24} \; ; \; \text{Re is the relative reynolds number}
\]

\[= \frac{\rho d_p |u_p - u|}{\mu}
\]

9- Heat transfer across the particle during evaporation:

\[m_p C_p \frac{dT_p}{dt} = h A_p (T_\infty - T_p) - \frac{dm_p}{dt} h_f g + A_p \varepsilon_p \sigma (\theta_R^4 - T_p)
\]

\[T_p \text{ is the particle temperature; } A_p \text{ is the surface area; } C_p \text{ is the specific heat at constant pressure; } h_f g \text{ latent heat of evaporation; } h \text{ is the heat transfer coefficient (W/m}^2\text{K)}
\]

The heat transfer coefficient from Ranz and Marshall Correlation which is given as:

\[Nu = \frac{hd_p}{K_\infty} = 2 + 0.6 Re_d^{(\frac{1}{2})} Pr^{(\frac{1}{3})}
\]

10- Heat transfer across the particle during char combustion:

\[m_p C_p \frac{d\theta_R}{dt} = h A_p (T_\infty - T_p) - \frac{dm_p}{dt} H_r + A_p \varepsilon_p \sigma (\theta_R^4 - T_p);
\]

\[f_h \text{ is the fraction of heat of reaction absorbed by particle during surface reaction. Its recommended value is 1.0 if the char combustion product is CO and 0.3 if it is CO}_2
\]

\[H_r \text{ is the heat of reaction released during surface reaction.}
\]

11- Discrete Phase/Continuous phase exchange of mass, momentum and heat

The momentum transfer from the continuous phase to discrete phase is calculated by examining the change in momentum of a particle as it passes through each control volume. Same thing happens with mass and heat.

\[\text{a) Momentum exchange: } F = \sum m_p du_p = \sum \left[ F_d(u - u_p) + g_x \frac{(\rho_p - \rho)}{\rho_p} + F_x \right] m_p \Delta t
\]

\[\text{b) Mass exchange: } M = \frac{\Delta m_p}{m_{p,o}} m_{p,o}
\]

\[\text{c) Heat Exchange:}
\]
\[ Q = \frac{m_{p,o}}{m_{p,o}} \left[ (m_{p,in} - m_{p,out})[-H_{lat,ref} + H_{pyrol}] - m_{p,out} \int_{T_{ref}}^{T_{out}} c_p dT \right. \\
\left. + \int_{T_{ref}}^{T_{in}} c_p dT \right] \\
\]

12- **Dilution assumption: Volumetric fraction of solid fuel should be \(< < 10\%\)**

Using mass flow rates of air and fuel with their true density volumetric fraction can be calculated as

\[ f_d = \frac{\left( \frac{m}{\rho} \right)_{fuel}}{\left( \frac{m}{\rho} \right)_{air}} \]

13- **Turbulent Dispersion model:** This model considers the turbulence in particle momentum due to the velocity fluctuation of the continuous phase. In Ansys Fluent, this can be calculated using one of the two models which are; the discrete random walk model (Stochastic model) or Cloud model.
Appendix B Virtual volatile compound

<table>
<thead>
<tr>
<th>Ultimate Analysis %</th>
<th>index</th>
</tr>
</thead>
</table>
| C                   | \[
\frac{(C\%)_12}{C\%_{12}} = 1
\] |
| H                   | \[
\frac{(H\%)_{1}}{C\%_{12}} = x
\] |
| O                   | \[
\frac{(O\%)_{16}}{C\%_{12}} = y
\] |
| N                   | \[
\frac{(N\%)_{14}}{C\%_{12}} = z
\] |
| S                   | \[
\frac{(S\%)_{28}}{C\%_{12}} = xx
\] |

\( CH_xO_yN_zS_{xx} \)
Appendix C Apparatus and TGA graphs

Figure C.1 1.5 W Knife mill, Model SM100, Retsch Inc. Newton, PA.

Figure C.2 Bomb calorimeter Parr 6100

Figure C.3 Thermogravimetric analysis (TGA) apparatus- Mining Department, UBC. 33 samples of RB, TB and CT can be loaded.
Figure C.4 TGA apparatus

Figure C.5 TGA curves of RB, TB and CT