**DETAILED STUDY OF WOOD COMBUSTION IN A FIXED BED
REACTOR UNDER OXY-FUEL CONDITION**

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**A THESIS SUBMITTED IN PARTIAL FULFILMENT OF THE
REQUIREMENTS FOR THE AWARD OF THE DEGREE OF DOCTOR
OF PHILOSOPHY IN MECHANICAL ENGINEERING IN THE
SCHOOL OF ENGINEERING OF DEDAN KIMATHI UNIVERSITY OF
TECHNOLOGY**

APRIL, 2020

DECLARATION

This thesis is my original work and has not been presented in any other University/Institution for a degree or for consideration of any certification.

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DEDICATION

This thesis is dedicated to my parents, my wife and my children.

ACKNOWLEDGEMENTS

The conception, design, implementation and execution of this PhD thesis would not have been possible without God's favour, mercy and grace.

The success of this research work is also greatly owed to my first supervisor, Prof. P. N. Kioni. He provided a deep insight, great support and invaluable guidance throughout the work. He also dedicated his time and provided valuable materials for this work. For all these, I am very grateful to him. I also like to thank my second supervisor, Prof. N. W. Karuri for the contribution, support and guidance throughout this work. I am also greatly indebted to my German Professor, Prof. Dipl. Ing. T. Mirre for not only guiding and supporting me throughout the work but also providing CFD software CD-Adapco (STAR CCM+ version 11.04) and hosting me in his laboratory while undertaking this research in Technische Hochschule, Wildau Germany. I would also like to thank Mr. M. Nowitzki for training me on STAR CCM+ software and his contribution while performing most of the computational work.

My gratitude also goes to many people who have contributed to the success of this work in one way or another. I can only mention but a few; to all others, my most sincere gratitude. I would like to particularly mention Prof. P. Muchiri and Prof. M. Herzog for their role in organizing successful research visits to Technische Hochschule, Wildau Germany. I would also like to thank Prof. Herzog for hosting me in his laboratory and allowing me to use some of his equipment like Atlas LOI equipment. I would also not forget Mr. E. Kornejew for providing me with laboratory instructional manuals and his valuable advice in this work.

I am also very grateful for the financial support of both Dedan Kimathi University of Technology (DeKUT), Kenya, and Technische Hochschule Wildau, Germany. Special thank also goes to the German Academic Exchange Service (DAAD) for granting me stipend while

undertaking this work at Technische Hochschule, Wildau, Germany. I would also thank my colleagues: Mr. Njeru, Mr. Mwangi, Mr. Kinyua, Mr. Nyakoe and Mr. Timothy of Advanced Design, Manufacturing Training Centre (ADMATC) for their assistance in the work that was done in DeKUT.

Finally, I fully appreciate the moral and spiritual support of my wife Fancy and my entire family throughout this period.

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ABBREVIATION

AMG	Algebraic Multi-Grid
ASU	Air Separation Unit
CCS	Carbon Capture and Storage
CFD	Computational Fluid Dynamics
CPU	Carbon Dioxide Purification Unit
DEM	Discrete Element Method
DNS	Direct Numerical Simulation
DOM	Discrete Ordinate Method
ESP	Electrostatic Precipitation
FGD	Flue Gas Desulphurization
FGR	Flue Gas Recycle system
LES	Large Eddy Simulation
PAHs	Polycyclic Aromatic Hydrocarbons
RANS	Reynold-Averaged Naviers Stoke
RTE	Radiative Transfer Equation
SD1	Eucalyptus sawdust with characteristic particle size diameter of 1.28 mm
SD2	Eucalyptus sawdust with characteristic particle size diameter of 2.91 mm
SCR	Selective Catalytic Reduction
SGS	Subgrid Scales
SIMPLE	Semi-Implicit Method for Pressure-Linked Equations
TC	Thermocouple
WC	Wood Chips

WS	Wood Spheres
WSGGM	Weight-Sum-of-Gray-Gas-Model

NOMECLATURE

The notations used in this thesis are grouped into Roman letters, Greek symbols, superscripts, subscripts, dimensionless parameters and operators.

Roman Letters

A	Arrhenius pre-exponential factor [$\text{s}^{-1} (\text{mol}/\text{m}^3)$]
A_b	Thermocouple bead surface area [m^2]
A_f	Flame surface area [m^2]
A_o	Thermocouple outermost shield surface area [m^2]
A_p	Char surface area [m^2]
A_s	Particle surface area [m^2]
a_κ	Weight factor [-]
C_l	Permeability [m^2]
C_2	Inertia loss coefficient [m^{-1}]
C_g	Overall gas concentration [mol m^{-3}]
C_{olg}	Oxidizer concentration [mol m^{-3}]
C_{pi}	Molar heat capacity of species i [$\text{J mol}^{-1} \text{K}^{-1}$]
$C_{\varepsilon 1}$	$k-\varepsilon$ model coefficient (take as 1.44) [-]
$C_{\varepsilon 2}$	$k-\varepsilon$ model coefficient (take as 1.92) [-]
$C_{\varepsilon 3}$	$k-\varepsilon$ model coefficient (take as 1 for $G_b \geq 1$ and 0 for $G_b < 0$) [-]
C_μ	$k-\varepsilon$ model coefficient (take as 0.9) [-]
c_p	Specific heat capacity [$\text{J kg}^{-1} \text{K}^{-1}$]
D	Diffusivity [$\text{m}^2 \text{s}^{-1}$]
D_b	Thermocouple bead diameter [m]

Deq	Diameter of the particle which is equal to that of volume-equivalent sphere [m]
D_{ij}	Binary diffusion coefficient for species i and j [$\text{m}^2 \text{s}^{-1}$]
$D_{T,i}$	Thermal diffusion coefficient for species i [$\text{kg m}^{-1} \text{s}^{-1}$]
d	Mesh size of the sieve [m]
$\bar{d}$	Characteristics size [m]
d_p	Particle diameter [m]
E	Activation energy [J mol^{-1}]
G	Incident radiative heat flux [W m^{-2}]
G_b	Production of turbulent kinetic energy, k due to buoyancy [$\text{m}^2 \text{s}^{-3}$]
G_k	Production of turbulent kinetic energy, k due to Reynolds Stresses [$\text{m}^2 \text{s}^{-3}$]
g	Gravity [m s^{-2}]
H	Molar enthalpy [J mol^{-1}]
H_i	Enthalpy of formation of species i [J kg^{-1}]
h_{ab}	Heat transfer coefficient between aspirating gas flow and bare thermocouple bead [$\text{W m}^{-2} \text{K}^{-1}$]
h_{as}	Heat transfer coefficient between aspirating gas flow and thermocouple shield [$\text{W m}^{-2} \text{K}^{-1}$]
h_{bg}	Heat transfer coefficient between external gas flow and bare thermocouple bead [$\text{W m}^{-2} \text{K}^{-1}$]
h_{gs}	Heat transfer coefficient between external gas flow and thermocouple shield [$\text{W m}^{-2} \text{K}^{-1}$]
h_c	Heat transfer coefficient [$\text{W m}^{-2} \text{K}^{-1}$]

h	Enthalpy [J kg^{-1}]
$I_{b\lambda}$	Black body intensity at wavelength λ [$\text{W m}^{-1} \text{sr}^{-1}$]
I_λ	Radiative intensity at wavelength λ [$\text{W m}^{-1} \text{sr}^{-1}$]
J	Diffusion mass flux [$\text{kg m}^{-2} \text{s}^{-1}$]
K	Total number of gray gases [-]
K_i	Rate constant for i^{th} reaction [$\text{s}^{-1} (\text{mol/m}^3)$]
K_{pl}	Rate constant for heterogeneous reaction [$\text{s}^{-1} (\text{mol/m}^3)$]
k	Turbulent kinetic energy [$\text{J kg}^{-1} \text{s}^{-1}$]
$k_{a\lambda}$	Absorption coefficient at wavelength λ [m^{-1}]
k_{cpl}	Mass transfer coefficient [-]
$k_{pa\lambda}$	Particle absorption coefficient at wavelength λ [m^{-1}]
$k_{ps\lambda}$	Particle scattering coefficient at wavelength λ [m^{-1}]
$k_{s\lambda}$	Scattering coefficient at wavelength λ [m^{-1}]
$\dot{m}_b$	Biomass burning rate [$\text{kg m}^{-2} \text{s}^{-1}$]
$\dot{m}_i$	Biomass ignition rate [$\text{kg m}^{-2} \text{s}^{-1}$]
$\dot{m}_m$	Mixture mass flow rate [kg s^{-1}]
m_p	Particle mass [kg]
N_g	Number of gas species [-]
n	Number of ordinates [-]
n_R	The parameter of Rosin-Rammler distribution [-]
p	Pressure [Pa]
Q	Volumetric flow rate [$\text{m}^3 \text{s}^{-1}$]
$Q_{a,p}$	Particle absorption coefficient [-]

q_R	Radiative heat flux [W m^{-2}]
q_{PR}	Radiative heat flux for particle [W m^{-2}]
R	Specific gas constant [$\text{J kg}^{-1} \text{K}^{-1}$]
R_R	Percentage of accumulated oversized mass (%)
R_u	Universal gas constant [$\text{J mol}^{-1} \text{K}^{-1}$]
r_b	Total reaction rate for biomass particle [kg s^{-1}]
r_c	Overall combined char reaction rate [kg s^{-1}]
r_p	Particle radius [m]
S_E	Energy source term [$\text{J m}^{-3} \text{s}^{-1}$]
S_i	Molar entropy of species i [$\text{J mol}^{-1} \text{K}^{-1}$]
S_m	Momentum source term [$\text{kg m}^{-2} \text{s}^{-2}$]
s	Distance in Ω direction [m]
s_i	Specific entropy of species i [$\text{J kg}^{-1} \text{K}^{-1}$]
T	Temperature [K]
T_b	Thermocouple bead temperature [K]
T_D	Display temperature [K]
T_M	Temperature at measuring point [K]
T_o	Temperature of thermocouple outermost shield [K]
T_∞	Average effective temperature of surrounding [K]
t	Time [s]
V_F	Flame front propagation speed [m s^{-1}]
V_p	Particle volume [m^3]
v	Velocity [m s^{-1}]

$\bar{v}_i$	Mean velocity component [m s ⁻¹]
v'	Fluctuating velocity component [m s ⁻¹]
W_g	Molecular weight for gas [kg mol ⁻¹]
W_{hp}	Molecular weight for char [kg mol ⁻¹]
W_i	Molecular weight of species i [kg mol ⁻¹]
w_i	Rate of production of species i [kg m ⁻³ s ⁻¹]
w_j	Quadrature weight [-]
X	Mole fraction [-]
x_i	Coordinate in i -direction [m]
x_j	Coordinate in j -direction [m]
Y	Mass fraction [-]

Greek Symbols

α	Exponent factor [-]
α_t	Total absorptivity of gray gas medium [-]
β	Thermal expansion coefficient [-]
β_λ	Extinction coefficient [-]
δ_{ij}	Kronecker delta [-]
ϵ	Emissivity [-]
ϵ_b	Thermocouple bead emissivity [-]
ϵ_i	Lennard-Jones potential well depth
ϵ_o	Thermocouple outermost shield emissivity [-]
ε	Turbulent dissipation rate [J kg ⁻¹ s ⁻¹]
ζ_{pl}	Particle pore area coefficient [-]

θ	Particle porosity [-]
κ	Total gray gas absorption coefficient [-]
κ_{κ}	Absorption coefficient of each gray gas [-]
λ	Wavelength [m]
λ_g	Thermal conductivity for gas-phase [W m ⁻¹ K ⁻¹]
λ_s	Thermal conductivity for solid-phase [W m ⁻¹ K ⁻¹]
μ	Dynamic viscosity [kg m ⁻¹ s ⁻¹]
μ_t	Turbulent viscosity [kg m ⁻¹ s ⁻¹]
ρ	Density [kg m ⁻³]
ρ_b	Bulk density [kg m ⁻³]
σ	Stefan-Boltzmann constant [W m ⁻² K ⁻⁴]
τ	Shear stress tensor [Pa]
$\bar{\tau}_{ij}$	Mean shear stress tensor [Pa]
χ	Region or bed porosity [-]
ψ	Sphericity [-]
Ω	Solid angle [sr]

Subscripts

0	Initial state of the particle
a	Air-fuel conditions
e	Effective
f	Flame
g	Gas
i,g	Gaseous species i

i,s	Solid-phase species i
ox	Oxy-fuel conditions
p	Particle
s	Solid

Superscripts

gs	Heterogeneous reaction
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Dimensionless Parameters

Bi	Biot number ($Bi = h_c d_p / \lambda_s$)
Nu	Nusselt number ($Nu = h_c d_p / \lambda_g$)
Pr	Prandtl number ($Pr = \mu c_p / \lambda_g$)
Pr_t	Turbulent Prandtl number ($Pr_t = \mu_t c_p / \lambda_g$)
Re	Reynold number ($Re = \rho v L / \mu$)

Operators

∇	Gradient operator
$\nabla \cdot$	Divergence operator

ABSTRACT

Biomass fuel is the major source of energy for a significant proportion of the world population. Conventionally, biomass is burned in combustors that use air as oxidizer. The need for efficiency and reduced emissions has led to development of clean combustion technologies such as oxy-fuel combustion. In oxy-fuel combustion technique, fuel is burnt in O_2/CO_2 environment instead of O_2/N_2 environment. In spite of biomass being used under oxy-fuel conditions using fixed bed furnaces, there is no detailed study of biomass combustion in fixed bed reactors under oxy-fuel condition. The studies only cover combustion under air-fuel condition. There is no report in the literature on important combustion parameters, viz., flame propagation speed, temperature profiles, ignition time, and species evolution in the fixed bed combustion under oxy-fuel conditions; the studies have been only in air. This work extends the research on biomass conversion to combustion under oxy-fuel conditions. To address these knowledge gaps, this PhD thesis focused on establishing and isolating the role of various CO_2 effects on biomass combustion properties using a laboratory fixed bed reactor through experiments and numerical modeling. The fixed bed reactor used in this study was operated in counter-current flame propagation mode. Oxidizer was a mixture of pure O_2 and N_2 or CO_2 . Measurement were made for air-fuel condition, oxy-fuel condition of different O_2/CO_2 mixtures and various initial bed porosity. In this work, all numerical simulations were carried out using a commercial CFD software CD-Adapco (STAR CCM+ version 11.04). Euler-Lagrange (CFD-DEM) approach was used to model biomass conversion in a packed bed. Solid particles and their conversion were modeled using DEM while fluid phase was modeled as a continuous phase using CFD. Biomass conversion was modeled by four sub-models, namely, drying, pyrolysis, gas-phase reactions and char oxidation models. These models were adopted and improved from previous research on wood combustion. To account for oxy-fuel combustion environment, reaction involving CO_2 which has been identified as the dominant reaction pathway as well as its associated chain-branching reactions were incorporated in homogeneous reaction sub-model. In order to separate effects of CO_2 on wood combustion, four different mixtures of O_2 and Ar/ CO_2/N_2 were designed and simulated. Temperature in O_2/CO_2 combustion environment was adjusted to be equal to that of O_2/N_2 environment by adding an appropriate amount of Ar while O_2 amount remained the same. The results showed that flame front propagation speed in oxy-fuel atmosphere reduced to 78% of that of the air-fuel condition with similar O_2 concentration. The CFD-DEM model agreed very well with experimental values for mass loss, propagation speed and flame front positions. However, peak temperatures were poorly predicted at lower oxygen concentrations. The accuracy of temperature prediction improved at higher oxygen concentrations. It was noted that oxy-fuel peak temperature is lower than air-fuel temperature by about 200 K. For oxy-fuel combustion, peak temperature value and propagation speed increases as O_2 concentration is increased. The results showed that at any given oxygen concentration, ignition time in oxy-fuel environment is almost twice that of corresponding air-fuel condition. It was established that the packing density affects combustion process by changing the burning conditions and limits. Furthermore, the study revealed that there is an optimum packing density, $\chi = 0.71$, beyond which the efficiency falls due to the onset of quenching in the spaces. It was concluded that dilution effect is the most influential parameter on the burning rate of wood combustion in an oxy-fuel system. In a future study, the model prediction could be improved by including ash inhibition sub-model and using a full chemical kinetic mechanism for hydro-carbon combustion. It was also recommended that a detail analysis of heat transfer in the bed could be investigated in a future study. The findings from this work are important and may be useful when designing burners which operate under oxy-fuel combustion conditions.

CHAPTER ONE

INTRODUCTION

1.1 Background of Study

Biomass fuel is the major source of energy for a significant proportion of the world population. Conventionally, biomass is burned in combustors that use air as oxidizer. The need for efficiency and reduced emissions has led to development of clean combustion technologies such as oxy-fuel combustion. In oxy-fuel combustion technique, fuel is burnt in O_2/CO_2 environment instead of O_2/N_2 environment. This is a clean energy technology where CO_2 is captured through recycling of flue gas and at the same time nitrogen oxides (NO_x) emissions are reduced. Even though oxy-fuel combustion of biomass is a clean combustion technology, it has been established that it reduces flame temperature (Pohlmann, Osório, Vilela, Diez, & Borrego, 2017), increases ignition delay time (Shan *et al.*, 2017) and reduces combustion rate (Riaza *et al.*, 2014).

Oxy-fuel combustion of coal has been extensively studied (Maffei *et al.*, 2013; Zhou *et al.* 2016). This is because coal still contributes to a large share of the world total electricity production as per International Energy Agency Report (2016). However, coal has significant impact on environmental pollution. In order to reduce this impact, coal demand in high income economies like United States and European Union is expected to decrease by 40% and 60%, respectively, by 2040. On the other hand, biomass is an attractive energy source as compared to coal because it is clean and affordable. In fact, most of the energy scenarios for the future indicates that it will increasingly be used to meet energy demand.

Combustion of coal and biomass in oxy-fuel environment have been investigated in previous studies. The studies range from laboratory research to tests in actual power plants. The tests

have been carried out in pilot scale, industrial scale and full scale power plant (Scheffknecht, Al-Makhadmeh, Schnell, & Maier, 2011). Large scale oxy-fuel coal power plant, which ranges between 30 and 300 MW_{th} have been established and installed worldwide (Scheffknecht *et al.*, 2011). Most of these power plants are coal-fired. Biomass-fired and co-fired power plants also exist in various parts of the world (Domenichini, Gasparini, Cotone, & Santos, 2011; Jiménez & Ballester, 2005). In addition, biomass-fired boilers are used for steam generation for use in process industries such as tea production. In Kenya, for example, most of tea industries use wood-fired boilers.

The studies on fundamental combustion phenomena occurring in oxy-fuel combustion such as transport, chemistry and thermodynamics processes are based on models and experiments on laboratory-scale devices. Such small-scale devices have been used previously by other researchers to study combustion in oxy-fuel environment; ignition delay time in coal (Shaddix & Molina, 2009), burnout, ignition temperature and NO_x generation in biomass/coal blends (Riaza *et al.*, 2012) and gaseous emissions from biomass/coal co-firing (Álvarez *et al.*, 2014). Such devices provide insights into combustion phenomena in practical oxy-fuel environment (Riaza *et al.*, 2012; Álvarez *et al.*, 2014). The presence of CO₂ in oxidizer alters gas properties such as density, heat capacity, diffusivity and gas emissivity with consequences on fuel reactivity, flame temperature and emissions. Unlike inert species such as argon and nitrogen which have thermal and dilution effects on combustion processes, addition of reactive species such as CO₂ results in chemical effect in addition to the first two effects. The dilution effect is the reduction of concentration of reactive species O₂ due to addition of CO₂ while thermal effect is the reduction of flame temperature due to addition of CO₂. On the other hand, chemical effect is the direct active participation through chemical reaction. The chemical effect is associated

with the dominant reaction pathway and important chain branching step in hydrocarbon combustion in which CO_2 plays an active role. These are, according to Liu *et al.* (2001), reaction Eqs (1.1) and (1.2) below.

The three roles played by CO_2 addition can be separated by adjusting the flame temperature to a value corresponding to a reference condition without change in oxidizer and fuel concentration (Al-Qurashi, Lueking, & Boehman, 2011; Du, Axelbaum, & Law, 1991). Figure 1.1 shows the various effects of CO_2 addition on specific oxidation rates of ethylene soot flame (Al-Qurashi *et al.*, 2011). This technique has been applied to study the effect of CO_2 on soot formation but it can also be applied on other combustion properties (Zhou *et al.*, 2016).

Figure 1.1: The isolated thermal, dilution, and chemical effects of CO_2 on the specific oxidation rate (R_{sp}) of the ethylene flame soot (Al-Qurashi *et al.*, 2011).

Biomass conversion to energy entails several processes, viz., drying, devolatilization/ pyrolysis, gas-phase reactions of volatile and heterogeneous reaction of char. The processes are coupled and occur simultaneously when biomass is burning. The overall kinetic model of biomass combustion constitutes these four processes.

Biomass contains a certain amount of water content that needs to be dried before combustion. Water in biomass exists in two forms: free water and bound water. Fibre saturation point is the criterion for distinguishing the two forms of water. There are three major ways of modeling drying: the first is thermal method where drying begins when fuel reaches a predefined temperature which is usually the prevailing boiling point, the second is use of algebraic expression for temperature as function of moisture content (evaporation temperature is not constant) and, the third is treating drying process as additional chemical reaction (first-order kinetic rate model). The third is the most common method where water and vaporization scheme is added to the overall kinetic scheme.

During combustion, dry wood decomposes into primary components char, tar and gas through pyrolysis or devolatilization processes. Devolatilization is the release of volatile matter by thermal decomposition under oxidizing atmosphere. On the other hand, if this process occurs in inert atmosphere, then it is referred to as pyrolysis. In both processes, CO_2 , H_2O , CO , H_2 , light hydrocarbon in gaseous form and heavy hydrocarbons in liquid form are released from biomass fuel. The kinetics of dry wood conversion into tar, char and gas have been developed and applied in Computational Fluid Dynamics (CFD) models (Di Blasi, 2000; Mahmoudi, Hoffmann, Markovic, Peters, & Brem, 2016). Tar may undergo secondary cracking reaction to release CO , CO_2 , H_2 , CH_4 and inert tar (Mahmoudi, Markovic, Peters, & Brem, 2015). Gas species considered in homogeneous gas-phase reactions are those generated from drying,

devolatilization, tar cracking and char heterogeneous reactions. Char consumption is through heterogeneous reactions. These reactions represent char oxidation and gasification by CO₂ and H₂O.

Several research studies have been geared toward understanding oxy-fuel combustion in biomass fuel. Shan *et al.* (2017) investigated the effects of CO₂ environment on ignition and combustion characteristics of single biomass pellets. The authors found out that CO₂ environment increased ignition delay time. A similar behaviour has been observed for oxy-coal combustion (Molina & Shaddix, 2007). This was attributed to a decrease in particle surface heating rate due to decreased co-flow temperature associated with the higher specific heat capacity of CO₂ than N₂ and low oxygen diffusion rate in CO₂. According to Molina & Shaddix (2007), other possible reasons for increased ignition delay time are radical formation suppression by CO₂ chemical effects and thermal decomposition of CO₂. It has been observed that internal ignition temperature of the pellet decreased with increased O₂ concentration (Shan *et al.*, 2017). However, they concluded that oxidation temperature effects on internal ignition temperature were more than oxygen concentration effects. In addition, volatile combustion time was increased (Riaza *et al.*, 2014; Shan *et al.*, 2017), while combustion temperature was reduced (Riaza *et al.*, 2014) when N₂ was replaced with CO₂ with 21% O₂ by volume. Riaza *et al.* (2014) reported that the intensity of combustion of a single biomass particle was reduced in CO₂ environment with 21% O₂ by volume. As O₂ was increased to 28-35%, combustion intensity attained a value similar to that of air.

Oxy-fuel combustion of biomass co-firing with coal has also been studied (Álvarez *et al.*, 2014; Farrow, Sun, & Snape, 2013; Yuzbasi & Selçuk, 2011). Co-firing of biomass with coal has been preferred because it reduces CO₂, NO_x and SO_x emission as compared to pure coal plant.

In addition, alkali metals present in biomass fuel provides catalytic effects on oxidation and gasification reactions (Farrow *et al.*, 2013). Indeed, the catalytic effect has been found to be more pronounced under oxy-fuel combustion conditions. In addition, Irfan *et al.* (2012) observed that there were improved ignition properties for coal/biomass blends in both oxy-fuel and air conditions. However, Gil *et al.* (2012a) work on kinetics and thermal reactivity of coal/biomass char blends in oxy-fuel combustion conditions did not show much effects of biomass.

Oxy-fuel combustion of pulverized biomass was studied by Pohlmann *et al.* (2016). They reported on the effects of O₂/CO₂ and O₂/N₂ environment on char reactivity and burnout of pulverized torrefied and carbonized biomass burned in a drop tube furnace. They found out that CO₂ environment increased the burnout of biomass fuel. In addition, char surface area was increased. Char particles from CO₂ devolatilization environment are small in size and have low reactivity (Gil, Riaza, Álvarez, Pevida, & Rubiera, 2015; Hanaoka, Sakanishi, & Okumura, 2012). Improved char burnout in CO₂ has been attributed to contribution from CO₂ gasification (Gubba *et al.*, 2011; Pohlmann *et al.*, 2016; Wang *et al.*, 2014). Even though the burnout time is high, the release of volatile matter is low under fast heating conditions in drop tube furnace operated under oxy-fuel environment (Heuer *et al.*, 2016; Pohlmann *et al.*, 2016). For entrained flow reactor, Gil *et al.* (2015) observed a high apparent volatile yield during devolatilization of biomass under CO₂ environment.

Flame propagation rate in biomass fixed bed gasifiers has been investigated under different operating conditions (Dasappa & Paul, 2001; Ryu *et al.*, 2006; Sakthivadivel & Iniyan, 2018; Yang *et al.*, 2005) although not in oxy-fuel environment. It is affected by various factors such as biomass fuel type, density, size, ultimate and proximate analysis and superficial velocity.

Based on superficial velocity, operation regimes have been classified either as two-regime (Fatehi & Kaviany, 1994) or three-regime (Porteiro *et al.*, 2010). In the two-regime classification, propagation speed increases in the fuel rich regime and decreases in the fuel lean regime. On the other hand, three-regime classification has fuel rich regime, fuel lean regime and convective cooling regime where propagation speed increases rapidly, gradually and decreases rapidly, respectively. Furthermore, the role of ash in flame propagation speed has been assessed (Varunkumar, 2012). Ash affects radiative heat transfer to the unburnt biomass, hence affecting the flame propagation. Although numerous works on flame propagation rate of biomass combustion in fixed bed have been done, none addresses an oxy-fuel environment.

Even though several contributions have been made on oxy-fuel combustion of biomass, the mechanisms through which CO₂ environment affects fundamental combustion phenomena such as flame propagation speed, burning rates, particulate matter characteristics and gas emissions have not been fully resolved. To address this knowledge gap, this work intends to establish and isolate the role of various CO₂ effects on wood combustion properties.

1.2 Problem Statement

Oxy-fuel combustion is a clean energy combustion technology that involves burning of fuels in O₂/CO₂ environment instead of O₂/N₂ environment. However, it has been established that oxy-fuel combustion of biomass reduces flame temperature, increases ignition delay time and reduces combustion rate. Furthermore, under oxy-fuel combustion environment, other flame parameters are negatively affected by the quenching effects of CO₂. If oxy-fuel combustion environment is not properly designed with regards to flame parameters and the operating conditions, the quenching effects of CO₂ cause a decrease in overall efficiency. In spite of biomass being used under oxy-fuel conditions using fixed bed furnaces, there is no detailed

study of biomass combustion in fixed bed reactors under oxy-fuel condition. The studies only cover combustion under air-fuel condition. There is no report in the literature on important combustion parameters, viz., flame propagation speed, temperature profiles, ignition time, and species evolution in the fixed bed combustion under oxy-fuel conditions; the studies have been only in air. This work extends the research on biomass conversion to combustion under oxy-fuel conditions. Appropriate chemical kinetic model that takes into account the presence of CO₂ in oxy-fuel combustion of biomass does not exist. In addition, the influence of particle packing density on combustion properties of oxy-fuel combustion of biomass have not been done. Furthermore, the roles and mechanisms through which CO₂ environment affects important combustion parameters have not been fully resolved.

1.3 Objectives

1.3.1 Main Objective

The main objective of this study was to establish and isolate roles and mechanisms through which CO₂ affects fundamental combustion properties of wood burning in a fixed bed operated under oxy-fuel environment.

1.3.2 Specific Objectives

The specific objectives were to

1. determine the influence of CO₂ environment on main combustion parameters, viz., temperature profiles, ignition time, burning rate, flame propagation speed and species evolution in the bed;
2. develop a kinetic model for wood pyrolysis, gasification and oxidation which can predict combustion behaviour in an oxy-fuel environment;

3. establish the influence of packing of fuel particle and bed porosity on combustion of wood in a fixed bed under oxy-fuel environment;
4. isolate the role of chemical, thermal and dilution effects of CO₂ on wood combustion properties through numerical simulation.

1.4 Scope

This study is focused on flame propagation speed under oxy-fuel conditions, particle packing density and separate effects of CO₂ in oxy-fuel combustion. A fixed bed combustion of wood is considered and other combustion technologies are beyond the scope of this work. The study is narrowed down to an investigation of combustion properties of a single type of wood, i.e., eucalyptus, in order to obtain detail information. The experimental investigation is limited to measurements of temperature and mass loss history but volume change in bed layers and species generation measurements are not possible in this study. However, all these combustion parameters are modelled through numerical technique. Furthermore, this study is limited to investigation of combustion parameters and does not consider formation of pollutants such as particulate matter, soot, nitrogen oxides and sulphur oxides.

1.5 Thesis Outline

This study deals with modeling and experimental work on oxy-fuel combustion of wood in a laboratory fixed bed reactor. These experiments and simulations have been done with an aim of establishing and isolating the role of various CO₂ effects on wood combustion properties in an oxy-fuel environment. In this chapter, background, problem statement, objectives and scope of the study have been presented.

A detailed literature review is presented in chapter two. First, a review of oxy-fuel combustion system and description of various components incorporated in biomass oxy-fuel power plant are presented. Biomass thermal conversion processes such as drying, devolatilization, homogeneous reactions and heterogeneous reactions are then discussed in detail. Subsequently, the effects of oxy-fuel conditions on combustion properties of biomass fuels are explained in detail. Secondly, a review on fixed bed combustion technologies. In addition, fixed bed operation and flame propagation modes are reviewed. Finally, modeling approaches for combustion of biomass in fixed bed are presented. Computational Fluid Dynamics – Discrete Element Method (CFD-DEM) modeling technique and shrinkage models are emphasized.

Experimental techniques used in determination of the fuel properties as well as in the laboratory test of wood combustion in a fixed bed under air and oxy-fuel environment are presented in chapter three. The techniques for determining combustion parameters, namely, mass history, temperature profiles, burning rates, ignition rates, bed porosity and flame front and propagating velocity are discussed. Experimental results are presented in the last section of chapter three.

Presented in chapter four are the numerical modelling techniques which were used in simulation of wood combustion in a fixed bed. The governing equations for both solid phase and gas phase as well as coupling equations are presented. Furthermore, other specific models which are required during computation such as turbulence models, radiation models, shrinkage models and kinetics models are also discussed. Finally, numerical solution methods employed, geometry and boundary conditions formulations and computational meshes are discussed.

In chapter five, numerical results of the three cases simulated in this study, viz., the effects of CO₂ environment on flame propagation speed and flames structures, the influence of particle packing density on combustion of wood in an oxy-fuel burning environment, and the separate

effects of CO₂ in oxy-fuel combustion are presented. The chapter begins by a description of the boundary conditions applied for each case. The mesh independent tests which were done to ensure independency of results on the grid size are then presented. Finally, the numerical results are presented.

Presented in chapter six are the CFD-DEM model validation results and discussions on the experimental and numerical study of wood conversion in a fixed bed under oxy-fuel environment. In the first section, CFD-DEM method and code validation are presented. Temperature distribution and species generation in the bed are discussed. The next section presents an investigation of wood combustion under oxy-fuel combustion environment using CFD-DEM numerical method. Effects of CO₂ combustion environment on mass loss history, flame propagation speed, flame fronts positions and flame structures are discussed. The influence of packing of fuel particle and bed porosity on combustion of wood in a fixed bed under oxy-fuel environment are then presented. Temperature history, ignition time, wood and char conversion rates and reaction zone thickness are discussed in detail. The last section presents the role of various CO₂ effects on burning rate. The overall and individual contribution of various CO₂ effects on wood conversion processes are discussed.

Chapter seven contains a summary of the main findings of this study; and conclusions arising out of the study. Future outlook of the study is in chapter eight.

CHAPTER TWO

LITERATURE REVIEW

2.1 Introduction

In this chapter, detailed review of oxy-fuel combustion system and description of various components incorporated in biomass oxy-fuel power plant are presented. Biomass thermal conversion processes such as drying, devolatilization, homogeneous reactions and heterogeneous reactions are also discussed in detail. Effects of oxy-fuel conditions on biomass combustion properties are then explained in detail. Fixed bed combustion technologies are also discussed. In addition, fixed bed operation and flame propagation modes are reviewed. Finally, modeling approaches for biomass combustion in fixed bed are presented. CFD-DEM modeling technique and shrinkage models are emphasized.

2.2 Oxy-Fuel Combustion

Oxy-fuel combustion technique in coal-power plants was first introduced in 1982 (Scheffknecht *et al.*, 2011). Since then, a lot of research have been done to understand the combustion phenomenon. This technique is also applicable to combustion of other fuels such as liquid and gas fuel. Special considerations are made when designing combustion device used for CO₂ rich environment due to the alteration of combustion processes introduced by replacing N₂ with CO₂ (Chui, Majeski, Douglas, Tan, & Thambimuthu, 2004). A typical atmospheric combustion system applied in a power plant that uses coal and operates in oxy-fuel environment is shown in Fig. 2.1 (Scheffknecht *et al.*, 2011). In addition to other devices used in air-fired systems, it consists of air separation unit (ASU), carbon dioxide purification unit (CPU) and flue gas recycle system (FGR). Pure O₂ is obtained from air by separating it from N₂ in ASU. Cryogenic distillation is normally used because it meets large scale demands for oxygen purity and amount. CPU consists of selective catalytic reduction (SCR) unit for removing nitrogen oxides,

NO_x, electrostatic precipitator (ESP)) unit for removing particulate matter and flue gas desulphurization (FGD) unit for removing sulphur oxides, SO_x. These units are connected to the exhaust gas port of the combustion chamber. FGR are positioned down stream of economizer such that flue gas is recycled either as wet or dry.

Figure 2.1: A typical atmospheric combustion system applied in a power plant that uses coal and operates in oxy-fuel environment (Scheffknecht *et al.*, 2011).

After purification, recycled flue gas which is mostly CO₂ and H₂O is compressed and stored in order to be utilized in oxy-fuel combustion system. The process of separating O₂ from N₂ in the air, purifying and compressing CO₂ takes a significant proportion of power from the system. Therefore, there is a decrease in the overall efficiency of the system. It has been established that the reduction in efficiency is about 8 to 12% (Scheffknecht *et al.*, 2011). Combustion properties of an oxy-fuel system is determined by the flue gas recycle ratio. In case of retrofitting existing air-fuel power plant to operate properly under oxy-fuel condition, it is important to match their combustion characteristics (Khare *et al.*, 2008). It has been shown that the adiabatic flame temperature similar to that attained in air-fuel conditions is achieved in oxy-fuel condition when it is operating at about 69% flue gas recycle ratio (Smart, O’Nions, Riley, & Jamieson, 2009).

2.3 Biomass Conversion

Thermo-chemical conversion of biomass by direct combustion is the process in which heat is released. It involves several chemical and physical processes. These include drying, devolatilization, homogenous and heterogeneous combustion. The entire conversion of biomass may either be continuous or batch depending on the design and the nature of application. For instance, wood combustion in a wood stove occurs in batch mode while a moving grate furnace is a continuous combustion mode where fuel is continuously fed into the combustion chamber. Homogenous and heterogeneous combustion may occur simultaneously, or consecutively with a degree of overlap. For small particles, the processes are more distinct as compared to those in large particles which have high degree of overlap between the various stages. These processes for small and large biomass particles are illustrated in Fig. 2.2 (Loo & Koppejan 2008) and Fig. 2.3 (He & Behrendt 2011), respectively, and discussed in subsequent subsections.

2.3.1 Drying

Biomass contain a certain amount of water, which may exist either as bound water or free water. The two forms of water are distinguished using the fibre saturation point criterion. The amount of water present in biomass need to be dried before combustion. Drying is the first step in biomass combustion. Drying is an endothermic process which absorb energy during combustion of biomass. Subsequently, it reduces the flame temperature in the combustion region and also lowers reaction rates of combustion. A very high amount of water in biomass inhibit combustion since it needs a lot of energy to evaporate it. It has been established that biomass with moisture content that exceeds 60% does not sustain (Goh *et al.*, 1999; Zakaria *et al.*, 2000).

Figure 2.2: Illustration of different conversion processes in a small biomass particle (Loo & Koppejan, 2008).

Figure 2.3: Illustration of different conversion processes in a large biomass particle (He & Behrendt, 2011).

There are three major ways of modeling drying: (1) thermal method where drying begins when fuel reaches predefined temperature which is usually 100 °C, (2) use of algebraic expression for

temperature as a function of moisture content and the evaporation temperature is not constant and, (3) treating drying process as additional chemical reaction and expressed as a first-order kinetic rate model. The latter is the most common method where water and vaporization scheme is added to the overall kinetic scheme. Reaction rate is expressed in first-order Arrhenius form:

2.3.2 Devolatilization

Devolatilization is the process of releasing volatile matter through thermal decomposition. Thermal decomposition of biomass starts at a temperature of about 500 K (Antal & Varhegyi, 1995; Pyle & Zaror, 1984; Shafizadeh, 1985). Devolatilization is also an endothermic process which absorbs energy from combustion. Thus it reduces flame temperatures and lowers combustion rates. As a result of devolatilization, combustible gases are released and the solid biomass particle remaining is char. The gases diffuse toward the surface of the particle where they are combusted within or in its vicinity. The composition and amount of volatiles and char depends on fuel type and chemical composition, decomposing temperature, particle sizes, pressure and heating rates.

Typical gases released are CO₂, H₂O, CO, H₂ and light hydrocarbons in gaseous form and heavy hydrocarbons in liquid form (Di Blasi, Branca, Santoro, & Gonzalez Hernandez, 2001; Piskorz, Majerski, Radlein, Scott, & Bridgwater, 1998; Scott, Piskorz, Bergougnou, Graham, & Overend, 1988). The latter are referred to as tar. The chemical composition of tar is a function of decomposition temperature and the time it stays in the combustion environment (Evans & Milne, 1997; Kinoshita, Wang, & Zhou, 1994; Meier, Oasmaa, & Peacocke, 1997). Tar are normally classified as primary, secondary and tertiary depending on their chemical composition. Primary, secondary and tertiary tar are oxygenated, hydrocarbon and aromatic

compounds, respectively. Primary tar is produced at low decomposition temperature of 673-773 K (Padban, Wang, Ye, Bjerle, & Odenbrand, 2000) while secondary tar is produced at 773-1173 K (Morf, Hasler, & Nussbaumer, 2002) and tertiary tar is produced at 1173-1273 K (Branca, Giudicianni, & Di Blasi, 2003).

Several biomass devolatilization models have been developed (Di Blasi, 2008). They are generally classified into three categories, namely, one-step global mechanism, one-step multi-reaction mechanisms and multi-step semi-global mechanisms. In one-step global mechanism, the products of biomass pyrolysis are char and volatiles. Alternatively, the products may be gases, tar and char, as shown in reactions Eqs. (2.2) and (2.3) (Di Blasi, 2000).

Arrhenius equation is used to express the reaction rate constant. The kinetic parameters, viz., pre-exponential factor, exponent and activation energy are evaluated through measurement data from experiments using devices such as thermogravimetric analysis (TGA) and tube furnace. The main short coming for this model is the inability to model the exact amount and percentage of volatiles constituents. In addition, all the components of original biomass are not accounted by the model. In one-step multi-reaction mechanism, biomass is converted into products which are then converted to volatiles and char, as illustrated in Eqs (2.4) and (2.5) (Caballero, Conesa, Font, & Marcilla, 1997; Varhegyi, Gronli, & Di Blasi, 2004) :

where j represents the individual products of biomass pyrolysis. The model does not include cracking of tar into light hydrocarbon gases that is experienced in high temperature and has long residence times.

In multi-step semi-global mechanism, biomass decomposes into active intermediate species with lower degree of polymerization which are further converted to other product, as illustrated in Fig. 2.4 (Di Blasi, 2008; Varhegyi, Szabo, & Antal, 1994).

Figure 2.4: Two-stage semi-global reaction mechanism for (a) cellulose; (b) wood (Di Blasi, 2008).

Tar from devolatilization may undergo secondary cracking reaction to release CO, CO₂, H₂, CH₄ and inert tar according to the reaction below (Mahmoudi *et al.*, 2015).

where γ_t , γ_{CO} , γ_{CO_2} , γ_{H_2} and γ_{CH_4} are mass fractions of CO, CO₂, H₂, CH₄ and inert tar whose amounts are 0.22, 0.564, 0.111, 0.017 and 0.088, respectively (Mahmoudi *et al.*, 2015; Wurzenberger, Wallner, Raupenstrauch, & Khinast, 2002).

2.3.3 Gas Phase Reactions

Volatile gases from devolatilization undergo chemical reactions with oxygen. Gas species considered in homogenous gas-phase reactions are those generated from drying, devolatilization, tar cracking and char heterogeneous reactions. In order to model emissions which normally occur in gas-phase such as nitrogen oxides (NO_x) and sulphur oxides (SO_x), chemical reaction sub-models that have their formation routes are required.

Gas-phase combustion of CO, H₂, CH₄ and other gas species, is modelled using appropriate reaction mechanism, which may be one-step global reaction, reduced reaction mechanism or detailed reaction mechanism. There are several detailed reaction mechanisms for modelling hydrocarbons. For instance, GRI Mech 3.0 mechanism (Smith *et al.*, 1999) and detailed chemical kinetic model (DCKM) suggested by Glarborg & Bentzen (2008). These mechanisms are usually applied to air-fuel combustion environment. They have also been shown to work well in oxy-fuel combustion environment (Chen, 2013). However, in order to model chemical effects of CO₂, these kinetic models require to be modified by adding relevant reactions.

Application of detailed reaction mechanism in CFD modelling of biomass combustion is usually challenging since they require high computational power. Reduced reaction mechanisms have been developed for modelling hydrocarbon combustion in oxy-fuel environment. These include two-step reaction mechanism suggested by Westbrook & Dryer (1981), three-step reaction mechanism suggested by Toporov *et al.* (2008) and four-step reaction mechanism suggested by Jones & Lindstedt (1988).

2.3.4 Char Oxidation

Char reaction with O_2 is referred to as oxidation while its reaction with other gases is referred to as gasification. Heterogeneous reactions are influenced by char structure, local temperature and pressure, local gas concentration and total active surface area. The overall scheme is defined by three main steps, namely, (1) heat and mass transfer by diffusion in the boundary layer of the particle, (2) heat and mass transfer by diffusion in the porous structure of char and, (3) heterogeneous reactions of gases and char surface. The heterogeneous reaction at the surface is expressed as follow:

There are three possible gases which react with char: O_2 , CO_2 and H_2O . Their reactions are given as follows:

The parameter Ω in reaction Eq. (2.8) control the ratio of CO_2 to CO emitted when char is burning.

The rate of char oxidation can either be treated as first order or half-order. For both cases, the oxidizer diffuses from the bulk gas phase to char surface where heterogeneous reaction take place. The rate limiting steps are the gas phase diffusion and heterogeneous reaction. For first order char oxidation, heterogeneous reactions are considered as first-order in the concentration

of the oxidizer at the surface. Overall combined char reaction rate, r_c is given by an implicit expression (CD-Adapco, 2017):

$$r_c = \frac{A_p^2 W_{hp} W_g \Omega K_{cpl} K_{pl} \zeta_{pl} C_{olg} C_g}{A_p W_g C_g (K_{pl} \zeta_{pl} + K_{cpl}) + r_b}, \quad (2.11)$$

where A_p is the char surface area, W_{hp} and W_g are molecular weight for char and gas mixture, respectively, K_{cpl} is the coefficient of mass transfer, ζ_{pl} is the coefficient of the particle pore area, C_{olg} is oxidizer concentration, C_g is the overall gas concentration, r_b is the total reaction rate for biomass particle and K_{pl} is the rate constant for heterogeneous reaction given by Arrhenius expression:

$$K_{pl} = AT_p^n \exp\left(-\frac{E}{R_u T_p}\right), \quad (2.12)$$

where A is the Arrhenius pre-exponential factor, T_p is the particle temperature, E is the activation energy, R_u is the universal gas constant.

For half order char oxidation, heterogeneous reactions are considered as half-order in the concentration of the oxidizer at the surface. Overall combined char reaction rate, r_c is expressed by an implicit equation (CD-Adapco, 2017):

$$r_c = \Omega K_{cpl} A_p W_{hp} \left[C_{olg} - \left(\frac{r_c}{\Omega K_{pl} A_p W_{hp} \zeta_{pl}} \right)^2 \right] \quad (2.13)$$

2.4 Effects of Oxy-Fuel Environment on Biomass Combustion Properties

CO₂ has different physical and thermal properties as compared to those of N₂. Therefore, combustion of biomass under CO₂ environment is different from N₂ environment. The

properties affected include heat transfer, ignition, drying, devolatilization, char formation and homogeneous reactions. They are discussed in the following subsections.

2.4.1 Heat Transfer

Radiative Heat Transfer

Radiation heat transfer is important when considering thermal conversion of biomass in a fixed bed combustion chamber. Flue gas compositions of biomass combustion under CO₂ burning conditions is not similar to that under air-fuel environment. Hence, radiative heat transfer is not the same in the two environments. The total radiative energy, q_R , from flame can be estimated by considering the whole flame as a uniform radiation source and may be expressed using Stefan-Boltzmann law, Eq. 2.14 (Chen, 2013).

$$q_R \propto \epsilon A_f \sigma T_f^4 \quad (2.14)$$

where A_f is the flame surface area, T_f is the flame temperature, ϵ is the average flame emissivity and σ is the Stefan-Boltzmann constant. Thus Eq. (2.14) shows that temperature has a significant effect since it is the highest order term. Therefore, temperature in oxy-fuel environment should be raised to match that of air-fuel environment so as to achieve the same amount of radiative heat transfer.

CO₂ and H₂O are the main products of combustion in an oxy-fuel environment. This is not the same as air-fuel environment where N₂ is also dominant in addition to these gases. CO₂ and H₂O are triatomic gases which make them not transparent to radiation (Chen, 2013). On the other hand, the emissivity and absorptivity of combustion gases in a CO₂ rich environment are higher because they have higher partial pressure as compared to air-fuel conditions under the same gas temperature (Chen, 2013). The overall effect is that radiative heat transfer is promoted

in a CO₂ rich environment. Since the absorptivity is not continuous over entire spectrum, its effective value for gas mixture is evaluated by integration of the governing equation over the entire spectrum. Thus it is difficult to achieve and requires high computing resources, hence, most CFD studies use gray gas.

Weighted-sum-of-gray-gas-model (WSGGM) is a widely used radiation model (Andersson & Johnsson, 2007). It was primarily developed for air-fuel conditions (Smith, Shen, & Friedman, 1982). However, under appropriate conditions, it can also be used in oxy-fuel environment. There have been several efforts to develop improved radiation heat transfer models for application in oxy-fuel environment. Among them are the following non-gray models: Statistical narrow band model (Johansson, Andersson, Leckner, & Thunman, 2010); exponential wide band model (Yin, Johansen, Rosendahl, & Kær, 2010); and empirical correlation (Krishnamoorthy *et al.*, 2010). Usage of these improved models significantly enhance prediction accuracy for oxy-fuel combustion. A comparison of radiative heat transfer behavior in a furnace in term of incident radiation flux, heat sources and temperature distribution predicted using gray and non-gray oxy-fuel WSGGMs and air-fuel WSGGM were reported by Yin (2012). There is a significant difference between prediction of non-gray and gray computation using the same oxy-fuel WSGGMs and is more pronounced than those in air-fuel WSGGM. Yin (2012) concluded that the difference observed in oxy-fuel WSGGMs is not very critical. However, non-gray oxy-fuel WSGGM model showed improved prediction accuracy for large-scale oxy-fuel furnace.

Convective Heat Transfer

The rate of convective heat transfer, $\dot{q}_{conv}$, is estimated using Newton law of cooling, Eq. 2.15.

$$\dot{q}_{conv} = h_c \Delta T, \quad (2.15)$$

where h_c is the convective heat transfer coefficient and ΔT is the temperature difference between flue gas and heated body. Convective heat transfer is expressed in terms of Nusselt number, Nu , which is a function of Reynolds number, Re , and Prandtl number, Pr . The correlation between these non-dimensional numbers are based on the shape of the heated body and the flow conditions (Incropera, DeWitt, Bergman, & Lavine, 2006; Whitaker, 1972). Consequently, h_c is a function of physico-chemical properties of gas such as density, thermal conductivity, viscosity and heat capacity. Based on non-dimensional numbers, convective heat transfer coefficients in CO₂ burning conditions, $h_{c,ox}$, and air-fuel conditions, $h_{c,a}$, may be compared using the following expression (Payne, Chen, Wolsky, & Richter, 1989):

$$\frac{h_{c,ox}}{h_{c,a}} = \left(\frac{Re_{ox}}{Re_a} \right)^m \left(\frac{Pr_{ox}}{Pr_a} \right)^n \left(\frac{\lambda_{ox}}{\lambda_a} \right), \quad (2.16)$$

where m and n are constants that depend on shapes of the heated body, λ is thermal conductivity and subscript ox and a represent oxy-fuel and air-fuel conditions, respectively. Physico-chemical properties of CO₂ are different from those of N₂, therefore, convective heat transfers are also different. Under the same conditions, CO₂ has a higher thermal conductivity and lower kinematic viscosity than those of N₂ (Nozaki, Takano, Kiga, Omata, & Kimura, 1997). Therefore, the overall effect is a higher convective heat transfer coefficient in a CO₂ rich environment. For coal burning in a CO₂ rich environment, $h_{c,ox}/h_{c,a}$ has been found to increase with increase in flue gas recycle ratio (Liu, Zailani, & Gibbs, 2005a, 2005b). Convective heat transfer coefficient of oxy-fuel environment may be matched to that in air-fuel by operating the power plant at appropriate flue gas recycle ratio (Smart, O’Nions, & Riley, 2010; Toftegaard,

Brix, Jensen, Glarborg, & Jensen, 2010). Therefore, existing air-fuel operated power plants may be retrofitted as oxy-fuel operated power plant without replacing the burners.

2.4.2 Drying under Oxy-fuel Environment

Drying of biomass particle in oxy-fuel combustion environment is different from an air-fuel burning environment because the two environments have different heat transfer processes. The rate of heating and drying of particles is influenced by heat transfer processes (Chen, Wu, & Agarwal, 2000; Topuz, Gur, & Gul, 2004; Wang, 2007). A simplified heat transfer model for the thermal conversion of a biomass particle is shown in Fig. 2.5 (Chen, 2013). The energy conservation in the biomass particle may be expressed as follows (Ceylan, Aktaş, & Doğan, 2007; Celma, Rojas, & Lopez-Rodríguez, 2008; Sander, 2007):

$$\frac{4}{3}\pi r_p^3 \rho_p c_p \frac{dT}{dt} = 4\pi r_p^2 h_c (T_g - T_p) + 4\pi r_p^2 \sigma (\epsilon_f T_f^4 - \epsilon_p T_p^4), \quad (2.17)$$

where c_p is the specific heat capacity for the particle, h_c is the convective heat transfer, r_p is the particle radius, T_f , T_g and T_p are the flame temperature, hot gas temperature and particle temperature, respectively, t is the time, ρ_p is the particle density, σ is the Stefan-Boltzmann constant, ϵ_f and ϵ_p are emissivity for gas and particle, respectively.

Equation (2.17) shows that flame and gas temperatures have a significant effect in the determination of the heating rate of a particle. In case of combustion in a CO₂ rich environment, flame temperatures have low values in comparison to those of air-fuel conditions with the same O₂ concentration. Subsequently, the heating rate of a particle in a CO₂ rich environment is expected to be lower than in air-fuel environment. In addition, convective heat transfer coefficient is also different in the two environments. This also affects the heating rate of CO₂ rich conditions.

Figure 2.5: Heat transfer processes for the thermal conversion of a biomass particle (Chen, 2013).

Chen, Yong & Ghoniem (2012) calculated drying times for particles conversion in O_2/N_2 and O_2/CO_2 environments using droplet evaporation model. It was observed that the drying time in both N_2 and CO_2 environments were similar. This is because the experiments were carried out at low Reynolds number flow conditions which makes thermal conductivity dominant over convective heat transfer. However, Chen (2013) concluded that combustion temperature plays a more significant role in influencing heating rate than the role of gas composition.

2.4.3 Biomass Ignition

There are two types of ignition for solid fuels, namely heterogeneous ignition and homogeneous ignition (Essenhig, Misra, & Shaw, 1989; Howard & Essenhig, 1967a, 1967b). Homogenous ignition occurs when volatiles and oxygen mixture are heated to auto-ignition temperature. For this case, ignition does not occur on the fuel solid surface. On the other hand, heterogeneous

ignition occurs on the solid surface for fuel with less volatiles and high oxygen concentration (Levendis, Joshi, Khatami, & Sarofim, 2011; Ponzio, Senthooorselvan, Yang, Blasiak, & Eriksson, 2008). For both types of ignition, the ignition time and temperature of biomass particles depends on the fuel properties, size, oxygen concentration, gas flow and heating rate.

Shan *et al.* (2017) investigated ignition and combustion characteristics of wood pellets in air-fuel and CO₂ rich environments. The investigations were done for different flow conditions, gas temperature and oxygen concentration. Ignition delay is higher in oxy-fuel environment than in air-fuel environment (Khatami, Stivers, Joshi, Levendis, & Sarofim, 2012; Liu, Geier, Molina, & Shaddix, 2011; Zhou, Lin, Hu, Hu, & Song, 2016). A similar behaviour has also been observed in coal combustion in oxy-fuel environment (Shaddix & Molina, 2009). This is attributed to the high heat capacity of CO₂ and low diffusivity of oxygen in CO₂ which results in slow heating rates of particles. For the same temperature, ignition delay decrease with increasing oxygen concentration. This is because as oxygen is increased, heat generation and transfer is enhanced, hence, ignition is also enhanced. When the gas flow is increased at the same temperature and oxygen concentration, ignition delay is reduced. A high gas flow increases turbulence which improves heat transfer and subsequently ignition of biomass fuels.

Internal ignition temperature of biomass fuels in N₂ and CO₂ environments have also been investigated (Kijo-Kleczkowska, Środa, Kosowska-Golachowska, Musiał, & Wolski, 2016; Kimura, Omata, Kiga, Takano, & Shikisima, 1995; Lu *et al.*, 2010). Under the same gas temperature and flow conditions, internal ignition temperature is inversely proportional to oxygen concentration changes. However, as oxygen concentration is increased beyond 50%, the decrease is minimal. For the same oxygen concentration and gas flow condition, increase in gas temperature decreases internal ignition temperature. In fact, Shan *et al.* (2017) concluded

that the influence of gas temperature on internal ignition temperature is more pronounced than that of oxygen concentration.

2.4.4 Biomass Devolatilization

When biomass is heated beyond 300 °C, it undergoes devolatilization whereby volatiles such as light gases, tar and vapour are released. Devolatilization is highly influenced by temperature change in the particle as it is an endothermic process. Moreover, it is also affected by pressure and gasifying agent (Gibbins-Matham & Kandiyoti, 1988; Ko *et al.*, 1989; Suuberg *et al.*, 1980). In addition, the amount and composition of volatiles released depend on biomass type and its chemical composition (Anthony, Howard, Hottel, & Meissner, 1976; Balat, Balat, Kırtay, & Balat, 2009a, 2009b).

Gasifying agents that can be used during biomass devolatilization include nitrogen, air and CO₂. Research work on devolatilization of biomass in CO₂ rich environment have been reported (Nakayama *et al.*, 1992; Tan, Croiset, Douglas, & Thambimuthu, 2006). Wijayanta *et al.* (2012) reported on the influence of different CO₂ concentration on major species and polyaromatics hydrocarbons (PAHs) production during biomass combustion. In general, volatiles yield is lower in N₂ burning environment than in CO₂ burning environment (Rathnam, Elliott, Wall, Liu, & Moghtaderi, 2009). It has been found out that there is a relatively higher amount of H₂ in N₂ burning environment than in oxy-fuel environment (Bautista, Russel, & Seville, 1986). On the other hand, the concentration of CO is high in oxy-fuel condition as compared to N₂ burning environment (Serio, Hamblen, Markham, & Solomon, 1987). This has been attributed to Boudouard reaction Eq. 2.9, whereby char is consumed by CO₂ to produce CO. In addition, for air-fuel environment reaction Eq. (2.18);

is a dominant chain branching step due to high amount of H₂ which break into H-atoms, while in oxy-fuel environment, reaction Eq. (2.19) is dominant because of high amount of CO₂ (Glarborg & Bentzen, 2008).

Reactions Eq. (2.18) and Eq. (2.19) show that for oxy-fuel conditions, H-atoms are competed for by O₂ and CO₂. Hence, for a high concentration of CO₂, a high amount of CO is produced through reaction Eq. (2.19). Moreover, the amount of CO in oxy-fuel environment is influenced by water-gas-shift reaction Eq. 2.20 (Glarborg & Bentzen, 2008).

2.4.5 Char Formation and Combustion

During combustion of biomass, char is a product of devolatilization process. Char properties, combustion and gasification characteristics is greatly influenced by its formation process, viz., the preceding devolatilization. Biomass char obtained from devolatilization under air-fuel environment is different from that from oxy-fuel environment because CO₂ plays a reactive role in the process whereas N₂ is inert. The properties of char that are affected include structure, porosity, surface area and morphology (Riaza *et al.*, 2011), all of which influence the reactivity of char (Pohlmann *et al.*, 2010).

Char formation under different devolatilization environments have been the subject of many researchers (Borrego & Alvarez, 2007; Gil *et al.*, 2012a; Li *et al.*, 2010). The studies have been done in different combustion systems, namely, drop tube furnace (Li *et al.*, 2010) and entrained flow reactor (Borrego & Alvarez, 2007; Gil *et al.*, 2012a). For these cases, chars were obtained at a wide range of operating temperatures; 800 - 1400 °C (Borrego *et al.*, 2009). These studies

showed that CO₂ reacts with char during high temperatures. Gil *et al.* (2012a) investigated the structure and morphology of biomass char obtained under N₂ and CO₂ environment. For char produced under N₂ environment, the particle swells and melts before releasing volatiles. They did not observe any evidence of swelling for char obtained from CO₂ devolatilization environment. They concluded that melting and fusion have greater impact on structural properties of char produced under oxy-fuel conditions than that of swelling. Consequently, char formed under CO₂ environment are spherical particles and have smooth surface. Conversely, char particles formed in N₂ environment have hollow surface (Brix, Jensen, & Jensen, 2010; Cetin, Moghtaderi, Gupta, & Wall, 2004).

According to Gil *et al.* (2012a), for all conversion values, reactivity of char produced under air-fuel devolatilization environment are higher than those of char produced in oxy-fuel environment. A decrease in the reactive part of char due to consumption by CO₂ causes a reduction in the reactivity. The effects of CO₂ on char reactivity is more pronounced at high temperatures (Naredi & Pisupati, 2011; Niu, Han, & Lu, 2011; Wang, Zhang, Liu, & Che, 2012) because of gasification of char through reaction Eq. 2.9.

Combustion characteristics of chars in CO₂ rich environment is different from those of air-fuel environment. Chen & Sheng (2016) investigated the effects of gas properties and CO₂ gasification on combustion characteristics of char in a CO₂ rich oxy-fuel environment. They demonstrated that changes in gas properties significantly reduces combustion temperatures. Oxy-fuel environment has low O₂ diffusivity and high thermal conductivity of gas mixture which result in temperature reduction (Bejarano & Levendis, 2008; Tolvanen & Raiko, 2014). They also showed that influence of O₂ diffusivity and high thermal conductivity of gas mixture are dominant at lower and higher O₂ concentration, respectively.

Char conversion by oxidation and gasification is also affected by the oxy-fuel environment. Haugen *et al.* (2015) investigated the effects of CO₂ concentration, carbon to mass ratio and equivalence ratio on char. They showed that for high equivalence ratio, char conversion takes longer time. On the other hand, char conversion in CO₂ gasification is faster. Conversion rate is affected by several factors such as temperature, oxidizer concentration, equivalence ratio (Croiset, Thambimuthu, & Palmer, 2000; Gonzalo-Tirado & Jiménez, 2015). For oxy-fuel environment, CO₂ gasification, which is an endothermic process greatly reduces the flame temperature in the combustion region. Low temperatures inhibit char conversion rate. But char conversion rate is enhanced through gasification with CO₂. The effect of the latter is more pronounced due to high amount of CO₂ in oxy-fuel environment. Subsequently, char conversion rate in oxy-fuel conditions are increased (Geier, Shaddix, Davis, & Shim, 2012; Mitchell, Kee, Glarborg, & Coltrin, 1991).

2.4.6 Chemical Effect of CO₂ on Homogeneous Reactions

Previous research (Kiga *et al.*, 1997; Suda, Masuko, Sato, Yamamoto, & Okazaki, 2007; Zhu, Egolfopoulos, & Law, 1989) have shown that CO₂ is not inert in gas-phase reactions, but undergo reaction with other species and affects combustion phenomena of the system. The dominant reaction through which CO₂ plays an active role in combustion is given by reaction Eq. (2.19). In addition to this reaction, chain branching step Eq. (2.18) is also important. Furthermore, the following reactions are also responsible for CO₂ active role in combustion but to a lesser extent (Liu *et al.*, 2001):

Through these reactions, CO₂ affects various combustion processes. For instance, addition of CO₂ to diffusion flames have been shown to reduce soot formation (Haynes & Wagner, 1981; McLintock, 1968; Schug, Manheimer-Timnat, Yaccarinc, & Glassman, 1980). According to McLintock (1968), CO₂ accelerates soot burnout when it is present at soot oxidation zone. Du *et al.* (1991) suggested that CO₂ decreases the formation of soot through thermal, chemical and dilution effects. CO₂ promotes production of oxygen atoms and hydroxyl which increases soot oxidation. Liu, Guo, & Smallwood (2003) investigated the influence CO₂ chemical effects on major species generation in a C₂H₄ diffusion flame. They observed a decrease of CO₂ concentration in fuel side which is an indication that it is consumed by chemical reactions. Mass fraction of CO and H₂O increases. Addition of CO₂ to oxidizer also has effects on burning velocities of gaseous fuel mixtures (Ju, Masuya, & Ronney, 1998; Masri, Dibble, & Barlow, 1992; Ruan, Kobayashi, Niioka, & Ju, 2001). Liu *et al.* (2001) isolated the role of CO₂ chemical effect on burning velocity of methane and hydrogen flames. They used a fictitious species, FCO₂, which has similar transport and thermal properties of CO₂ but is not allowed to participate in reactions. The difference between the results of CO₂ and FCO₂ addition show the role played through chemical reaction. They showed that CO₂ significantly reduce burning velocity of the flames through chemical reactions.

2.5 Fixed Bed Combustion

A typical fixed bed combustion system consists of a primary air supply port, grate, fuel bed, secondary air supply port and exhaust port, as illustrated in Fig. 2.6 (Loo & Koppejan, 2008). Fixed bed reactors usually operate with superficial velocity of between 0.3 to 1.2 m/s (Mathekga, Oboirien, & North, 2016). Fuel particles located in the fuel bed undergo various processes of biomass thermal conversion, namely, drying, devolatilization, gas-phase reactions and char combustion. Primary air is supplied at the bottom through grate to the fixed bed. Homogeneous reactions take place in region above fixed bed, also known as freeboard region. Secondary air may be supplied in this region for complete combustion of pyrolysis gases.

Figure 2.6: A typical fixed bed combustion furnace.

Combustion of wood in a fixed bed is favourable because of its simplicity. Consequently, this technique has been applied in most biomass power plants all over the world (Hermansson & Thunman, 2011). This has created a lot of research interests which is aimed at improving

combustion efficiency and reduction of emission (Costa *et al.*, 2014; Guo *et al.*, 2017; Yahaya, Somalu, Muchtar, Sulaiman, & Daud, 2019). Over the past, studies of a wide range of biomass fuels have been carried out in a fixed bed operated with air as the oxidizer (Abrego, Atienza-Martínez, Plou, & Arauzo, 2019; Chen, Annamalai, Ansley, & Mirik, 2012; Meng *et al.*, 2018; Plis & Wilk, 2011). However, there has been a growing interest for combustion of biomass in a CO₂ rich burning environment.

Typical devices used in a fixed bed combustion system includes grate furnaces and underfeed stokers. The choice of combustion technology depends on fuel type and properties. Careful consideration is required in order to obtain optimum efficiency and reduced exhaust emissions. Grate furnace type has a grate through which primary air is supplied to fuel bed. The design of the grate is use to differentiate the various types of grate furnaces which may be moving, fixed, rotating, traveling or vibrating. Grate furnace is suitable for fuel with high moisture content, wide particle variation and high ash content (Yang, Sharifi, & Swithenbank, 2004; Yang, Goh, Zakaria, Nasserzadeh, & Swithenbank, 2002). On the other hand, underfeed stoker is a furnace where fuel particles are fed into the burning region using a screw conveyor located at the bottom where it is transferred upward using a grate which is either on the outer or inner side. They are suitable for small and medium scale power plant with capacity of up to 60 MW_{th} (Hermansson & Thunman, 2011).

In practice, wood particles of different shapes and sizes are normally burned in a fixed bed. The packing and arrangement of fuel particles affect bed porosity. Bed porosity is a complex parameter which is not only affected by this factor but also changes as combustion progresses due to bed shrinkage (Khodaei, Al-Abdeli, Guzzomi, & Yeoh, 2015; Porteiro, Granada, Collazo, Patiño, & Morán, 2007).

Thermal conversion of biomass in a fixed bed is affected by fuel particle size and shape. The shape influence is through the following four ways: particle overlapping; grain direction; geometry and packing in the bed. Particles with flat or concave surface may overlap in the bed. On the other hand, surface with convex surface like a sphere do not overlap. Overlapping of surfaces reduces effective surfaces for fluid flow and chemical reactions. The influence of particle overlapping is analyzed by defining a particle surface availability (Trudel & Hallet, 2017). Alternatively, its effect is determined using a shape factor included in heat and mass transfer correlations (Glaser & Thodos, 1958).

Biomass fuels are made of fibres which are normally arranged along one another. It has been shown that pyrolysis rate is faster along the fibres than across them (Larfeldt, Leckner, & Melaaen, 2000). Volatiles also flow faster along the fibres as compared to movement across them (Henriksen, Hindsgaul, Qvale, Fjellerup, & Jensen, 2006). Char produced through pyrolysis under low heating rates have fibres arrangement similar to those of raw biomass since they are not destroyed (Trudel *et al.*, 2018). Consequently, porosity is high across the fibres. This cause a higher gas permeability along the grain (Larfeldt *et al.*, 2000). It has been observed that char conversion rate is higher on surface normal to the fibres (Trudel *et al.*, 2018). Thus aspect ratio plays an important role in wood and char gasification (Pattanotai, Watanabe, & Okazaki, 2015).

The geometry of a particle affects biomass conversion through surface area. Most biomass particles utilized in power plants have wide ranges of shapes which are normally irregular. The shape of a particle is defined in terms of sphericity. It has been shown that sphericity of particles have correlation with ignition rate and bed porosity (Horttanainen, Saastamoinen, & Sarkomaa,

2002). Particles with high sphericity have decreased surface area which impact negatively on burning times (Huff, 1985).

The shape and the size of fuel particles also have great impact on the packing of the bed. Consequently, hydrodynamics of flow, heat and mass transfer in the bed are affected. In fact, theories and correlations for pressure loss, heat and mass transfer are based on hydraulic diameter of bed (Comiti & Renaud, 1991; Whitaker, 1972). The size of fuel particles affects wood conversion in a packed bed through convective and radiation heat transfer, gas species and energy dispersion by turbulence, mass transfer and mixing rate of volatiles and air in the bed. Subsequently, it affects the amount of volatiles released (Yang, Ryu, Khor, Sharifi, *et al.*, 2005), reaction zone thickness (Yang, Ryu, Khor, Yates, *et al.*, 2005), operational limit of air flow rate (Horttanainen *et al.*, 2002), burning rate (Ryu *et al.*, 2006) and ignition front velocity (Porteiro *et al.*, 2010).

Operation mode of the fixed bed is classified as either updraft or downdraft (La Villetta, Costa, & Massarotti, 2017; Mahapatra, Kumar, & Dasappa, 2016; Martínez, Mahkamov, Andrade, & Silva Lora, 2012). These classification depends on the flow direction of oxidizer relative to fuel movement. The various fixed bed operation modes are illustrated in Fig. 2.7. Updraft operation mode is where air is supplied at the bottom and moves upward while the fuel is supplied at the top. Downdraft operation mode is where oxidizer is supplied at the top and moves downward (Pérez, Melgar, & Tinaut, 2014). Fuel is also filled up from the top side of the bed. This configuration of fixed bed is useful when generating devolatilization gases, viz., CO, H₂ and CH₄ which can be used in internal combustion engines (Lapuerta, Hernández, Pazo, & López, 2008; Melgar, Pérez, Laget, & Horillo, 2007; Tinaut, Melgar, Pérez, & Horillo, 2008).

Despite the significance of fixed bed combustion technology in power generation, there are no studies of oxy-fuel combustion of biomass in a fixed bed. The effects of bed porosity on wood conversion in a fixed bed under oxy-fuel environment have not been reported.

2.6 Flame Propagation in a Fixed Bed

Flame propagation mode in a fixed bed may be classified as either co-current or counter current as illustrated in Fig. 2.7. For co-current flame propagation mode, flame front moves in the same direction as the air movement. On the other hand, counter-current flame propagation is where flame front moves in the opposite direction as air movement. When calculating effective flame speed propagation, bed movement due to shrinkage is taken into consideration. The rate of flame front propagation in biomass fixed bed reactors have been investigated by several researchers, (Dasappa & Paul, 2001; Ryu *et al.*, 2006; Sakthivadivel & Iniyen, 2018). It is affected by various factors such as biomass fuel type, density, size, ultimate and proximate analysis and superficial velocity (Gort & Brouwers, 2001; Horttanainen *et al.*, 2002; Mahapatra, 2016; Thunman & Leckner, 2005). Flame front speed have been shown to increase with increase in air mass flux up to a peak point where it starts to decrease (Dasappa & Paul, 2001). Typical range of flame front speed for various biomass fuels burned under different conditions are summarized in Table 2.1.

Operation regimes of fixed bed reactor have great impact on flame front propagation rate. Based on superficial velocity, operation regimes have been classified either as two-regime (Fatehi & Kaviany, 1994; Shin & Choi, 2000) or three-regime (Porteiro *et al.*, 2010). In the two-regime classification, propagation speed increases in the fuel rich regime and decreases in the fuel lean regime, as illustrated in Fig. 2.8 (Fatehi & Kaviany, 1994). In this case, flame front propagation

are estimated using classical asymptotic analysis analogous to a premixed flame (Dosanjh, Pagni, & Fernandez-Pello, 1987).

Figure 2.7: Fixed bed operation modes: (a) downdraft – co-current; (b) downdraft – countercurrent; (c) updraft – countercurrent; (d) updraft – co-current.

Table 2.1: Typical range of flame front speed for various biomass fuels burned under different conditions

Fuel type	Air flow rate (kg/m²/s)	Propagation speed (mm/s)	Source
Casuarina wood	0.06 - 0.20	0.04 - 0.089	Mahapatra <i>et al.</i> (2016).
Char particles	0.015 - 0.28	0.06 - 0.30	Dasappa & Paul (2001)
Pine wood	0.1	0.24	Yang <i>et al.</i> (2005).
Straw	0.013 - 0.062	0.94 - 3.58	Khor <i>et al.</i> (2007)
Switch grass	0.017 - 0.070	0.83 - 2.89	Khor <i>et al.</i> (2007)
Reed canary grass	0.017 - 0.046	0.39 - 1.47	Khor <i>et al.</i> (2007)
Coconut shells	not provided	0.063	Sakthivadivel & Iniyen (2018)
Prosopis juliflora	not provided	0.071	Sakthivadivel & Iniyen (2018)
Tamarind seed pellets	not provided	0.05	Sakthivadivel & Iniyen (2018)

On the other hand, three-regime classification has fuel rich regime, fuel lean regime and convective cooling regime where propagation speed increases rapidly, gradually and decreases rapidly, respectively. This is illustrated in Fig. 2.9 (Porteiro *et al.*, 2010). A different three-

regime classification which is based on exit gas composition was presented by Rönnbäck *et al.* (2008). In this classification, the three regimes are sub-stoichiometric combustion with incomplete consumption of oxygen where flame front speed increases rapidly, stoichiometric combustion regime with complete consumption of oxygen where flame front speed increases gradually and over stoichiometric combustion regime where flame front speed decreases. Furthermore, the role of ash in flame propagation speed has been assessed (Cooper & Hallett, 2000; Ryan & Hallett, 2002; Varunkumar, 2012). Ash affects radiative heat transfer to the unburnt biomass, hence affecting the flame propagation.

Figure 2.8: Two-regime classification of fixed bed combustion (Fatehi & Kaviany, 1994).

Although numerous works on flame propagation rate of biomass combustion in fixed bed have been done, none addresses an oxy-fuel environment.

Figure 2.9: Three-regime classification of fixed bed combustion (Porteiro *et al.*, 2010).

2.7 Modeling Approaches for a Fixed Bed

Modeling of the various thermal conversion of biomass in a fixed bed have been approached differently. One approach is the consideration of fixed bed as a continuous system made of two phases: a gas phase and a solid phase. Using one-dimensional models, different researchers (Fatehi & Kaviany, 1994; Saastamoinen & Taipale, 2000), have studied the propagation of ignition front and the reactions for biomass fuels burning in a fixed bed combustion chamber. In these cases, 1D and transient conservational equations for solid and gaseous phases are used to model fixed bed combustion. Since these models do not consider individual particles, they do not accurately predict thermal conversion of fixed bed and requires experimentally determined empirical correlation.

Another approach is single particle model, where the sum of individual particles processes constitutes the conversion of the packed bed. Ha & Choi (1994) investigated the effects of initial relative velocity, free stream oxygen concentration, the particle size, pre-exponential factor and

particle entrainment on conversion of a single particle using 2D, unsteady, laminar conservation equations. Similarly, Lee, Yetter & Dryer (1995) used a fully transient formulation to compute oxidation of a single carbon particle with focuses on flow field at the boundary layer. Peters (2002) developed a 1D transient particle model which addresses reactions and temperature distribution in the particle. Haseli, Oijen & Goey (2011) also developed a 1D model for thermal conversion of a wood particle in which they assumed that biomass pyrolysis is by three independent reactions that yield gas, tar and char, respectively. Recently, three-dimensional models for simulating combustion in fixed bed have been developed (Collazo, Porteiro, Patiño, & Granada, 2012; Mahmoudi, Hoffmann, Markovic, *et al.*, 2016). Collazo *et al.* (2012) simulated fixed bed reaction using 3D model for both solid and gaseous phases. However, the model did not consider the shrinkage of fuel bed which normally occur in the last phase of combustion. A model that consider bed movement was proposed by Mahmoudi *et al.* (2015). In the model, gas phase was modeled in three-dimensional, while solid phase was model in one dimension. The model was tested in a fixed bed for various characteristics of biomass combustion including self-heating and self-ignition in a packed bed (Mahmoudi, Hoffmann, Markovic, *et al.*, 2016). Furthermore, Mahmoudi, Hoffmann, & Peters (2016) propose a model that has improved flow field description by fully resolving solid phase and semi resolving gas phase. The gas phase is described on a length scale smaller than solid particle. The model was implemented on Euler-Lagrange simulation framework.

2.8 Modeling Shrinkage in Biomass Combustion

During biomass combustion, shrinking or local collapse occurs in the fuel bed. There are several methods of modeling shrinkage in biomass combustion. These models determine the behavior in which a particle that burns internally changes through the course of the particle reaction.

Consequently, it represents the way the particle losses mass, that is, by either increase in particle porosity or decrease in the diameter. Shrinkage models have been developed for both single particle and fixed bed combustion. For a single particle, a model where the particle density remains constant while the mass reduces was implemented by Villiermaux *et al.* (1986). This model does not take into consideration the porosity change that take place in actual particle combustion. In case of a fixed bed, a model which considers constant porosity while particles shrink have been implemented by Cooper & Hallett (2000), Shin & Choi (2000) and Zhou *et al.* (2005). The problem with this model is that it does not consider heterogeneities produced by combustion. Collazo *et al.* (2012) presented a model in which particle porosity varied but with no contraction in the bed. Consequently, the bed size remained almost the same. A model which considered both bed shrinkage and porosity change was implemented by Hermansson & Thunman (2011). Even though the model had improved accuracy, it didn't consider local shrinkage of the bed. To address this issue, Gomez *et al.* (2014) presented a model which considered both local consumption of particle leading to the change in porosity and local shrinkage of bed caused by collapsing of areas due to combustion. This model showed an improved accuracy in prediction of some of the combustion parameters.

As combustion progresses, bed shrinkage is affected by packing and arrangement of fuel particles. Consequently, bed porosity also varies during combustion. Although there are numerous studies on fixed bed shrinkage, the influence of particle packing density on combustion properties of oxy-fuel combustion of biomass have not been done.

2.9 Deduction

Different aspects of biomass combustion in a fixed bed have been studied through both experimental and numerical modeling. These studies reported cases where biomass is burnt

conventionally under air-fuel conditions. The properties investigated include ignition time and temperature, mass loss history, species history, temperature profiles and emission characteristics of single biomass pellets, biomass co-fired with coal and pulverized biomass. But these properties have not been studied in oxy-fuel environment. Chemical kinetics for biomass conversion have also been well developed. The need for efficiency and reduced emissions has led to development of clean combustion technologies such as oxy-fuel combustion. Even though several contributions have been made on oxy-fuel combustion of biomass, there are several knowledge gaps that need to be studied. The following knowledge gaps are to be addressed in study:

- In spite of biomass being used under oxy-fuel conditions using fixed bed furnaces, there is no detailed study of biomass combustion in fixed bed reactors under oxy-fuel condition. The studies only cover combustion under air-fuel condition.
- There is no report in the literature on important combustion parameters, viz., flame propagation speed, temperature profiles, ignition time, and species evolution in the fixed bed combustion under oxy-fuel conditions; the studies have been only in air. This work extends the research on biomass conversion to combustion under oxy-fuel conditions.
- Appropriate chemical kinetic model that takes into account the presence of CO_2 in oxy-fuel combustion of biomass does not exist.
- Although there are numerous studies on fixed bed shrinkage, the influence of particle packing density on combustion properties of oxy-fuel combustion of biomass have not been done.

- The roles and mechanisms through which CO₂ environment affects fundamental combustion phenomena such as flame propagation speed, temperature profiles, ignition time, burning rates and species evolution have not been fully resolved.

CHAPTER THREE

LABORATORY EXPERIMENTS AND RESULTS

3.1 Introduction

Presented in this chapter are the experimental techniques used in determination of the fuel properties as well as in the laboratory test of wood combustion in a fixed bed under air and oxy-fuel environment. The techniques for determining combustion parameters, namely, mass history, temperature profiles, burning rates, ignition time, bed porosity and flame front propagating velocity are discussed. Experimental results are presented in the last section of this chapter.

3.2 Wood Sample Preparation

In this work, the biomass fuel is eucalyptus wood. Eucalyptus is the main source of fuel for wood-fired boilers used for steam generation in process industries such as tea production in Kenya. Eucalyptus tree is an attractive source because it takes a short time to mature. Ash, volatile matter, gross calorific value and moisture contents of the fuels were determined in accordance to European standards CEN-TS 14775: 2009, CEN-TS 15148:2009, CEN-TS 14918:2009, CEN-TS 14774-2:2009, respectively, and presented in Table 3.1. In addition, ultimate analysis for the samples is presented in Table 3.1.

For studies on packing density, fuel sample sizes were determined in accordance to BS EN 15149 – 2:2010 (2010). The samples were sieved using Fritsch vibratory sieve shaker. In every sieving conducted, an amplitude of 3 mm and time of 15 min was used.

The fuel particles were grouped into four categories according to their sizes, viz., sawdust 1 (SD1), sawdust 2 (SD2), wood chips (WC) and wood spheres (WS), as shown in Fig. 3. 1. The

characteristic size, $\bar{d}$, of each group was best fitted using Rosin-Rammler distribution, Eq. (3.1) (Williams *et al.*, 2016).

$$R_R(d) = 100 \left(\exp \left(-\frac{d}{\bar{d}} \right)^{n_R} \right) \quad (3.1)$$

where d is the particle diameter or mesh size, n_R is the parameter of Rosin-Rammler distribution and R_R is the percentage of accumulated oversize mass. n_R was determined according to the method on Brezáni & Zeleňák (2010). More details about Rosin-Rammler distribution are provided in Appendix A.

Table 3.1: Proximate and ultimate analysis of fuel sample.

Proximate Analysis	(wt %)	Standards
Moisture	10.3	CEN-TS 14774-2:2009
Volatile matter (wt% dry basis)	84.9	CEN-TS 15148:2009
Fixed carbon (wt% dry basis) - by difference	14.9	-
Ash (wt% dry basis)	0.2	CEN-TS 14775:2009
Ultimate Analysis	(wt % dry basis)	Standards
C	50.87	CEN-TS 15104:2011
H	5.73	CEN-TS 15104:2011
N	0.3	CEN-TS 15104:2011
O (by difference)	43.1	-
Gross calorific value (MJ/kg)	19.3	CEN-TS 14918:2009

The size and shape of the particle were used to determine its sphericity, ψ (Trudel *et al.*, 2018) which is expressed as follows:

$$\psi = \frac{\pi D_{eq}^2}{A_s} = \frac{\pi^{1/3} (6V_p)^{2/3}}{A_s}, \quad (3.2)$$

where A_s is the particle surface area, V_p is the particle volume, D_{eq} is the particle diameter which is equivalent to that of a sphere with the same volume. D_{eq} is expressed as follows:

$$D_{eq} = \left(\frac{6V_p}{\pi} \right)^{1/3}. \quad (3.3)$$

(a) Wood spheres (WS)

(b) Wood chips (WC)

(c) Sawdust 2 (SD2)

(d) Sawdust 1 (SD1)

Figure 3.1: Wood fuel samples.

Bed porosity, χ , was determined from the measured fuel bed density, ρ_b , and density of wood particle, ρ_p , which were related through Eq. (3.4) (Horttanainen *et al.*, 2002):

$$\chi = 1 - \frac{\rho_b}{\rho_p} \quad (3.4)$$

The sphericity, equivalent diameters and bed porosity of different fuel samples used in this study are presented in Table 3.2.

Table 3.2: Properties of wood samples and fixed bed.

Fuel type	ρ_b (kg/m ³)	ρ_p (kg/m ³)	D_{eq} (mm)	ψ (-)	χ (-)
Wood chips (WC)	597	1220	5.25	0.30	0.51
Sawdust 1 (SD1)	321	1220	1.28	0.25	0.74
Sawdust 2 (SD2)	477	1220	2.91	0.29	0.61
Mixture of WC and SD1 (25% of WC)	390	1220	3.27	0.28	0.68
Mixture of WC and SD2 (50% each)	537	1220	4.08	0.30	0.56

3.3 Experimental Set-Up

A schematic diagram of the experimental set up and a photo of the laboratory setup used in this work are shown in Fig. 3.2 and 3.3, respectively.

Figure 3.2: Schematic diagram of the experimental set-up.

It is a laboratory fixed bed reactor, which has provision for regulating the ratio of O₂/CO₂ and O₂/N₂ during combustion. It has an internal diameter of 40 mm and a height of 200 mm. It has

provisions for thermocouple insertions located at 10 mm intervals. Internal and external parts are made of stainless steel and between them is a 20 mm thick refractory cement for insulation. Thermal conductivity of refractory cement is 0.34 W/m.K (Lienhard IV & Lienhard V, 2003). Critical insulation radius for this material, considering typical values of convective heat transfer coefficient for air in natural convection as 10-20 W/m².K (Incropera *et al.*, 2006) lies between 17 and 34 mm. An external radius of 40 mm used in this reactor is, therefore, sufficient for heat insulation. Fuel bed is held by a stainless steel grate.

Figure 3.3: A photo of laboratory set-up.

The reactor was operated in counter-current flame propagation mode. Top fuel was ignited initially and the flame front propagates downward into the virgin fuel. Oxidizer was supplied from the bottom. For this arrangement, there is no fuel bed movement. The fuel bed was ignited using methane gas flame with a flow rate of 0.051 m³/h. Ignition time was about 10 s. The amount of methane used in ignition was estimated to be 94 mg and released a total amount of

heat of 4719 J. It was expected that this amount of heat ignites a top layer of wood of about 2.26 g, therefore, wood temperature during ignition was raised to about 1182 °C.

Oxidizer was a mixture of pure O₂ and N₂ or CO₂ in various composition. The different gas components were supplied independently through a perforated bottom plate of a 100 mm long mixing chamber made of brass. The chamber was filled with 8 mm long hollow glass with internal diameter of 4 mm for settling and generating a relatively uniform flow. A constant mass flow rate of 0.1 kg/m²/s was used for all the tests carried out. Gas flow rates were measured using variable area flowmeters (rotameters) in-build in Atlas LOI equipment with a tolerance of ±2%. The flow rate of the mixture for various O₂ concentration was calculated based on Eqn. (3.5) and tabulated in Table 4.3.

$$\dot{m}_m = Q_{O_2} \left(\frac{p}{RT} \right)_{O_2} + Q_D \left(\frac{p}{RT} \right)_D \quad (3.5)$$

where p is the supply pressure, T is the supply temperature, $\dot{m}_m$ is the mixture mass flow rate (kg/s) and Q_{O_2} and Q_D are volumetric flow rate of O₂ and diluent, N₂ or CO₂, respectively.

Table 3.3: Volumetric flow rates for O₂/N₂ and O₂/CO₂ supplied at $T = 295$ K, $p = 5$ bar and operating condition of $\dot{m} = 0.1$ kg/m²/s.

O₂ composition (% vol)	O₂/N₂ mixture		O₂/CO₂ mixture	
	O₂ flow rate (l/min)	N₂ flow rate (l/min)	O₂ flow rate (l/min)	CO₂ flow rate (l/min)
21	0.057	0.213	0.039	0.148
25	0.067	0.201	0.047	0.142
30	0.080	0.186	0.058	0.135
35	0.093	0.172	0.068	0.127
40	0.105	0.158	0.079	0.119
45	0.117	0.143	0.091	0.111
50	0.130	0.130	0.102	0.102

During combustion, the reactor was placed on a weighting balance in order to obtain mass loss history. The weighing balance has an accuracy of ± 0.01 g. Temperature in the fuel bed was monitored by five Type K thermocouples. They are connected to a data acquisition system that records temperature every second. Temperature measurement and data acquisition using Type K thermocouples were done in accordance to ASTM MNL12 (Park *et al.*, 1993). In this regard, temperature measurement uncertainty and calibration of thermocouples were done. Uncertainty of thermocouple data acquisition system is dependent on combustion zone temperature. For the whole range of thermocouple measurement, it is between ± 2.184 °C and ± 6.630 °C (for more details see Appendix B). In addition, temperature measured by thermocouple may differ significantly from the true gas temperature because of radiation heat loss from the thermocouple surface to the cooler surrounding walls. Error due to radiation loss was corrected according to the methodology developed by Blevins & Pitts (1999) and have been applied by other researchers (Brohez, Delvosalle, & Marlair, 2004; Rashidian, Al-Abdeli, Yeoh, Patiño, & Guzzomi, 2017; Roberts, Coney, & Gibbs, 2011). In this method, maximum and minimum measurement error which occur when using bare bead and single shielded aspirated thermocouple (TC), respectively, are used to estimate the error in sheathed thermocouple with the same bead size (for more details see Appendix C).

Measurement of combustion properties were made for different O₂/CO₂ mixtures which varied in composition of O₂ in CO₂ from 21% to 50% by volume. For comparison purposes, measurements of combustion properties were made for air-fuel condition. The gaseous mixtures were supplied at room temperature (295 K). Each test was done in three replicate to check repeatability.

3.4 Determination of Combustion Parameters

3.4.1 Burning History

Burning history for the fuel bed was monitored by temperature and mass loss measurement. A 6 cm fuel bed were combusted. For each test, bulk density of the bed was determined. Despite using the same particle size and bed height, there were slight variations of the bulk density, ± 2 kg/m³, because of random fuel and void arrangement in the bed. For all the particle type studied, a bulk density of 402 to 597 kg/m³ were recorded during experiments.

Temperature at five equidistant vertical locations, 10 mm apart, were measured using type K thermocouple. A data acquisition device was used to record temperature with respect to time. The mass of the bed was continuously monitored using a weighting balance.

3.4.2 Flame Front Propagation Speed

The flame front propagation speed, V_F , is estimated from distance and time data of temperature measuring points (Sakthivadivel & Iniyar, 2018; Yang, Ryu, Sharifi, & Swithenbank, 2006). It is calculated as follows:

$$V_F = \frac{\Delta x}{\Delta t}, \quad (3.6)$$

where Δx is the distance between two thermocouples and Δt is the time between the abrupt increase in temperature of thermocouples from ambient value to peak value.

Another parameter that was used to quantify combustion in the bed is reaction zone thickness. It is regarded to be the physical distance in the flame front where the bed temperature rises from ambient value to peak value. A stiff temperature rise represents a thin reaction front whereas a gradually changing temperature rise represents a thick reaction front.

3.4.3 Ignition Time

Ignition time is considered to be the time at which devolatilization starts where a sustainable combustion is achieved. In this work, ignition of fuel at any part of the bed was assumed to take place when there is an abrupt increase of temperature from ambient value to peak value.

3.4.4 Burning Rate

Burning rate, $\dot{m}_b$, represent the rate of biomass consumption which include both devolatilization and char combustion. It is defined as the rate of mass loss per unit cross-sectional area (Khor *et al.*, 2007; Yang, Ryu, Khor, Yates, *et al.*, 2005). It was determined by considering the amount of fuel burnt, given by the measured change in weight of the column, and the total time of combustion;

$$\dot{m}_b = \frac{\text{Fuel weight (kg)}}{\text{Combustion time(s)} \times \text{Cross sectional area(m}^2\text{)}} \quad (3.7)$$

The difference between burning rate and ignition rate is the rate of mass accumulation above the ignition front.

3.5 Experimental Results

Presented in this section are the experimental results of temperature profiles, mass loss history, ignition times, flame front propagation speeds and burning rates. The results are for combustion of wood in different O₂/N₂ and O₂/CO₂ mixtures and for various bed porosity. In all the results presented, error bars are the standard deviations.

Figure 3.4 shows the mass loss history measured during entire combustion period for wood combustion in a fixed bed at 21% O₂/79% N₂ and 21% O₂/79% CO₂ mixtures. In both cases, the graph clearly depicts three phases of wood conversion, namely, drying phase represented

by the first region of slow mass loss, devolatilization phase represented by a slightly fast mass loss, and char combustion phase with the slowest changes in mass. The deviation of experimental values of mass loss from their respective mean values ranges between 2% and 17%. Thus the experimental values showed a good repeatability.

Figure 3.4: Measured mass loss history for wood combustion in fixed bed at 21% O₂/79% N₂ and 21% O₂/79% CO₂ mixtures.

Temperature distributions at different height above the grate were measured and recorded by thermocouples. Fig. 3.5 presents results of temperature for combustion of spherical wood particles in a fixed bed in 21% O₂/79% N₂ mixture and 21% O₂/79% CO₂ mixture while Fig. 3.6 presents results of temperature for combustion of wood in 21% O₂/79% CO₂ with various bed porosity; $\chi = 0.51$ to $\chi = 0.74$. In Fig. 3.5, the graph shows that the temperature profile for both N₂ and CO₂ environment have two distinct temperature peaks. The peak temperature is lower

in CO_2 environment as compared to N_2 environment. Low porosity beds have two distinct temperature peaks, Figs 3.6(a) and (b), while high porosity beds have single temperature peak, Figs 3.6 (a)-(c). Furthermore, high porosity beds attained relatively higher values of temperature at the peak than those for the first peaks of low porosity beds. For each case, errors are shown for data of a representative thermocouple. The deviation of experimental values of temperature from their respective mean values for all points ranges between 1.8% and 7.7%. This also indicates a good repeatability.

Figure 3.5: Measured temperature profiles at various distances from the bed bottom for wood combustion in (a) 21% O_2 /79% N_2 mixture and (b) 21% O_2 /79% CO_2 mixture.

The ignition times for fixed bed combustion of spherical wood measured in various O_2/N_2 and O_2/CO_2 mixtures are shown in Fig. 3.7 while for various bed porosity is shown in Fig. 3.8. In both N_2 and CO_2 environments, the graph shows that ignition times decrease with increase in O_2 concentration. The ignition times at corresponding oxygen concentration are higher in CO_2 environment than in N_2 environment. The standard deviations of experimental values of ignition times from their corresponding mean values ranges from 2.2% to 18%.

Figure 3.6: Measured temperature profiles at various heights above the grate for particle types (a) WC ($\chi = 0.51$), (b) WCS D2 ($\chi = 0.56$), (c) SD2 ($\chi = 0.61$), (d) WCS D1 ($\chi = 0.68$) and (e) SD1 ($\chi = 0.74$).

Figure 3.7: Measured ignition time for fixed bed combustion of wood in N_2 and CO_2 environments.

Figure 3.8: Measured ignition time for wood combustion in 21% O_2 /79% CO_2 mixture for different initial bed porosity.

The flame front propagation speed for fixed bed combustion of spherical wood measured in various O_2/N_2 and O_2/CO_2 mixtures are shown in Fig. 3.9 while for various bed porosity is

shown in Fig. 3.10. The graph shows that flame front propagation speed is directly proportional to O_2 concentration in both N_2 and CO_2 environments. The flame front propagation speed at corresponding oxygen concentration are higher in N_2 environment than in CO_2 environment. The standard deviations of experimental values of flame front propagation speed from their corresponding mean values ranges from 3% to 12.6%. The lower flame speed observed in CO_2 environment could be attributed to its higher specific heat capacity which reduces its flame temperature. As a result, the heating rates of the fuel particles in the bed is decreased and lead to a decrease in flame speed.

Figure 3.9: Measured flame front propagation speed for fixed bed combustion of wood in N_2 and CO_2 environments.

The burning rates for fixed bed combustion of spherical wood measured in various O_2/N_2 and O_2/CO_2 mixtures are shown in Fig. 3.11. The graph shows that burning rates increase with increase in O_2 concentration in both N_2 and CO_2 environments. The burning rates at corresponding oxygen concentration are higher in N_2 environment than in CO_2 environment. The standard deviations of experimental values of burning rates from their corresponding mean values ranges from 2.9% to 10.8%. The burning rate of a fuel is highly depended on the

combustion temperature which affects the heating rate of the particles. The lower burning rates in CO_2 environment is associated to its lower combustion temperature, as noted in Fig. 3.5. Furthermore, O_2 diffusivity in CO_2 environment is low since CO_2 is a heavy gas (Suda *et al.*, 2007). Therefore, the reduced amount of O_2 at the particles' reactive surface causes a decrease in its consumption as well as the burning rate.

Figure 3.10: Measured flame front propagation speed for wood combustion in in 21% O_2 /79% N_2 and 21% O_2 /79% CO_2 mixtures for different initial bed porosity.

Figure 3.11: Measured burning rate for fixed bed combustion of wood in N_2 and CO_2 environments.

In overall, the experimental results showed a good repeatability with most of the points having a standard deviation from their respective mean values being below 18%.

CHAPTER FOUR

NUMERICAL MODELLING

4.1 Introduction

Presented in this chapter are the numerical simulation of wood combustion in a fixed bed. The governing equations for both solid phase and gas phase as well as coupling equations are presented. Furthermore, specific models for the various physico-chemical processes, viz., turbulence, radiation, fuel shrinkage and chemical kinetics are also discussed. Numerical solution methods employed, geometry and boundary conditions formulations and computational meshes are also presented.

4.2 Governing Equations

A fixed bed of solid fuel consists of particles which interact with one another in terms of heat exchange by conduction and radiation. They also interact with gas phase surrounding them in the void spaces. In addition, they undergo conversion through several processes, viz., drying, pyrolysis and char oxidation. All these processes are illustrated in Fig. 4.1. To model particles conversion in a fuel bed, all these processes must be accounted. This section presents governing equations for both solid phase and gas phase as well as coupling equations and other specific models which are required during computation of wood combustion in a fixed bed.

In this work Euler-Lagrangian model have been used to model biomass conversion in a fixed bed. Computational Fluid Dynamics - Discrete Element Method (CFD-DEM) simulation method was used in this study. Solid particles and their conversion have been modeled using DEM while fluid phase have been modeled as a continuous phase using CFD. The two phases are coupled together. The interaction between the phases is enabled by two-way coupling equations.

Figure 4.1: Processes of a fuel bed thermal conversion.

4.2.1 Merits and Demerits of CFD-DEM Code

In this work, numerical simulations of wood conversion in a fixed bed using CFD-DEM approach were implemented through a commercial software STAR CCM+ version 11.04 (CD-Adapco, 2017). CFD-DEM code considers the conversion of each particle, which are sum to obtain the conversion in the bed. The code has the following merits and demerits:

4.2.1.1 Merits

- Solid-phase is modeled using single particle technique. Detailed information for mass, species and energy are captured for each particle. Therefore, the prediction accuracy of the entire fuel bed conversion is improved.

- Empirical correlations which are experimentally determined are not required since the conversion of each particle is considered. Hence, the method is independent of particular experimental conditions.
- Shrinkage of fuel bed is easily implemented in this method by considering a suitable particle shrinkage model.

4.2.1.2 Demerit

The method requires high computing power. This is because it solves transport equations of energy, mass and species for each particle. In addition, it requires a computer with a large storage that is capable of storing all information for mass, species and energy for each particle.

4.2.2 Model Considerations

To model a fixed bed combustion, the following main considerations have been made:

1. Wood fuel is considered to be spherical particles. Each particle is modeled as thermally thin, that is, it has low Biot number, $Bi < 0.1$, which causes negligible internal temperature gradient. Therefore, each particle is assumed to be internally homogeneous. The physical properties of the wood and char used in simulations are presented in section 4.8.
2. Fuel bed is considered as a porous media where the pressure loss is accounted for by Ergun equation (Mehrabian, Shiehnejadhesar, Scharler, & Obernberger, 2014). This is incorporated as a source term in gas-phase momentum equation.
3. For the conditions tested in this study, the Reynolds Number, Re , for the gas flow in the bed was evaluated to be in the range of 3200 to 4820, which is in the turbulent flow regime. Therefore, turbulent combustion model was considered in the simulation.

4. Gas phase and solid phase interact by exchanging mass, species and energy. Heat is exchanged between solid-phase and gas-phase by convection and radiation while within solid phase is by conduction and radiation.
5. Porosity of the particle, denoted by θ , is assumed to vary during bed thermal conversion as a result of local consumption of solid phase. Therefore, the particle diameter slightly shrinks producing a slight change in the bed size during entire combustion period.

These considerations are discussed here below.

4.2.3 Gas-Phase Equations

The conservation equations governing multi-component, chemically reacting, gas mixtures applicable to a fixed bed are presented below (CD-Adapco, 2017; Mehrabian, 2013; Wehinger, 2016):

- Mass conservation equation:

$$\frac{\partial}{\partial t}(\chi \rho_g) + \nabla \cdot (\rho_g \mathbf{v}_g) = \sum_{i,g} w_{i,g}^{gs}; \quad (4.1)$$

- Momentum conservation equation:

$$\frac{\partial}{\partial t}(\chi \rho_g \mathbf{v}_g) + \nabla \cdot (\rho_g \mathbf{v}_g \mathbf{v}_g) = -\nabla p + \nabla \cdot \tau + \rho_g g + S_m, \quad (4.2)$$

where is S_m momentum source term given as;

$$S_m = -\left(\frac{\mu}{C_1} \mathbf{v}_g + C_2 \rho_g |\mathbf{v}_g| \mathbf{v}_g\right); \quad (4.3)$$

- Energy conservation equation:

$$\begin{aligned} \frac{\partial}{\partial t}(\chi \rho_g h_g) + \nabla \cdot (\rho_g \mathbf{v}_g h_g) = \frac{\partial}{\partial t}(\chi p) + \nabla \cdot \left(\lambda_{g,e} \nabla T_g - \sum_{i=1}^{N_g} h_{i,g} J_{i,g} \right) \\ + \nabla \cdot (\mathbf{v}_g p) - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}_g) + S_E; \end{aligned} \quad (4.4)$$

where S_E is energy source term given as;

$$S_E = A_s h_c (T_s - T_g) - \sum_{i,g} w_{i,g}^{gs} H_{i,g} + q_R; \quad (4.5)$$

- Species conservation equation for a species i, g :

$$\frac{\partial}{\partial t}(\chi \rho_g Y_{i,g}) + \nabla \cdot (\rho_g \mathbf{v}_g Y_{i,g}) = \nabla \cdot (\rho_g D \nabla Y_{i,g}) + w_{i,g}^{gs}; \quad (4.6)$$

In Eqs (4.1) - (4.6), A_s is the particle surface area, C_1 is the permeability, C_2 is the inertia loss coefficient, D is the diffusivity, g is the gravity, $H_{i,g}$ is the enthalpy of formation of gas-phase species i , h_c is the heat transfer coefficient, h_g is the enthalpy of gas-phase mixture, $h_{i,g}$ is the enthalpy of gas-phase species i , $J_{i,g}$ is the diffusion mass flux of gas-phase species i , N_g is the number of gas species, p is the hydrostatic pressure, q_R is the radiant heat flux vector, T_g is the gas-phase temperature, t is the time, T_s is the solid-phase temperature, $\mathbf{v}_g$ is the gas-phase velocity vector, $\lambda_{g,e}$ is the effective gas-phase thermal conductivity, μ is the coefficient of dynamic viscosity, ρ_g is the gas-phase mass density, χ is the void fraction, $\boldsymbol{\tau}$ is the shear stress tensor, $Y_{i,g}$ is the mass fraction of gaseous species i, g and $w_{i,g}^{gs}$ is the rate of production of gaseous species i, g heterogeneous chemical reactions.

4.2.4 Solid-Phase Equations

In this thesis, fixed bed is treated as a collection of particles and conversion of each particle is modeled using DEM. Conversion of the bed is equal to the summation of all the particles processes.

Conservation equations for a multi-component solid particle employed in STAR CCM+ are summarized below (CD-Adapco, 2017; van Kuijk, 2008):

- Mass conservation:

$$\frac{\partial}{\partial t}((1 - \chi)\rho_s) = \sum_{i,s} w_{i,s}^{gs}; \quad (4.7)$$

- Species conservation:

$$\frac{\partial}{\partial t}((1 - \chi)\rho_s Y_{i,s}) = w_{i,s}^{gs}; \quad (4.8)$$

- Energy conservation:

$$\begin{aligned} \rho_s c_{ps} (1 - \chi) \frac{\partial T_p}{\partial t} = & \underbrace{\nabla \cdot (\lambda_{s,e} \nabla T_s)}_1 + \underbrace{A_s h_c (T_g - T_s)}_2 \\ & + \underbrace{\frac{A_s}{4} Q_{a,p} (G - 4\sigma T_s^4)}_3 + \underbrace{\sum_{i,s} w_{i,s}^{gs} H_{i,s}}_4; \end{aligned} \quad (4.9)$$

where term 1 in Eq. (4.9) is the heat transfer by conduction within the particle, term 2 is the heat flux at the particle surface due to convection, term 3 is the radiation heat flux at the particle surface and term 4 is the energy change due to enthalpy of formation of species i .

In Eqs (4.7) – (4.9), besides the symbols defined earlier, ρ_s is the particle density, $Y_{i,s}$ is the mass fraction of solid-phase species i,s , $w_{i,s}^{gs}$ is the rate of production of solid-phase species i,s by heterogeneous chemical reactions, c_{ps} is the specific heat capacity of the particle, T_p is the particle temperature, $\lambda_{s,e}$ is the effective solid phase thermal conductivity, $Q_{a,p}$ is the absorption efficiency of the particle, G is the incident radiative heat flux, and σ is the Stefan-Boltzmann constant, $H_{i,s}$ is enthalpy of formation of solid-phase species i .

The heat transfer coefficient, h_c is given in terms of the particle Nusselt number, Nu_p :

$$Nu_p = \frac{h_c d_p}{\lambda_g}, \quad (4.10)$$

where d_p is the particle diameter. Nu_p for spherical particles in flows of up to Reynolds number, $Re_p \cong 5000$ can be defined using Ranz-Marshall correlation (Incropera *et al.*, 2006):

$$Nu_p = 2(1 + 0.3Re^{1/2}Pr^{1/3}), \quad (4.11)$$

where Pr is the Prandtl number of the continuous phase.

4.2.5 Two-way coupling equations

Two-way coupling equations allow particle phase to exchange mass, species and energy with the continuous phase. These equations are described below (CD-Adapco, 2017):

- Mass conservation:

$$\sum_{i,g} w_{i,g}^{gs} = - \sum_{i,s} w_{i,s}^{gs}; \quad (4.12)$$

- Species conservation equation for species i,s :

$$w_{i,g}^{gs} = -w_{i,s}^{gs}; \quad (4.13)$$

- Energy conservation - The interaction between solid-phase and gas-phase in terms of convective and radiation heat transfer is enabled by a source term added to solid phase energy equation, Eq. (4.9), and subtracted in gas-phase energy equation, Eqs. (4.4) and (4.5).

4.3 Turbulence Model

There are three main frameworks for computing turbulent flows which are reactive, viz.; (1) Reynolds-Averaged Naviers Stokes (RANS), (2) Direct Numerical Simulations (DNS) and, (3) Large Eddy Simulation (LES). In DNS the three-dimensional unsteady governing equations are fully solved with regard to time, velocity and the scalar fields. The time and length scales are

fully solved. Therefore, it requires trillions of grids points and very numerous number of time steps. Current state of the art DNS is able to compute problems with domain which are very close to actual systems, i.e., with one order of magnitude less than the practical combustion devices. The main challenge of DNS is the temporal integration of conservation equations.

In LES, contribution of large eddies is considered through spatial filtration of governing equations. In this method, scale separation approach is utilized. Scale separation is made on large eddies that have energy and small eddies or subgrid scales (SGS) which dissipate energy. The advantage of LES is that it takes into consideration large scale information in the governing equations. Consequently, the importance of large scale eddies on mixing and reactions rates is realized in LES.

RANS is based on time or ensemble averaged of instantaneous transport equations for mass, momentum and reactive scalars. Turbulent motion and combustion are not resolved in time and length scales. This method requires closure models in order to address unresolved terms.

In this work RANS modeling approach has been used. RANS equations are obtained by decomposing instantaneous transport equations for various conservation quantities into two components, i.e., mean and fluctuating parts. As a results of Reynold decomposition, an additional term arises in momentum transport equation. This new term is referred to as Reynold stress, as illustrated in the Reynold-averaged momentum equation (Wehinger, 2016):

$$\frac{\partial}{\partial t}(\rho_g \bar{v}_i) + \frac{\partial}{\partial x_j}(\rho_g \bar{v}_i \bar{v}_j + \rho_g \overline{v'_i v'_j}) + \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} = \rho_g g_i, \quad (4.14)$$

where $\bar{v}_i$ and $\bar{v}_j$ are the mean velocity component in i and j direction, v'_i and v'_j are the fluctuating velocity component in i and j direction, x_i and x_j are the Cartesian co-ordinates, $\bar{p}$ is the mean pressure, $\bar{\tau}_{ij}$ is the mean stress tensor and $\rho_g \overline{v'_i v'_j}$ is the Reynolds stresses. $\rho_g \overline{v'_i v'_j}$ is modeled using Boussinesq approximation (Echekki & Mastorakos, 2011; Wehinger, 2016):

$$-\rho_g \overline{v'_i v'_j} = \mu_t \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{2}{3} \left(\rho_g k + \mu_t \frac{\partial v_i}{\partial x_i} \right) \delta_{ij}, \quad (4.15)$$

where μ_t is the turbulent viscosity, k is turbulent kinetic energy and δ_{ij} is the Kronecker delta which is unity for $i = j$ else zero.

Closure models utilized in STAR CCM+ are eddy viscosity models and Reynolds stress transport models. Eddy viscosity models use the concept of a turbulent viscosity, μ_t to model the Reynolds stresses as a function of mean flow quantities, for example Boussinesq approximation Eq. (4.15). Other models in this category which require additional transport equations includes $k - \varepsilon$ models, $k - \omega$ models and Spalart-Allmaras models (Knaus *et al.*, 2000; Shur, Spalart, Strelets, & Travin, 2008). In this work, $k - \varepsilon$ model was used. In this model, the additional transport equations required are for turbulent kinetic energy, k and turbulence dissipation rate, ε . Various forms of $k - \varepsilon$ model exists, for example, standard, standard two-layer, standard low-Re and realizable model. Standard $k - \varepsilon$ model was used in this work because it is easy to implement and suitable at all Reynolds numbers.

In standard $k - \varepsilon$ model, the additional equations used are those which were proposed by Jones & Launder (1972) and coefficients proposed by Launder & Sharma (1974). These equations are expressed as follows:

$$\frac{\partial}{\partial t}(\rho_g k) + \frac{\partial}{\partial x_i}(\rho_g v_i k) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho_g \varepsilon, \quad (4.16)$$

$$\frac{\partial}{\partial t}(\rho_g \varepsilon) + \frac{\partial}{\partial x_i}(\rho_g v_i \varepsilon) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} [G_k + (1 - C_{\varepsilon 3}) G_b] - C_{\varepsilon 2} \rho_g \frac{\varepsilon^2}{k}, \quad (4.17)$$

where G_k is the production of turbulent kinetic energy, k due to Reynolds stresses;

$$G_k = -\rho_g \overline{v'_i v'_j} \frac{\partial v_j}{\partial x_i}, \quad (4.18)$$

G_b is production of turbulent kinetic energy, k due to buoyancy;

$$G_b = -\beta g_i \frac{\mu_t}{Pr_t} \frac{\partial T_g}{\partial x_i}, \quad (4.19)$$

Pr_t is the turbulent Prandtl number, β is the thermal expansion coefficient and $C_{\varepsilon 1}, C_{\varepsilon 2}$ and $C_{\varepsilon 3}$ are model coefficients which are taken as $C_{\varepsilon 1} = 1.44$, $C_{\varepsilon 2} = 1.92$,

$$C_{\varepsilon 3} = \begin{cases} 1 & \text{for } G_b \geq 0 \\ 1 & \text{for } G_b < 0 \end{cases} \quad (4.20)$$

Turbulent viscosity is computed as follows:

$$\mu_t = \rho C_\mu kT, \quad (4.21)$$

where C_μ is a constant taken as 0.09.

4.4 Radiation Model

In this work, radiation energy exchange between continuous region and particles have been considered. A participation media radiation model (Fiveland, 1988) also known as Discrete Ordinate Method (DOM) have been implemented. The model simulates thermal radiation exchange between diffuse/specular surfaces which forms a closed set. The radiative properties of the surface are specified in terms of diffuse/specular reflectivity, emissivity and radiation temperature. The region between the surfaces are filled with media which absorb, emit and scatter radiation. The media include both the fuel particles and the gases. Therefore, apart from surface's optical properties and thermal boundary conditions, the amount of radiation emitted and received by the surface depends on this effect.

The presence of high concentration of H_2O and CO_2 gases in an oxy-fuel combustion environment alters radiative gas properties. The choice of the property model affects the accuracy of the overall radiation model. Some models use oversimplified approach, for

example, gray gas model, while others use comprehensive approach, for example, wavelength dependent property models. A widely used model is weighted-sum-of-gray-gas-model (WSGGM) which works well in an air-fuel combustion environment (Smith *et al.*, 1982). There have been some efforts, for instance Yin *et al.* (2012), to modify WSGGM so as to improve its accuracy in predicting radiation in an oxy-fuel combustion environment. It has been noted that modified WSGGM model has significant improvement on the accuracy when considering large scale reactors (Álvarez *et al.*, 2014; Park *et al.*, 2012). A minimal change of less than 1% on temperature was noted when applied on a small scale reactor (Álvarez *et al.*, 2014). The reactor used in this study is small, therefore, unmodified WSGGM was implemented with an expectation that it would not significantly affects the results.

In WSGGM model, the radiative properties of the medium are considered to be constant in the entire spectrum. The method assumed that the medium is made up of different amount of gray gases with different absorption coefficients. In WSGGM method, H₂O and CO₂ are the only gases considered because they are the main products of combustion with significant influence on absorption and emission of radiation.

Bouguer-Lambert law (Malinin & Yoe, 1961) defines the relationship between the total gray gas absorption coefficient, κ and the total absorptivity for a gray medium, α_t :

$$\alpha_t = 1 - e^{-\kappa s}, \quad (4.22)$$

where s is the optical path length.

A weighted-sum of several gray gases is use to approximate the total absorptivity:

$$\alpha_t \approx \sum_{\kappa=0}^K a_{\kappa} (1 - e^{-\kappa_{\kappa} s}), \quad (4.23)$$

where K is the total number of gray gases, a_κ is the weight factor and κ_κ is the absorption coefficient of each gray gas. The total gray gas absorption coefficient, κ , which is represented in RTE Eq. (D.1) as k_a , Appendix D, is obtained by solving Eqs (4.22) and (4.23).

4.5 Shrinkage Model

In this thesis, the porosity of the particle, θ was modeled according to Eqs (4.24) and (4.25):

$$\frac{d_p}{d_{p,0}} = \left(\frac{m_p}{m_{p,0}} \right)^{\frac{\alpha}{3}}, \quad (4.24)$$

$$\theta = 1 - \left(\frac{m_p}{m_{p,0}} \right)^{1-\alpha}, \quad (4.25)$$

where d_p is the particle diameter, m_p is the particle mass, α is the exponent factor ($0 \leq \alpha \leq 1$) and 0 is the initial state of the particle.

The particle volume, V_p , is obtained from the following expression:

$$V_p = \frac{m_p}{(1 - \theta)\rho}, \quad (4.26)$$

and the diameter, d_p is evaluated using Eq. (3.3). And the apparent density, $\rho_{apparent}$ is evaluated as follows:

$$\rho_{apparent} = (1 - \theta)\rho, \quad (4.27)$$

The diameter of the particle is then used to evaluate the surface area of the particle, A_s . When the surface area of a particle changes, the overall reaction rate is affected. Through Eqs (4.24) and (4.25), the following shrinkages models are possible:

1. Particles can lose mass by increasing porosity yet maintaining the original diameter ($\alpha = 0$), as illustrated in Fig. 4.2.
2. Particles can lose mass by decreasing in diameter yet maintaining zero porosity ($\alpha = 1$), as illustrated in Fig. 4.3.
3. Particles can lose mass by decreasing in diameter and increasing porosity ($0 < \alpha < 1$), as illustrated in Fig. 4.4.

Figure 4.2: Shrinkage model where particle porosity increases while the original diameter is maintained.

Figure 4.3: Shrinkage model where particle diameter decreases while maintaining zero porosity.

Figure 4.4: Shrinkage model where particle porosity increases while the diameter decreases.

In this work a model which considered both shrinkage of particles and porosity variation was implemented, i.e., $0 \leq \alpha \leq 1$. In this model local consumption of particle leads to the change in porosity and local shrinkage of bed is caused by collapsing of areas due to combustion. The model was chosen because of its improved accuracy in prediction of the combustion parameters (Gómez, Porteiro, Patiño, & Míguez, 2014).

4.6 Chemical Kinetic Model

Biomass conversion was modeled by four sub-models, namely, drying, pyrolysis, gas-phase reactions and char oxidation models. The overall kinetic model used in this work is presented in Table 4.1. Drying of the wet wood was modeled by a first-order kinetic rate model, shown in reaction R(1) (Johansson, Thunman, & Leckner, 2007).

Dry wood decomposed into primary components char, tar and gas through pyrolysis process. The kinetics of dry wood conversion into tar, char and gas is given by reactions R(2)-R(4) while the tar cracking is reaction R(5). The mass fractions for gas species from wood pyrolysis in reaction R(2) were specified according to Mahmoudi *et al.* (2016) and Di Blasi (2000). The components of tar cracking reaction R(5) are inert tar, CO, CO₂, H₂ and CH₄ whose mass fractions amounts are 0.22, 0.564, 0.111, 0.017 and 0.088, respectively (Mahmoudi *et al.*, 2015; Wurzenberger *et al.*, 2002).

Table 4.1: Biomass kinetic model.

Drying		Rate expression		Source
R(1)	Wet wood $\rightarrow$ Dry wood + H ₂ O (g)	$R_{dry} = Y_m \rho_{b,wet} 1.6 \times 10^{27} \exp(-25000/T_s)$		Johansson <i>et al.</i> (2007)
Pyrolysis Reactions		Rate expression, $K_i = A_i T^n \exp(-E_i/RT)$	Kinetics: A (s ⁻¹), E(kJ/mol)	Source
R(2)	Dry wood $\rightarrow$ gas	$\dot{w}'_b = K_2 \rho_{b,dry}$	$A_2 = 111 \times 10^9$, $E_2 = 177$	Gómez <i>et al.</i> (2016)
R(3)	Dry wood $\rightarrow$ Tar	$\dot{w}'_b = K_3 \rho_{b,dry}$	$A_3 = 9.28 \times 10^9$, $E_3 = 149$	Gómez <i>et al.</i> (2016)
R(4)	Dry wood $\rightarrow$ char	$\dot{w}'_b = K_4 \rho_{b,dry}$	$A_4 = 30.5 \times 10^9$, $E_4 = 125$	Gómez <i>et al.</i> (2016)
R(5)	Tar $\rightarrow \gamma_t \text{Tar}_{inert} + \gamma_{CO} \text{CO} + \gamma_{CO_2} \text{CO}_2 + \gamma_{H_2} \text{H}_2 + \gamma_{CH_4} \text{CH}_4$	$\dot{w}'_{Tar} = K_5 \rho_{Tar}$	$A_5 = 9.55 \times 10^4$, $E_5 = 93.37$	Mahmoudi <i>et al.</i> (2016)
Homogeneous Gas-Phase Reactions		Rate expression, $K_i = A_i T^n \exp(-E_i/RT)$	Kinetics: A (s ⁻¹), E(kJ/mol)	Source
R(6)	2CO + O ₂ $\rightarrow$ 2CO ₂	$R_{CO} = K_6 [\text{CO}] [\text{O}_2]^{0.25} [\text{H}_2\text{O}]^{0.5}$	$A_6 = 2.24 \times 10^{12}$, $n = 0$, $E_6 = 167.36$	Mahmoudi <i>et al.</i> (2016)
R(7)	CH ₄ + 2O ₂ $\rightarrow$ CO ₂ + 2H ₂ O	$R_{CH_4} = K_7 [\text{CH}_4]^{0.7} [\text{O}_2]^{0.8}$	$A_7 = 11.58 \times 10^{13}$, $n = 0$, $E_7 = 202.5$	Mahmoudi <i>et al.</i> (2016)
R(8)	2H ₂ + O ₂ $\rightarrow$ 2H ₂ O	$R_{H_2} = K_8 [\text{H}_2] [\text{O}_2]$	$A_8 = 2.19 \times 10^9$, $n = 0$, $E_8 = 109.2$	Mahmoudi <i>et al.</i> (2016)
R(9)	Tar + 2.9O ₂ $\rightarrow$ 6CO + 3.1H ₂	$R_{Tar} = K_9 [\text{Tar}]^{0.5} [\text{O}_2]$	$A_9 = 9.2 \times 10^6$, $n = 0$, $E_9 = 80.2$	Mahmoudi <i>et al.</i> (2016)
R(10)	CO + OH $\rightarrow$ CO ₂ + H	$R_{CO} = K_{10} [\text{CO}] [\text{OH}]$	$A_{10} = 4.76 \times 10^7$, $n = 1.3$, $E_{10} = 0.293$	Smith <i>et al.</i> (1999)
R(11)	H + O ₂ $\rightarrow$ O + OH	$R_H = K_{11} [\text{O}] [\text{OH}]$	$A_{11} = 2.65 \times 10^{16}$, $n = -0.671$, $E_{11} = 71.347$	Smith <i>et al.</i> (1999)
R(12)	H ₂ + O ₂ $\rightarrow$ OH + OH	$R_{H_2} = K_{12} [\text{H}_2] [\text{O}_2]$	$A_{12} = 2.51 \times 10^{12}$, $n = 0$, $E_{12} = 163.075$	Westbrook <i>et al.</i> (1984)
R(13)	H ₂ O + CO $\rightarrow$ CO ₂ + H ₂	$R_{H_2O} = K_{13} [\text{H}_2\text{O}] [\text{CO}]$	$A_{13} = 2.78$, $n = 0$, $E_{13} = 12.55$	Gómez <i>et al.</i> (2016)
R(14)	CO ₂ + H ₂ $\rightarrow$ H ₂ O + CO	$R_{CO_2} = K_{14} [\text{CO}_2] [\text{H}_2]$	$A_{14} = 93.69$, $n = 0$, $E_{14} = 46.594$	Gómez <i>et al.</i> (2016)
Heterogeneous Reactions		Rate expression, $K_i = A_i T^n \exp(-E_i/RT)$	Kinetics: A (s ⁻¹), E(kJ/mol)	Source
R(15)	$\Omega \text{C} + \text{O}_2 \rightarrow 2(\Omega - 1) \text{CO} (2 - \Omega) \text{CO}_2$	$\dot{w}'_{char,O_2} = K_{15} P_{O_2} S_{a,char}$	$A_{15} = 2.54 \times 10^{-3}$, $E_{15} = 74.8$	Mahmoudi <i>et al.</i> (2016)
R(16)	C + CO ₂ $\rightarrow$ 2CO	$\dot{w}'_{char,CO_2} = K_{16} P_{CO_2} S_{a,char}$	$A_{16} = 1.81 \times 10^{-2}$, $E_{16} = 130$	Mahmoudi <i>et al.</i> (2016)
R(17)	C + H ₂ O $\rightarrow$ CO + H ₂	$\dot{w}'_{char,H_2O} = K_{17} P_{H_2O} S_{a,char}$	$A_{17} = 1.81 \times 10^{-2}$, $E_{17} = 130$	Mahmoudi <i>et al.</i> (2016)

Gas species considered in homogenous gas-phase reactions R(6)-R(14) are those generated from drying, H₂O, devolatilization, i.e., CO₂, H₂O, CO, H₂, CH₄, tar cracking and char heterogeneous reactions. Oxidation of CO, CH₄, H₂ and tar are represented by reactions R(6)-R(9). For the purpose of checking the chemical effect in oxy-fuel environment reaction R(10), which has been identified as dominant reaction pathway (Liu *et al.*, 2003; Liu *et al.*, 2001) is incorporated into the mechanism. Important chain-branching steps of H₂ (R(11), R(12)) relevant

to this reaction are included. Furthermore, the forward and reverse reactions R(13) and R(14) for H₂O and CO have been considered (Gómez *et al.*, 2014; Johansson *et al.*, 2007).

Char consumption is represented by heterogeneous reactions R(15)-R(17). Char oxidation is given by reaction R(15) while its gasification by CO₂ and H₂O is by reactions R(16) and R(17), respectively. Char combustion rate were evaluated based on partial pressure of O₂, CO₂ and H₂O available at its surface (Evans & Emmons, 1977). The parameter Ω in reaction R(15) control the ratio of CO₂ to CO emitted when char is burning. It is expressed as a function of char surface temperature (Johansson *et al.*, 2007; Thunman, Leckner, Niklasson, & Johnsson, 2002):

$$\Omega = \frac{2 \left(1 + 4.3 \exp \left[-\frac{3390}{T_{particle}} \right] \right)}{2 + 4.3 \exp \left[-\frac{3390}{T_{particle}} \right]}. \quad (4.28)$$

4.7 Thermodynamic and Transport Properties of Gas-Phase

4.7.1 Thermodynamic Properties

Gas thermodynamic properties required during computation of biomass combustion in a fixed bed are the frozen specific heat capacities at constant pressure of the pure species i , c_{pi} , the frozen specific heat capacity at constant pressure of the gas mixture, c_p , and the enthalpy, h_i , for pure species i .

The polynomial curve fits of NASA type are used to calculate the gas thermodynamic properties (Burcat & Ruscic, 2005). Specifically, the properties are given as follows:

- Molar heat capacity at constant pressure, C_{pi} :

$$\frac{C_{pi}}{R_0} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4; \quad (4.29)$$

- Molar enthalpy, H_i :

$$\frac{H_i}{R_0} = a_6 + a_1 T + \frac{a_2}{2} T^2 + \frac{a_3}{3} T^3 + \frac{a_4}{4} T^4 + \frac{a_5}{5} T^5; \quad (4.30)$$

- Molar entropy, S_i :

$$\frac{S_i}{R_0} = a_7 + a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4; \quad (4.31)$$

Here $a_1 - a_7$ are polynomial coefficients. The thermodynamic database has two set of polynomial coefficients; the first set is for the high temperature range, 1000-6000 K, and the second set for the low temperature range of 300-1000 K. The molar quantities C_{pi} , H_i and S_i are related to the respective mass-based quantities through $C_{pi} = c_{pi} W_i$, $H_i = h_i W_i$ and $S_i = s_i W_i$. The mass-based mixture frozen specific heat capacity, enthalpy and entropy are given by the following expressions:

$$c_p = \sum_i^N Y_i c_{pi}, \quad h = \sum_i^N Y_i h_i, \quad \text{and} \quad s = \sum_i^N Y_i s_i, \quad (4.32)$$

4.7.2 Transport Properties

The transport properties required during computation of biomass combustion in a fixed bed are the dynamic viscosity, μ , of the gas mixture, the thermal conductivity, λ , of the gas mixture, and the ordinary mixture-averaged and thermal diffusion coefficients for species i , D_i , and D_{Ti} , respectively.

A detailed modeling of molecular transport data as presented in CD-Adapco (2017) may be summarized as follows:

- Dynamic viscosity of species i , μ_i :

$$\mu_i = \frac{5}{16} \frac{\sqrt{\pi m_i K_B T}}{\pi \sigma_i^2 \Omega^{(2,2)*}}, \quad (4.33)$$

where σ is the Lennard-Jones collision diameter, m_i is the mass of the molecule, K_B is the Boltzmann constant, $\Omega^{(2,2)*}$ is collision integral, which is a function of the reduced temperature, T^* and dipole moment, δ^* . The quantities T^* and δ^* are given as: $T^* = T_i^* \equiv (K_B T / \epsilon_i)$ and $\delta^* = \delta_i^* = (1/2)(d_i^2 / \epsilon_i \sigma_i^3)$, here d_i is the dipole moment of species i , ϵ_i is its Lennard-Jones potential well depth.

- Dynamic viscosity of the mixture, μ :

$$\mu = \frac{1}{2} \left(\sum_{i=1}^N X_i \mu_i + \frac{1}{\sum_{i=1}^N (X_i / \mu_i)} \right); \quad (4.34)$$

- Thermal conductivity of species i , λ_i :

$$\lambda_i = \frac{\mu_i}{W_i} (f_{trans} C_{v,trans} + f_{rot} C_{v,rot} + f_{vib} C_{v,vib}); \quad (4.35)$$

where f_{trans} , f_{rot} , and f_{vib} are the species' translational, rotational and vibrational degrees of freedom, respectively, and $C_{v,trans}$, $C_{v,rot}$, $C_{v,vib}$ are the respective contribution to the molar heat capacity at constant volume, C_v , of species i .

- Thermal conductivity of the mixture, λ :

$$\lambda = \frac{1}{2} \left(\sum_{i=1}^N X_i \lambda_i + \frac{1}{\sum_{i=1}^N (X_i / \lambda_i)} \right); \quad (4.36)$$

- Binary diffusion coefficient, D_{ij} :

$$D_{ij} = \frac{3}{16} \frac{\sqrt{2\pi K_B^3 T^3 / W_{ij}}}{p \pi \sigma_{ij}^2 \Omega^{(1,1)*}}. \quad (4.37)$$

Besides the quantities defined before, $W_{ij} = 2W_iW_j/(W_i + W_j)$ is the reduced molar mass for the pair of species, i, j , and σ_{ij} is the average collision diameter. The mixture average diffusion coefficient, D_i is given as

$$D_i = \frac{1 - X_i}{\sum_{j=1, j \neq i}^N (X_j/D_{ij})}. \quad (4.38)$$

- Thermal diffusion coefficient of species i , D_{Ti} :

$$D_{Ti} = \frac{\theta_i D_i}{X_i}, \quad (4.39)$$

where θ_i is the thermal diffusion ratio of species i .

4.8 Thermodynamic and Transport Properties of Solid-Phase

The physical, thermodynamics and transport properties required during computation of biomass combustion in a fixed bed are the density, ρ_s , the porosity, θ , the specific heat capacity at constant pressure, $c_{p,s}$, and the thermal conductivity, λ_s . The physical, thermodynamics and transport properties of the wood and char used in this work are presented in Table 4.2.

Table 4.2: Physical properties of wood.

Eucalyptus wood	
Density, ρ (kg/m ³)	1220
Porosity, θ	0.64
Specific heat, c_p (J/kgK)	$1500 + T_s$
Conductivity, λ_s (W/mK)	0.2
Char	
Density, ρ (kg/m ³)	250
Porosity, θ	0.85
Specific heat, c_p (J/kgK)	$420 + 2.09T_s - 6.85 \times 10^{-4} T_s^2$
Conductivity, λ_s (W/mK)	0.1

4.9 Numerical Solution Methods

Numerical simulations of combustion of biomass in fixed bed were carried out using a commercial CFD software CD-Adapco (STAR CCM+ version 11.04), CD-Adapco (2017). Unsteady state solver was employed to solve the governing equations in which the pressure-velocity coupling was enabled by using Pressure Implicit with Splitting of Operators (PISO) algorithm. The PISO algorithm is suited for transient cases. PISO is faster than Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) at short time-steps, though both algorithms have the same level of temporal accuracy (Issa, Gosman, & Watkins, 1986).

Second-order upwind scheme was used for the discretization of momentum, species, energy and radiation transport equations, as described in Appendix D. The transient terms were discretized using a second-order implicit scheme.

The criterion of convergence of solution was enabled by setting residual values for continuity, species, momentum, energy and radiation. The residuals for all the variables were set to converge at 10^{-6} . Under-relaxation factor (URF) was adjusted in order to accelerate convergence of numerical stable solutions. Appropriate values of URF for each equation were selected by performing several trials and also by reference to previous research (Kangwanpongpan, 2013). URFs for various equations which improved convergence of numerical stable solutions were as follows: for density = 0.85; for momentum = 0.85; for turbulence = 0.85; for radiation = 0.85; for species = 0.95.

4.10 Mesh and Grid Refinement

Computational domain representing the burner was meshed into highly-refined unstructured grids which ensured grid independent solutions. The burner was considered to have double

symmetry. Therefore, a quarter of the burner with the dimensions described in section 3.3 was used in all simulated cases in order to reduce the computational time.

Mesh independent test was carried out to determine appropriate number of cells. The cells were dense in the fuel bed region in order to improve the accuracy of the solution, Fig 4.5(a). The cells were made of polyhedral elements and prismatic layers near the wall, as shown in Fig. 4.5(b). Based on the mesh independent test results (Chapter five), a computational mesh with 200,0000 cells was selected for all the cases computed.

4.11 Boundary Conditions

4.11.1 Inlet Boundary Conditions

The inlet boundary was at the bottom of the fixed bed. At this boundary, mass flow rate, species mass fraction, temperature, pressure, turbulence intensity and turbulence viscosity ratio were specified using Dirichlet boundary condition as follows:

$$\dot{m} = \dot{m}_L, T = T_L, p = p_L, Y_i = Y_{i,L}, \text{ for } i = 1, \dots, N, I = I_L \text{ and } \mu_r = \mu_{r,L}.$$

where subscript L represent the value at the inlet boundary. Turbulent kinetic energy, k and turbulent dissipation rate, ε in this boundary are calculated using the specified turbulence intensity I and turbulent viscosity ratio, μ_r using Eqs. (4.40) and (4.41), respectively.

$$k \approx \frac{3}{2} (I\vartheta)^2. \quad (4.40)$$

$$\varepsilon \approx \frac{\rho C_\mu k^2}{\mu_r \mu} \quad (4.41)$$

where $\mu_r = \mu_t/\mu$, ϑ is the turbulent velocity scale and C_μ is the coefficient of the model.

Figure 4.5: Computational mesh for the fixed bed; (a) highly refined mesh in fuel bed and grate; (b) prismatic layers near the wall.

4.11.2 Outlet Boundary Conditions

The outlet boundary was at the top of the fixed bed. At this boundary, pressure, turbulence intensity and turbulence viscosity ratio were specified using Dirichlet boundary conditions as in the case for inlet boundary conditions. However, species mass fraction and temperature were specified using Neumann boundary condition as follows:

$$\partial T / \partial x_j = 0 \text{ and } \partial Y_i / \partial x_j = 0, \text{ for } i = 1, \dots, N.$$

where x_j is the direction normal to the outlet boundary.

4.11.3 Walls

A stationary wall with no-slip conditions was considered; the tangential velocity at the wall was explicitly set to zero. Thermal boundary condition at the walls were modeled as a mixture of convective and radiation heat transfer. Convective heat flux at the wall was selected, which requires a specification of heat transfer coefficient. Similarly, to account for radiation heat transfer, a specification of emissivity at the wall is required and computed.

At walls, a Neumann boundary condition is used for the turbulent kinetic energy, k , that is $\partial T / \partial \eta|_w = 0$.

4.12 Code Input and Output

4.12.1 Code Input

Code input includes:

1. Geometrical model – the first step in simulating combustion in STAR CCM+ code is to input the geometry of the burner. The code provides two ways of inputting the geometry, namely, importing a geometrical model prepared previously in a CAD package into the

code and direct creation of a geometrical model using 3D-CAD module within the code.

Fig. 4.6(a) shows a geometrical model details.

Figure 4.6: Illustration of details input in the code for (a) geometrical model and (b) mesh specification.

2. Mesh details specification and generation – the geometrical model is meshed by specifying the type, size and number of cells. An example of mesh details input in the code is shown in Fig. 4.6(b).
3. Physics model – the physics model defines the primary variables of the simulation such as temperature, pressure and velocity and the type of mathematical formulation to be used to generate the solution. In this work, the flow involves a turbulent, compressible, multiphase flow whose components are reacting chemically.
4. Material properties – material properties of the gas mixture and solid phase species that are to be input in the model are required. Method of determining dynamics viscosity

and thermal conductivity of the gas mixture as a whole is specified. Then the method of calculating specific heat for each gas component is set. An interface for material properties selection in the code is shown in Fig. 4.7(a).

Figure 4.7: Specification of material properties and reactions in a multiphase flow for (a) multi-component gas and (b) multi-component solid.

5. Reactions - reaction involves in both phases, gas-phase and solid-phase, are input in the model. The code has provision for specifying the reactants, products and rate constants for each reaction. Fig. 4.7(b) shows specification of the reaction for the solid phase components.
6. Initial conditions for species, temperature, turbulence and pressure are specified and input in the code.
7. The boundary conditions at the walls, inlet and outlet are defined and input in the code.
8. Solvers parameters such as type of the solver, URF, convergence criterion, order of accuracy are defined and input in the model.

4.12.2 Code Output

Code output includes:

1. Report – it defines the quantity of interest and the region where it is being monitored.
2. Monitor – it is use to dynamically monitor any quantity while the solution develops.
3. Plot – x-y graph plots are created for any quantity defined, for instance, temperature and CH₄ shown in Fig. 4.8. Plots may be exported as graphs or tabulated data.

Figure 4.8: x-y graph plots for temperature and CH₄ created in STAR CCM+ code.

4. Scene – allows the user to visualize the model. A scene is a summary of the complete representation of the components that are required to generates an image or animation including: lights, cameras, parts, properties, transformation, geometry and texture. An example of the scene is the image of grids shown in Fig. 4.5.

CHAPTER FIVE

NUMERICAL RESULTS

5.1 Introduction

In this chapter, numerical results of the three cases simulated in this study, viz., the effects of CO₂ environment on flame propagation speed and flames structures, the influence of particle packing density on combustion of wood in an oxy-fuel burning environment, and the separate effects of CO₂ in oxy-fuel combustion are presented. The chapter begins by a description of the boundary conditions applied for each case. The mesh independent tests which were done to ensure independency of results on the grid size are then presented. Finally, the numerical results are presented.

5.2 Boundary Conditions

Three cases were simulated in this study, namely, the effects of CO₂ environment on flame propagation speed and flames structures, the influence of particle packing density on combustion of wood in an oxy-fuel burning environment, and the separate effects of CO₂ in oxy-fuel combustion. In all the cases, the inlet boundary was at the bottom of the fixed bed. At this boundary, mass flow rate, species mole fraction and temperature were specified using Dirichlet boundary condition. The mass flux of the mixture at the inlet was 0.1 kg/m²/s while mass fraction of O₂ and N₂ or CO₂ were specified according to the case tested and was supplied at a temperature of 295 K. The mass fraction of O₂ and N₂ or CO₂ for each case are described here below.

For the numerical simulation of wood combustion in a fixed bed on the effect of CO₂ environment on flame propagation speed and flame structures, a summary of the composition of the oxidizer mixture is presented in Table 5.1.

Table 5.1: Composition of the oxidizer mixture for different oxy-fuel conditions.

Cases	Mixture 1		Mixture 2		Mixture 3		Mixture 4		Mixture 5	
	O ₂	N ₂	O ₂	CO ₂	O ₂	CO ₂	O ₂	CO ₂	O ₂	CO ₂
Concentration (% vol)	21	79	21	79	30	70	40	60	50	50

In the second case where the influence of particle packing density on fixed bed combustion of wood in an oxy-fuel burning environment is investigated, the oxidizer mixture constituted of 21% O₂ and 79% CO₂, by volume.

Finally, for the numerical simulation of the role of various carbon dioxide effects on the burning rate, the concentration of oxygen and N₂/CO₂/Ar were set in accordance to the required pre-designed conditions. In the first set of experiments, O₂ concentration by volume was varied between 21% and 50% with diluent as either N₂ or CO₂. In addition, four mixtures were designed to separate the effects of CO₂ environment. The four mixtures were denoted by letters A, B, C and D and their composition by volume were: 21% O₂/79% N₂; 21% O₂/22.5% CO₂/56.5% Ar; 40% O₂/60% CO₂; and 40% O₂/47% CO₂/13% Ar, respectively.

In all the cases, the outlet boundary was at the top of the fixed bed. At this boundary, species concentration and temperature gradients were set to zero using Neumann boundary condition. A stationary wall with no-slip conditions was considered; the tangential velocity at the wall was explicitly set to zero. Thermal boundary conditions at the wall was modeled as a mixture of convective and radiation heat transfer. Typical values of convective heat transfer coefficient for air in natural convection is 10 – 20 W/m².K, Incropera *et al.* (2006). Therefore, convective heat flux at the wall was selected with an adopted heat transfer coefficient of 10 W/m².K. An emissivity of 0.8 was adopted because the wall was made from stainless steel, Incropera *et al.* (2006).

5.3 Mesh Independent Tests

Computations were done on an unstructured grid that consisted of cells which were made of polyhedral elements. The cells closest to the walls were made of prism layers. Solutions which are independent of grid size were ensured by performing a mesh independent test. Consequently, the choice of mesh size was based on this test whose results are shown in Figs 5.1 – 5.4.

Figure 5.1: Comparison of temperatures profiles along axial length of the reactor for wood combustion in 21% O₂/79% CO₂ mixtures at (a) 450 s and (b) 600 s when applying different computational mesh sizes.

The prediction of temperature profiles along axial length of the reactor for oxy-fuel environment at two different times applying different computational mesh sizes are shown in Figs 5.1(a) and (b). In both cases, there was a significant change in results when mesh size was increased from 100,000 to 200,000 cells. But the predictions using 200,000, 300,000 and 400,000 cells did not have much differences. The prediction of tar mass fraction along axial length of the reactor at two different times applying different computational mesh is shown in Figs 5.2(a) and (b). The behaviour is similar to that of temperature predictions, i.e., there is a

significant change in prediction for 100,000 to 200,000 cells but there are no much differences for 200,000, 300,000 and 400,000 cells.

Figure 5.2: Comparison of tar mass fraction along axial length of the reactor for wood combustion in 21% O₂/79% CO₂ mixtures at (a) 450 s and (b) 600 s when applying different computational mesh sizes.

Temperature profiles along the axial length of the bed for combustion of fuel type WC and SD1 predicted using different mesh sizes is shown in Figs 5.3(a) and (b), respectively. In both fuel types, temperature predicted using a mesh size with 100,000 cells showed a significant difference from that predicted using a mesh size of 200,000 cells. However, changing of mesh size to 300,000 and 400,000 cells, respectively, did not significantly changed prediction when compared to that of 200,000 cells.

The predicted temperature profile at 5 cm from bed bottom under oxy-fuel condition is shown in Fig. 5.4. The graph show that the temperature is significantly different when using a mesh that consists of 100,000 cells as compared to that of 200,000 cells. The difference in temperature profiles is negligible for mesh that consist of 200,000, 300,000 and 400,000 cells, respectively. Therefore, a computational mesh with 200,000 cells was selected for all the cases computed.

Figure 5.3: Comparison of temperature profiles along the axial length of the bed for particle type (a) WC ($\chi = 0.51$) and (b) SD1 ($\chi = 0.74$) when reaction front is at 4 cm from the grate applying different computation mesh sizes.

Figure 5.4: Predicted temperature profiles at 5 cm from the bed bottom for wood combustion under oxy-fuel environment for different mesh sizes.

5.4 Results

Numerical results of mass loss history, temperature profiles, species concentration profiles, ignition times, burning rates and flame front propagation speed are presented. Fig. 5.5 shows

the mass loss history predicted by the model for spherical wood combustion in a fixed bed under both N_2 and CO_2 environments. The graph reveals that the rate of consumption of wood in a N_2 environment is faster than in a CO_2 environment. Consequently, the drying time, devolatilization time and char combustion time are relatively longer in a CO_2 environment. The low rate of consumption of wood particles in oxy-fuel environment is linked to higher molecular weight of CO_2 gas. O_2 diffusivity to the active surface of the particle in CO_2 gas is decreased because it is a heavy gas. Therefore, the rate of consumption of the fuel particle by oxidation is lowered in CO_2 than in N_2 environment.

Figure 5.5: Predicted mass loss history for wood combustion in fixed bed at 21% O_2 /79% N_2 and 21% O_2 /79% CO_2 mixtures.

Figure 5.6 shows the temperature profiles predicted by the model at various heights above the grate for different bed porosity; $\chi = 0.51$ to $\chi = 0.74$. Temperature profiles in low porosity

Figure 5.6: Predicted temperature profiles at various heights above the grate for particle types (a) WC ($\chi = 0.51$), (b) WCSD2 ($\chi = 0.56$), (c) SD2 ($\chi = 0.61$), (d) WCSD1 ($\chi = 0.68$) and (e) SD1 ($\chi = 0.74$).

beds, Figs 5.6(a) and (b), have two distinct peaks which are achieved during ignition propagation phase and char combustion phase, respectively. On the other hand, high porosity

beds, Figs 5.6(d) and (e) have a single temperature peak which indicates that devolatilization and char combustion phases occur concurrently. The transition from two temperature peak points to a single peak point occurs at a bed porosity of 0.61.

Concentration of major combustion species – tar, CO and H₂ – predicted by the model in the bed during the entire combustion time is shown in Fig. 5.7. The products of combustion, CO₂ and H₂O as well as O₂ predicted by the model are also shown in the graph. The species are plotted at 4 cm from the grate for wood combustion in 21% O₂/79% CO₂ mixture and a bed porosity of 0.51. At this location, the flame front passes at 410 s, devolatilization phase ends at 1210 s and char combustion phase ends at 1550 s.

Figure 5.7: Predicted species concentration and temperature during entire combustion time in 21% O₂/79% CO₂ taken at 4 cm from the grate for particle type WC ($\chi = 0.51$).

Flame structures along axial length of the bed for wood combustion in 21% O₂/79% N₂ and 21% O₂/79% CO₂ mixtures are shown in Figs 5.8 and 5.9, respectively. The flame front positions are clearly indicated by both graphs. For 21% O₂/79% N₂ mixture, the flame front

passes through (a) 5 cm point at 200 s, Fig. 5.8(a), (b) 4 cm point at 300 s, Fig. 5.8(b) and, (c) 3 cm point at 400 s Fig. 5.8(c). On the other hand, for 21% O₂/79% CO₂ mixture, the flame front passes through (a) 5 cm point at 300 s, Fig. 5.9(a), (b) 4 cm point at 450 s, Fig. 5.9(b) and, (c) 3 cm point at 600 s Fig. 5.9(c). The fuel bed is entirely under char combustion phase at 1000 s in 21% O₂/79% N₂ mixture, Fig. 5.8(d) and at 1100s in 21% O₂/79% CO₂ mixture, Fig. 5.9(d).

Figure 5.8: Predicted species and temperatures profiles along axial length of the reactor for wood combustion in 21% O₂/79% N₂ mixture at different times: (a) 200 s, (b) 300 s (c) 400 s and (d) 1000 s.

Figs 5.8 and 5.9 show that the flame front moves faster in N_2 environment than in CO_2 environment. This is associated to the higher heat capacity of CO_2 and low O_2 diffusivity in it. These two effects have negative impact on heating rate of the particle and consequently decreases the flame front movement.

Figure 5.9: Predicted species and temperatures profiles along axial length of the reactor for wood combustion in 21% O_2 /79% CO_2 mixture at different times: (a) 300 s, (b) 450 s (c) 600 s and (d) 1100 s.

Figure 5.10 shows ignition time predicted by the model for fixed bed combustion of wood in various O_2/N_2 and O_2/CO_2 mixtures. In both mixtures, ignition time is inversely proportional to the O_2 concentration. Under the same O_2 concentration, ignition time is higher in CO_2 environment than in a N_2 environment. CO_2 environment has low heating rates due to its higher heat capacity and low O_2 diffusivity. Therefore, it takes a longer time for the particle to release enough volatiles for ignition. The effect of bed porosity on ignition time is shown in Fig. 5.11. As bed porosity is increased ignition time decreases. However, beyond a porosity of 0.68, ignition time increases with increase in bed porosity. As bed porosity increases, more void spaces are available in the bed. Hence, there is excess O_2 in the bed. Therefore, there is quick oxidation of volatiles released from the particle, which decreases the ignition time. But beyond a porosity of 0.68, flame quenching due to excess CO_2 occurs and causes an increase in ignition time.

Figure 5.10: Predicted ignition time for fixed bed combustion of wood in N_2 and CO_2 environments.

Figure 5.11: Predicted ignition time for wood combustion under oxy-fuel condition for different initial bed porosity.

The flame front propagation speed predicted by the model for fixed bed combustion of wood in various O_2/N_2 and O_2/CO_2 mixtures are shown in Fig. 5.12. In both cases, the flame front propagation speed increases with increase in O_2 concentration. Under the same O_2 concentration, the flame front propagation speed is higher in a N_2 environment than in a CO_2 environment. This is associated to the retarded ignition time in CO_2 environment as noted in Fig. 5.10. In addition, the lower heating rates of the particles in CO_2 environment contribute to reduction in its flame speed. Fig. 5.13 presents numerical results of predicted flame front propagation speed with respect to bed porosity. The graph shows that the flame front propagation speed increases as bed porosity is increased up to an optimum point where it starts to decrease. The optimum point occurs at $\chi = 0.61$ in 21% $O_2/79\%$ N_2 mixture and at $\chi = 0.71$ in 21% $O_2/79\%$ CO_2 mixture.

Figure 5.12: Predicted flame front propagation speed for fixed bed combustion of wood in N_2 and CO_2 environments.

Figure 5.13: Measured and predicted flame front propagation speed for wood combustion in N_2 and CO_2 environments for different initial bed porosity.

Figure 5.14: Predicted burning rates for fixed bed combustion of wood in N₂ and CO₂ environments.

The burning rates predicted by the model for fixed bed combustion of wood in various O₂/N₂ and O₂/CO₂ mixtures are shown in Fig. 5.14. The burning rates are directly proportional to O₂ concentration. Under the same O₂ concentration, the burning rate is higher in a N₂ environment than in a CO₂ environment. The burning rate reduction observed in CO₂ environment could be attributed to its lower thermal diffusivity as compared to that of N₂, (Suda *et al.*, 2007). Furthermore, CO₂ absorb radiative heat more than N₂. The overall impact of these thermal properties of CO₂ gas is a decrease in burning rate.

CHAPTER SIX

CFD-DEM MODEL VALIDATION, RESULTS AND DISCUSSIONS

6.1 Introduction

This chapter presents CFD-DEM model validation results and discussions on the experimental and numerical study of wood conversion in a fixed bed under oxy-fuel environment. In the first section, CFD-DEM method and code validation are presented. Temperature distribution and species generation in the bed are discussed. The next section presents an investigation of wood combustion under oxy-fuel combustion environment using CFD-DEM numerical method. Effects of CO₂ combustion environment on mass loss history, flame propagation speed, flame fronts positions and flame structures are discussed. Results of the influence of packing of fuel particle and bed porosity on combustion of wood in a fixed bed under oxy-fuel environment are then presented and discussed. Temperature history, ignition time, wood and char conversion rates and reaction zone thickness are discussed in detail. The last section presents the role of various CO₂ effects on burning rate. The overall and individual contribution of various CO₂ effects on wood conversion processes are discussed.

6.2 CFD-DEM Method and Code Validation

In this section, numerical simulation of wood combustion in a laboratory-scaled fixed bed under air-fuel condition is presented. The main aim was to validate CFD-DEM approach in predicting temperature distribution and species generation in combustion of wood in a fixed bed.

6.2.1 Temperature Distribution

The model results were validated by comparing predicted and measured temperature at corresponding positions in the fuel bed. Shown in Fig. 6.1 is the temperature history at 5 cm from bed bottom. A good agreement between predicted and measured temperature values is

achieved. The graph shows that the temperature profile has two peaks; the first peak is about 1200 K while the second peak is about 1400 K. As the flame front passes the position where measurement is done, temperature rises rapidly up to the first peak. Then it gradually decreases to about 900 K where it starts to rise again. This phase of combustion is characterized by both exothermic and endothermic processes. Exothermic reactions of the volatiles increase the temperature while drying and pyrolysis which are endothermic processes decrease the temperature. The second part of the graph where temperature rises signifies the end of endothermic processes. The volatiles transported from lower part of the bed burn in this phase. The last regime where temperature decrease is characterized by char gasification and oxidation. Whereas char oxidation increases the temperature, char gasification with H_2O and CO_2 decreases the temperature. Overall decrease in temperature indicates that gasification is the dominant process in this regime.

Figure 6.1: Measured and predicted temperature profiles at 5 cm from fuel bottom for wood combustion at 21% O_2 /79% N_2 .

Presented in Fig. 6.2 are the gas-phase and particle surface temperatures at different times. The figures clearly reveal the movement of reaction front from top to bottom as combustion proceeds. Temperature distribution at the same cross section is non-uniform. Some particles have higher temperature than others located within the same height. Uneven distribution of temperature in the same height could be attributed to random packing in the bed, which causes variation of flow field at various points in the same cross section. This affects the conversion process of the particle in terms of the associated heat and mass transfer.

Initially, the bed is ignited at the top. During ignition, heat is absorbed by the particles in drying and pyrolysis which occur simultaneously. The bed temperature does not increase significantly as illustrated in Figs. 6.2(a) and 6.2(b). Once pyrolysis products are released, they react with O_2 and release more heat which increases the temperature, as shown in Fig. 6.2(c). Heat spreads to other particles by radiation, convection and conduction. As reaction front moves downward, more pyrolysis products are released. These products are not completely combusted at their point of production. Some are transported downstream (freeboard region) where they react and generate more heat which significantly increases the temperature, as shown in Figs. 6.2(d) and 6.2(e).

Movement of the reaction front from top to bottom results in devolatilization of all particles in fuel bed. As a result, the fuel bed slightly shrinks as shown in Fig. 6.2(f). The remaining biomass is now pure char which undergoes heterogeneous reactions with O_2 , H_2O and CO_2 . The overall temperature decreases because char reactions with H_2O and CO_2 are dominant in this phase and they are endothermic. It is also noted that in the vicinity of the grate, temperatures are lower than in the other region of the bed. The cause of this is convective cooling associated with incoming cold air.

Figure 6.2: Gas-phase and particle surface temperature distribution in the wood fuel bed burning at 21% O_2 /79% N_2 at different times.

6.2.2 Major Species Generation

Illustrated in Figs. 6.3 and 6.4 are the mass fraction distribution of the major combustible species of pyrolysis: tar and CO. Likewise to temperature distribution, the species mass fraction distribution at a given cross section is also non-uniform. Nonetheless, the flame front propagation is clearly depicted. Significant amount of tar and CO are produced in fuel bed from ignition up to about 750 s, as shown in Figs. 6.3 and 6.4. During this period, devolatilization is the dominant process. At 1000 s, Figs. 6.3 and 6.4, traces of the volatiles are noticeable in the bed. This indicates that at this time devolatilization is complete and the bed is undergoing char combustion.

Figure 6.3: Tar mass fraction distribution in the wood fuel bed burning at 21% O_2 /79% N_2 at different times.

Volatiles released from the bed burn within or outside the bed. As shown in Fig. 6.5, for the tested flow rate oxidant is high enough to oxidize all the volatiles. As flame front moves

downward, the amount of tar and CO released at its position decreases. This could be attributed to non-uniformity of flame front movement. Some particles at the same level get heated and pyrolyzed faster than others.

Figure 6.4: CO mass fraction distribution in the wood fuel bed burning at 21% O_2 /79% N_2 at different times.

Shown in Fig. 6.6 is water vapour (H_2O) mass fraction distribution in fuel bed. H_2O is a gaseous product arising from particle evaporation. It is also one of the pyrolysis product. In addition, H_2O in the bed is due to oxidation of CH_4 and H_2 . During initial stages of combustion, for instance ignition up to 300 s, most of H_2O is confined to fuel bed. This is because during this period H_2O is mostly from particle evaporation and pyrolysis. As combustion proceeds, e.g. from 400 s to 1000 s, H_2O generated in fuel bed is spread to freeboard region by convection. It is important to note that at this time, all the aforementioned sources participate in its production making it more pronounced than earlier stage. H_2O together with CO_2 are the main products of

combustion that radiate heat. As a result, its effects on temperature distribution is seen in Fig. 6.2.

Figure 6.5: O₂ mass fraction distribution in the wood fuel bed burning at 21% O₂/79% N₂ at different times.

Figure 6.6: H₂O mass fraction distribution in the wood fuel bed burning at 21% O₂/79% N₂ at different times.

Presented in Fig. 6.7 is mass fraction distribution of CO₂ in the burner. CO₂ is a product which arises from pyrolysis as well as oxidation of CO, CH₄ and char. Its production is also contributed to by tar cracking reactions. During initial stage of combustion, 100 s to 300 s, it is observed that CO₂ production is minimal and restricted to the fuel bed. CO₂ generation is more pronounced in the last stage of combustion, 750 s and 1000 s. This is char combustion stage where char is oxidized into CO and CO₂ which increases its amount in the burner.

Figure 6.7: CO₂ mass fraction distribution in the wood fuel bed burning at 21% O₂/79% N₂ at different times.

Flame structures at different positions from fuel bed bottom are presented in Figs. 6.8. The graphs show that in the freeboard region flame structures at different positions have similar profiles but differ in magnitude. Since the fixed bed that was tested was operated in batch mode under unsteady conditions, amount of heat released changed with respect to time. At 10 cm, intense heat is released between 170 s and 600 s, while at 15 cm it is at 200 s to 600 s. These

periods fall within devolatilization stage where volatiles transported to these positions react and generate heat. Temperature then decreases gradually until the end of combustion. During this time, heat present in these positions is by convection and radiation from fuel bed.

Figure 6.8: Major species and temperatures profiles at different position from fuel bed bottom for wood combustion at 21% O₂/79% N₂.

In summary, this section presented modeling of fixed bed combustion of wood using CFD-DEM approach. The modeling results were validated with measurement done in a laboratory-scaled fixed bed. A good agreement between model and experimental results were achieved. It was established that temperature profile at a given position in the bed has two peaks; the first peak is about 1200 K while the second peak is about 1400 K. Temperature distribution at the same cross section is non-uniform. Some particles have higher temperature than others located within the same height. Likewise, species mass fraction distribution at a given cross section is also non-uniform. Nonetheless, the flame front propagation is clearly depicted. In freeboard region, flame structures at different positions have similar profiles but differ in magnitude. Therefore, it was proven that CFD-DEM is a good tool in analysis of fixed bed furnace.

6.3 Flame Structure of Fixed-Bed Wood Combustion under Oxy-Fuel Conditions

This section presents an investigation of wood combustion in a laboratory-scaled fixed bed with an aim of establishing the effect of CO₂ environment on flame propagation speed and flame structures. Results show that flame front propagation speed in oxy-fuel atmosphere reduced to 78% of that of the air-fuel condition with similar O₂ concentration. This is attributed to the transport and thermodynamics properties of CO₂ gas as well as its chemical effects. For oxy-fuel conditions, propagation speed increased with increase in O₂ concentration. The CFD-DEM model agrees very well with experimental values for mass loss, propagation speed and flame front positions. However, peak temperatures are poorly predicted at lower oxygen concentrations. The accuracy of temperature prediction improves at higher oxygen concentrations. During initial and devolatilization stage, mass fraction of tar predicted in CO₂ environment are smaller than in N₂ environment, while the amount of CO predicted is almost equal in both environments. However, during char combustion stage a high amount of CO is observed in oxy-fuel conditions.

6.3.1 Mass Loss History

Validity of the model is checked by comparing mass loss history, peak temperatures and flame propagation speed obtained from simulations to corresponding experimental data. Shown in Fig. 6.9 is the mass loss history for wood combustion in 21% O₂ concentration under both N₂ and CO₂. The model agrees very well with experimental values. The curve for oxy-fuel condition is less steep with a longer devolatilization stage when compared with N₂ atmosphere. A slightly long char stage is also observed in CO₂ atmosphere. In overall, combustion of the same amount of wood takes a longer time for oxy-fuel condition than for air-fuel condition. This suggest a slow fuel consumption and burning rate in CO₂ atmosphere.

Figure 6.9: Mass loss history for wood combustion in fixed bed at 21% $O_2/79\%$ N_2 and 21% $O_2/79\%$ CO_2 mixtures.

Presented in Figs 6.10, 6.11 and 6.12 are temperature maps in the fuel bed at different times for different combustion atmospheres. The simulated and measured peak temperatures attained in the bed are compared in Fig. 6.13. Temperatures are poorly predicted at lower oxygen concentrations. The accuracy of prediction improves at higher oxygen concentrations. Temperatures corrected for radiation losses are also plotted in Fig. 6.13. Indeed, their agreement with predicted values are better than those of uncorrected values. Consequently, this emphasize the importance of considering radiation losses when validating a model.

It is important to note that after ignition, different conversion processes such as drying, devolatilization, char combustion and homogenous reactions takes place simultaneously at various heights of the bed. Since some processes are endothermic and others are exothermic, the temperatures at various regions are strongly dependent on the dominant process as discussed below. In the model used in this study, gaseous species released from biomass, depending on availability of oxidative species, either react within fuel bed or are transported to freeboard

region where they react and produce heat. For all the cases studied, it is observed that during initial stages of combustion, freeboard temperatures are almost equal to bed temperatures. For 21% O₂ concentration, the period extended up to 300 s, Fig. 6.10, and 450 s, Fig. 6.11, for N₂ and CO₂ environments, respectively. As O₂ concentration is increased in oxy-fuel condition, the period reduces from 450 s to 300 s, Fig. 6.12. During this stage, heat release by homogeneous reactions is absorbed by downstream particles which are still undergoing devolatilization. At the same time, immediate upstream particles take up heat for drying.

Figure 6.10: Temperature distribution in the wood fuel bed burning at 21% O₂/79% N₂ at different times.

As combustion progresses downward which is clearly depicted by propagation of reaction front, for example, between 400 -750 s, in Figs 6.10, 6.12, and 600 - 950 s, in Fig. 6.11, more volatiles are released. During this period, freeboard temperatures are higher than bed temperatures. At this time, particles adjacent to freeboard have probably completely undergone endothermic

processes (drying and devolatilization). In addition, these particles are in char combustion stage which releases more heat. Heat released from homogeneous reaction and char combustion is transported from bed to freeboard by convection of combustion products which are dominated by H_2O and CO_2 .

Figure 6.11: Temperature distribution in the wood fuel bed burning at 21% O_2 /79% CO_2 at different times.

After some time, reaction front reaches the bottom of the reactor and, at this point, all volatiles have been released. After this point, combustion in the bed is dominated by char combustion, for example, at 1000 s of Figs 6.10, 6.12 and 1100 s in Fig. 6.11. Freeboard temperatures decrease during this period. This is because homogeneous reactions which release intense heat is almost complete.

Figure 6.12: Temperature distribution in the wood fuel bed burning at 30% O₂/70% CO₂ at different times.

Figure 6.13: Predicted and measured peak temperatures in the wood fuel bed burning at different CO₂ atmospheres.

Even though the temperature distribution in fuel bed under both conditions exhibit the same behavior, the magnitudes are different. At 21% O₂ concentration, air-fuel has a peak temperature of 1497 K while oxy-fuel has 1388 K. As shown in Fig. 6.13, as O₂ concentration is increased, temperature also increases. A value of temperature close to that of 21% O₂/79% N₂ mixture is achieved at around 30% O₂/70% CO₂ mixture. Low values of temperatures in oxy-fuel conditions are associated with higher specific heat capacity of CO₂ gas than that of N₂ gas. This applies for all the temperatures above 650 K where specific heat capacity of CO₂ gas is higher than that of N₂ gas.

6.3.2 Flame Front Propagation Speed

The flame front propagation speed is estimated from distance and time data of temperature measuring points (Sakthivadivel & Iniyan, 2018). For both experiment and model, flame front passes through a point when there is an abrupt increase in temperature from ambient value to a peak value (Ryu *et al.*, 2006). The exact position of predicted and measured reaction front for wood combustion in 21% O₂ concentration under both N₂ and CO₂ is shown in Fig. 6.14. For air-fuel conditions at 21% O₂ concentration, a higher value of flame speed is observed. In general, propagation speed for air-fuel condition reported in literature (Dasappa & Paul, 2001; Yang, Ryu, Khor, Yates, *et al.*, 2005), are higher than those observed in oxy-fuel conditions of the current study. However direct comparison cannot be done because flame front propagation speed is dependent on several factors such as air mass flux, fuel properties, particles size, reactor operation mode, et cetera. Flame front speed have been shown (Dasappa & Paul, 2001; Mahapatra *et al.*, 2016; Ryu *et al.*, 2006; Sakthivadivel & Iniyan, 2018) to increase with increase in air mass flux up to a peak point where it starts to decrease. Mahapatra *et al.* (2016) reported a peak value of 0.089 mm/s for air flow rate of 0.132 kg/m²/s and casuarina wood as

fuel. While studying char combustion in a packed bed, Dasappa & Paul (2001) reported a peak value of 0.30 mm/s for air mass flux of 0.1 kg/m²/s. Yang, Ryu, Khor, Yates, *et al.* (2005) showed that flame speed decreased from 0.24 mm/s for 10 mm sized particles to 0.21 mm/s for 35 mm sized particles. In a recent study, Sakthivadivel & Iniyan (2018) obtained a flame speed of about 0.05 - 0.07 mm/s for different fuels tested in air-fuel environment.

Figure 6.14: Predicted and measured flame front position for wood combustion in fixed bed at 21% O₂/79% N₂ and 21% O₂/79% CO₂ mixtures. Fuel bed top is taken as datum.

In order to have a proper comparison, investigation of flame propagation speed for the same wood fuel with the same particle size burning in air-fuel conditions was conducted. Fig. 6.14 shows that the gradient (propagation speed) is steeper in N₂ environment than in CO₂ environment. Indeed, it is observed that flame speed in oxy-fuel atmosphere reduced to 76% (model) and 78% (experiment) of that of the air-fuel condition with similar O₂ concentration. It is also noted that ignition delay is longer in CO₂ environment. Reduction in speed could be attributed to transport and thermodynamic properties of CO₂ gas and chemical effects associated with it. The chemical reactions involving consumption of CO₂ include reverse water

gas shift reaction R(14) and Bourdoudard reaction R(16). The reaction rates of both reactions are several orders of magnitude smaller than those of homogeneous reactions R(6)-R(13). Therefore, their contribution to flame speed is quite small. On the other hand, CO₂ gas has a higher specific heat capacity than N₂ gas (1.5 times higher than that of N₂). In addition, CO₂ is a heavy gas and O₂ diffusivity in it is lower. Consequently, the overall effect is reduction of temperature and heating rates of fuel particles. Thus a reduced flame speed is observed in CO₂ environment. It is also noted that mass fraction of combustible volatiles released in CO₂ environment are smaller. This also contribute to reduction in flame speed and is discussed in subsequent paragraphs.

Figure 6.15: Predicted and measured flame front propagation speed in the wood fuel bed burning at different CO₂ atmospheres.

Shown in Fig. 6.15 are plots of flame front propagation speed in fuel bed operated at different oxy-fuel conditions. The curves show good agreement between the predicted and measured values. Flame speed increased from 0.06 mm/s at 21% O₂/79% CO₂ to 0.21 mm/s at 50% O₂/50% CO₂. As O₂ concentration is increased, gas mixture properties also change. This means

a reduced portion of CO_2 in which O_2 diffusivity is improved. As a result, an increase in temperature is seen (Fig. 6.13) and also heating rates of particles is increased. Hence, the flame speed also increases.

6.3.3 Species Generation under Oxy-Fuel Conditions

Presented in Figs 6.16-6.19 are the flames structures of wood combustion in both environments at different combustion stages. The main species mass fraction and temperature profiles at a given time are plotted against axial length of the reactor. Fig. 6.16 illustrates flame structures in oxy-fuel and air-fuel conditions when reaction front is at 5 cm from the bottom of reactor. Because each case has a different flame speed it occurs at different times: at 200 s in 79% N_2 , Fig. 6.16(a); and 70% CO_2 , Fig. 6.16(c); and at 300 s in 79% CO_2 , Fig. 6.16(b). In all the cases, reaction zone covers a region of depth between 4 cm to 7 cm. The particles within this region are mainly undergoing drying and pyrolysis. Homogeneous reactions of pyrolysis products, tar, CO , CH_4 , H_2 , with O_2 are exothermic. It is observed that gaseous species react within the fuel bed and are also transported to freeboard region. Some of the heat released is absorbed by particles because pyrolysis is an endothermic reaction while the remaining amount is convected to freeboard region. Although the flame structures depict similar profiles, the magnitude of species and temperature are different. Highest amounts of tar and steam are observed in 79% N_2 environment while lowest amounts of these species are seen in 79% CO_2 environment. The amount of CO is almost equal in all the 3 cases. The high amount of tar and steam in 79% N_2 environment is attributed to high temperature which enhance pyrolysis process. Low amount of tar in oxy-fuel condition affirms the influence on flame propagation speed.

Figure 6.16: Species and temperatures profiles along axial length of the reactor for wood combustion in O_2/N_2 and O_2/CO_2 mixtures when reaction front is at 5 cm from fuel bottom: (a) 79% N_2 at 200 s, (b) 79% CO_2 at 300 s and (c) 70% CO_2 at 200 s.

As the flame front propagates downward, the positions of the peak values of species also change, Figs. 6.17 and 6.18. The position where peak temperatures occur, however, remain just approximately at the fixed bed top. This is because particles in this region have completed pyrolysis process and no longer absorb heat released by homogeneous reactions. Furthermore, at this stage, the heat transfer through convection is high enough to raise the exit temperature.

Figure 6.17: Species and temperatures profiles along axial length of the reactor for wood combustion in O₂/N₂ and O₂/CO₂ mixtures when reaction front is at 4 cm from fuel bottom (a) 79% N₂ at 300 s, (b) 79% CO₂ at 450 s and (c) 70% CO₂ at 300 s.

Very low amounts of tar and CO and high amounts of CO₂ and H₂O in this region reflect an increase in consumption rate of volatiles. For oxy-fuel cases, the amount of CO₂ from combustion adds to the supplied amount and hence dominates the combustion products, Figs 6.17(b) and 6.17(c). Just like in the initial stage, flame front in CO₂ environment arrives at 4 cm, Fig. 6.17(b), and 3 cm, Fig. 6.18(b), later than in air-fuel condition. For the flow condition

tested, tar and CO are completely consumed within the fuel bed. As seen in the figures, O_2 is sufficient for complete oxidation of these species. The amount of tar and CO at reaction front decreases as it moves downward, Fig. 6.18. As shown in Figs 6.18(a)-(c), the mass fraction of these species are almost equal in the three cases.

Figure 6.18: Species and temperatures profiles along axial length of the reactor for wood combustion in O_2/N_2 and O_2/CO_2 mixtures when reaction front is at 3 cm from fuel bottom: (a) 79% N_2 at 400 s, (b) 79% CO_2 at 600 s and (c) 70% CO_2 at 400 s.

Figure 6.19: Species and temperatures profiles along axial length of the reactor for wood combustion in O_2/N_2 and O_2/CO_2 mixtures during char combustion stage: (a) 79% N_2 at 1000 s, (b) 79% CO_2 at 1100 s and (c) 70% CO_2 at 1000 s.

After the flame front reaches the bottom of the bed, the fuel bed is completely in char combustion stage. Major species generation and temperature profiles during this stage, for each of the three cases, are shown in Fig. 6.19. Absence of tar indicates that devolatilization stage has ended. As in the previous combustion stages, it is also noted that this stage occurs at a later time in CO_2 environment than in N_2 environment. Temperatures in the bed are relatively lower

than in the previous combustion stages. As expected, temperatures in oxy-fuel conditions, Figs 6.19(b) and (c), are lower than that in air-fuel case, Fig. 6.19(a). Low temperatures in all cases are attributed to absence of homogeneous reactions of volatiles which reduces rate of heat release. The only heat release is in char and CO oxidation. In addition, char gasification with CO_2 and H_2O is an endothermic reaction. Moreover, heat is lost by convective heat transfer to freeboard region. Because of cold air inlet, cooling effect results in relatively low temperatures in the grate. For char combustion stage, char is converted to CO and CO_2 . A high amount of CO is observed in oxy-fuel condition which is as a result of gasification of char in the CO_2 environment.

In this section, a comprehensive study of the effect of CO_2 combustion atmosphere on flame propagation speed and flame structures in wood combustion in a laboratory-scaled fixed bed operated under counter-current mode was presented in this section. CFD-DEM approach was used to simulate wood conversion in a packed bed and the results compared to experimental data. Computational results agree very well with experimental values except temperature which showed poor prediction at low O_2 concentration. For mass loss history and flame propagation speed, the deviation of most of the model data from experimental data were less than 10%. The agreement of temperatures corrected for radiation losses with predicted values are better than those of uncorrected values. Hence, it was established that prediction accuracy of CFD-DEM is not the same in different O_2/CO_2 mixtures. Furthermore, it was observed that flame speed in oxy-fuel atmosphere reduced to 78% of that of the air-fuel condition with same O_2 concentration. This was determined both by experiment and through computation. Reduced flame speed was attributed to a higher heat capacity of CO_2 and lower O_2 diffusivity in CO_2 whose overall effect is reduction of temperature and heating rates of fuel particles. Low mass

fraction of combustible volatiles predicted in the CO₂ environment also contribute to a reduced flame speed. Flame structures have similar profiles but differ in value of temperature and species quantities. As expected, temperatures in the CO₂ environments were lower than those in the N₂ environments. During initial stages of combustion, the amount of tar and steam is observed to be highest in 79% N₂ environment and lowest in 79% CO₂ environment, as shown in Fig. 6.16. The amount of CO was almost equal in both environments during pyrolysis, $Y_{CO} \approx 0.05$ as shown in Fig. 6.16, but high amounts were predicted in oxy-fuel environments during char combustion stage, as shown in Fig. 6.19.

6.4 Particle Packing Density

Presented in this section is an investigation of the impact of particle packing density on fixed bed combustion of wood in an oxy-fuel burning environment. The packing density, which determines the region porosity, is influenced by fuels' geometry. Size and shape were determined directly from fuel particles and used to evaluate the particle sphericity which is an input in the computational model. Euler-Lagrange method was used to model conversion of wood in a fixed bed. A comprehensive analysis of wood conversion in terms of temperature profiles, gas species generation and conversion rates in the entire possible operation range of bed porosity were investigated. Furthermore, the computational model was validated by performing experiments in a fixed bed using wood of different shapes and sizes, viz., fixed bed of different porosity. It was established that the packing density affects combustion process in an oxy-fuel environment by changing the burning conditions and limits. The operational range with respect to porosity was decreased in an oxy-fuel burning condition due to higher quenching effects of CO₂. Furthermore, the study revealed that there is an optimum packing density, $\chi = 0.71$, beyond which the efficiency falls due to the onset of quenching in the spaces.

6.4.1 Temperature History

The CFD-DEM model results were validated by data obtained from experiment. Fig. 6.20 presents a validation of temperatures at various heights in the bed for different fuel particle types. In general, deviations of 10% or less between the model and measured data indicate a good agreement. Particle type WC, WCSD2 have two distinct temperature peaks, Figs 6.20(a)-(b), while particle type WCSD1 and SD1 have a single temperature peak, Figs 6.20(d) and (e). Particle type SD2 is a transition case with a distinct first temperature peak and the temperature plateaus off in the second peak, Fig. 6.20(c). The first peak is attained during ignition front propagation phase while the second peak is attained during char oxidation phase (Khor *et al.*, 2007). Figs 6.20(a)-(b) indicate that less porous beds have substantial amount of char remaining in the bed after devolatilization. The char combustion phase peak temperatures for these fuel particle types are higher than ignition front propagation phase peak temperatures. In particle type SD2, some of the char produced are oxidized in the first peak region leading to a higher flame temperature being attained. Subsequently, its second peak region has a low temperature value. In case of porous beds, Figs 6.20(d) and (e), they have a single peak temperature point with relatively higher values than those for the first peaks of the less porous beds. It is also observed that in all the fuel particles investigated the bed temperatures are relatively less than those for air-fuel environment in comparable burning conditions as discussed in section 6.5. Temperature in a O₂/CO₂ mixture is reduced by its higher heat capacity.

6.4.2 Ignition Time

Presented in Fig. 6.21 is the ignition time for the different fuel particles. Bed ignition time was considered to be the time in which the reaction front takes to start at the top surface of the bed. Ignition time decreases with increase in initial bed porosity. For the entire range, the

Figure 6.20: Measured and predicted temperature profiles at various heights above the grate for particle types (a) WC ($\chi = 0.51$), (b) WCSD2 ($\chi = 0.56$), (c) SD2 ($\chi = 0.61$), (d) WCSD1 ($\chi = 0.68$) and (e) SD1 ($\chi = 0.74$).

ignition time values are higher than those reported for wood combustion under N_2 environment in the same conditions, as seen later in section 6.5. Higher ignition time in CO_2 environment could be due to its decreased flame temperature and heating rates. Furthermore, chemical reactions of CO_2 through reactions R(14) and gasification of char, R(16), contribute to retardation of ignition time. Reaction R(16) is endothermic and results in decreasing the amount of heat in the bed. Consequently, it increases the ignition time delay in the fuels.

Figure 6.21: Measured and predicted ignition time for wood combustion under oxy-fuel condition for different initial bed porosity. Error bars are the standard deviations.

The impact of porosity on air to fuel stoichiometry and flame front propagation speed is presented in Fig. 6.22. The values are compared to those obtained in N_2 environment under similar operating conditions. The equivalence ratio presented are the averaged values based on the total combustion time, fuel chemical composition and air flow rates. The actual equivalence ratio varies at different combustion stages as noted later in the analysis of gas species generation in the bed: It is higher during pyrolysis phase and lower during char consumption phase. For

both cases, flame front propagation speed increases with increases in bed porosity. It is correspondingly lower in CO₂ environment.

Figure 6.22: Measured and predicted flame front propagation speed for wood combustion in N₂ and CO₂ environments for different initial bed porosity. Error bars are the standard deviations.

Figure 6.22 also shows that as bed porosity is increased the burning condition is shifted from fuel-rich to fuel-lean side. Under the same air flow rate and O₂ volumetric concentration, this shift is more toward the porous region in a O₂/CO₂ mixture than in a O₂/N₂ mixture as a result of differences in molecular weight. Furthermore, as noted in the flame front propagation speed, the operational range with respect to porosity is narrowed in a CO₂ environment. This is due to its high heat capacity which causes earlier quenching effects than in N₂ environment.

6.4.3 Wood Conversion and Char Formation Rates

Drying, pyrolysis, homogeneous reactions and char conversion in the bed occurs simultaneously. Overlapping of these processes depends on the burning conditions. Dry wood particles with the same amount of mass initially located at 4 cm from the grate for different particle types were tracked in order to monitor their conversion progression. Fig. 6.23(a) presents the conversion of these particles in the bed with respect to time. The mass of dry wood remains constant until the onset of pyrolysis. Amongst the cases investigated, the onset of pyrolysis in particle type WCSD1 occurred at 180 s, which is earlier than any other particle. Pyrolysis in particle type WC started to occur at 390 s and took longer a time to complete, 1110 s. This indicate that as porosity of the bed is increased, pyrolysis process takes a shorter time. Though it is observed that there is an optimum point at which pyrolysis times begins to increase even with increase in porosity. This optimum point occurs when porosity is about 0.71. This is as a result of combustion conditions becoming too lean and the flame starts to be quenched by excess CO₂ through convection cooling.

Figure 6.23: Predicted (a) wood conversion and (b) char formation of the particles with the same amount of mass initially located at 4 cm from the grate for different fuel particle types.

The amount of char produced in the bed decreases with increase in porosity, Fig. 6.23(b). Higher amount of char in less porous bed indeed confirms the second peak temperatures attained in these particle types seen in Figs 6.20(a)-(b), which arise from combustion of char that is left in the bed after devolatilization. Char, which is in essence carbon, is produced and consumed within a shorter period of time as bed porosity increases. The amount of char presented in Fig. 6.23(b) is the net amount at a given time for particle tracked. Char is produced from pyrolysis of dry wood through reaction R(4). Once it is produced, it is consumed through reactions R(15)-R(17) depending on bed temperature and availability of O₂, CO₂ and H₂O.

The actual rates for conversion of dry wood particles are presented in Fig. 6.24(a). Particle type WCSD1 and WC attained the fastest and slowest pyrolysis rate of 4.78 and 2.13 kg m⁻³ s⁻¹, respectively. The trend of influence of porosity is similar to what was observed before; pyrolysis rate increases with increase in porosity up to the optimum point, 0.71, where it starts to decrease. As porosity is increased, there is a quick release of volatiles. Oxidation of combustible volatiles through reaction R(6)-R(10) releases intense heat which increases the conversion rate. Since the conversion processes are fast, ignition is quick and flame propagation is also fast as noted in Figs 6.21 and 6.22, respectively. In low porosity beds, volatiles are slowly released, heating rate is low and consequently, a slow conversion rate. Subsequently, low porosity beds have higher ignition time and low flame front propagation speed. Net char formation and consumption for the particles with respect to time are presented in Fig. 6.24(b). Just like wood pyrolysis rate, net char formation rates, positive values, increases as porosity is increased up to an optimum value, then it starts to decrease. However, the net consumption rates, negative values, have no optimum value. Particle type WC, WCSD2 and SD2 attained almost the same peak consumption rates. Char consumption rate is directly proportional to the

char specific surface area, $S_{a,char}$ as indicated in reactions R(15)-R(17). Thus, the high specific surface area for char in porous bed increases their consumption.

Figure 6.24: Predicted rate of (a) wood conversion and (b) char formation of the particles with the same amount of mass initially located at 4 cm from the grate for different fuel particle types.

6.4.4 Flames Structures

Gas species concentration and temperature predicted during entire conversion of wood at a particular height is shown in Fig. 6.25. The values presented are taken at 4 cm from the grate for different particle types. The figures clearly depict the three distinct stages of wood combustion; drying, pyrolysis and char consumption. In all the cases, drying starts when the temperature reaches about 50 °C, as evident in the drying front which is always slightly ahead of the ignition front. The decrease in CO_2 mole fraction at the onset of drying is due to introduction of water vapour in the bed and should not be viewed as a consumption. The absolute amount of CO_2 only changes in the reaction zone as it is a product of oxidation of char and volatiles which contain carbon in their molecular structure. Alternatively, its amount may change through its participation in gasification of char, through reaction R(16) and in the forward and backward reactions of H_2O and CO , in R(13) and R(14).

Figure 6.25: Predicted species concentration and temperature during entire combustion time taken at 4 cm from the grate for particle types (a) WC ($\chi = 0.51$), (b) WCS2D ($\chi = 0.56$), (c) SD2 ($\chi = 0.61$), (d) WCS2D1 ($\chi = 0.68$) and (e) SD1 ($\chi = 0.74$).

During pyrolysis, particles at a local point absorb heat energy from oxidation of volatiles released by adjacent particles located in the upper side through radiation and conduction. Once

the particle attains devolatilization temperature, then the volatiles are rapidly released. Combustible volatiles, are oxidized through reactions R(5)-R(10) releasing intense heat which rapidly increases the temperature to the first peak point, as seen in Fig. 6.25 for all the cases. During this period, O_2 decreases gradually but does not go to zero immediately. Under the same oxidizer mixture mass flux as used in this study, the extent to which O_2 concentration falls depends on the bed porosity. For particle type WC and WCSD2, Figs 6.25(a) and (b), as pyrolysis progresses downward, the volatiles release at the lower part of the bed consume all the O_2 . Consequently, O_2 is not able to reach the upper region. Since the wood fuels in this region are still undergoing pyrolysis, which is endothermic, the local temperature decreases. During this time, volatiles in upper region are not oxidized and their concentration remains almost constant. Similarly, char produced is not oxidized during this time. For this particle types, during devolatilization time, char is only consumed by gasification H_2O and CO_2 . As a result, the amount of char is higher than for SD1, SD2 and WCSD1, as observed in Fig. 6.23(b).

Once the entire bed is completely pyrolyzed, volatiles in the lower region are the first to be completely oxidized since O_2 is supplied from the bottom. This is evident in the steep increase in temperature of thermocouple located close to grate, Figs 6.20(a) and (b). After complete oxidation of volatiles in the lower region of the bed, excess O_2 is convected upward. The volatiles remaining in the bed are oxidized progressively from bottom to the top, as depicted in steep temperature rise at the end of devolatilization stage in Figs 6.20(a) and (b). At a given height, CO_2 concentration sharply increases at the end of devolatilization stage. This is partly due to oxidation of CH_4 , CO and tar. Its increase is also caused by depletion of other species through complete oxidation. Complete oxidation of volatiles end at 1200 s and 860 s for particle type WC and WCSD2, respectively, Figs 6.25(a) and (b). After this point, there is excess O_2 in

the bed and char oxidation through reaction R(15) starts. Concurrently, char is consumed by CO_2 through Boudouard reaction R(16). In overall, the amount of CO_2 decreases while that of CO increases. Finally, CO is completely oxidized to CO_2 toward the end of char combustion.

Pyrolysis and char consumption in particle types SD2, WCSD1 and SD1 proceed in almost a similar way. They all operate under lean conditions throughout conversion process as depicted by excess O_2 in their reaction zones, Figs 6.25(c)-(e). As a result, oxidation of volatiles continues in the upper part of the bed as pyrolysis progresses downwards. This is evident in the low concentration of tar, CH_4 , H_2 and CO in these particles as compared to those of particle types WC and WCSD2. In addition, char is oxidized concurrently with volatiles. This explains the high temperatures in the first peak of the porous fuels seen in Figs 6.20(c)-(e). The low amount of char in the porous bed noted in Fig. 6.23(b) is also accounted for by this fact. For particle types SD1 and WCSD1, the heat release from oxidation of the char remaining in the bed after complete devolatilization is not sufficient to raise the temperature to a second peak, Figs 6.25(d) and (e). However, particle type SD2 still has a substantial amount of char whose oxidation is sufficient to increase the temperature to a second peak. Though it is not as high as for particle types WCSD2 and WC1.

Flame structures along axial length of the bed for different particle types when the reaction front is at 4 cm from the grate are presented in Fig. 6.26. The graphs clearly illustrate the thickness of the reaction front for various fuel particles. Thickness of the reaction front was considered to be the axial length in the bed in which the temperature changes from ambient value to maximum as flame front passes (Yang *et al.*, 2003). It is affected by several factors which include burning rates, flame front propagation speed and fuel particle size. In general, it was observed that reaction front thickness increases as porosity increases; the lowest and

highest values being 21 mm and 35 mm for particle types WC and SD1, respectively. Thin reaction front indicates that the particles at a given height burn uniformly. For this case, higher amounts of volatiles are present at a given height, Figs 6.26(a)-(c). On the other hand, a thicker reaction front as seen in Figs 6.26(d) and (e) is associated with a high flame front propagation speed, high burning rates and fast pyrolysis. In this case, fuel particles at a lower region start releasing small amount of volatiles which are immediately oxidized. Consequently, the amounts of volatiles are not as high as for cases with thin reaction front thickness. Furthermore, radiation energy in less porous beds have short penetration into fuel particles in unreacted region. Therefore, their flame front propagation moves slowly as seen in Fig. 6.22, and the reaction zone is thin. This is opposite to porous bed which allows deep penetration of radiation energy to unreacted particles in the lower part of the bed making them to have high flame front propagation speed and a thicker reaction zone.

Volatiles released when the reaction front is at 4 cm from the grate, for all the cases, are not completely oxidized in the fuel bed, Fig. 6.26. Unreacted volatiles do not stay in the bed but instead, they are transported to freeboard region, height above 6 cm, where they are reacted as indicated by their decreasing levels. Unlike in the bed region, there are no endothermic processes, pyrolysis and gasification, in freeboard region. Therefore, oxidation of volatiles results in higher freeboard temperature in all the cases. It is noted that for fuels with thick reaction zone thickness, Figs 6.26(c)-(e), H_2 is the dominant volatile in the low temperature region of about 300 to 800 K. A high amount of H_2 in these fuels is as a result of reaction R(13). This is supported by low amount of CO in this region. Furthermore, this reaction has been reported to have better prediction and works well in fuel lean conditions under which these fuels were operated (Andersen *et al.*, 2009; Jones & Lindstedt, 1988).

Figure 6.26: Predicted major species concentration and temperature along axial length of the bed for particle types (a) WC ($\chi = 0.51$), (b) WCSD2 ($\chi = 0.56$), (c) SD2 ($\chi = 0.61$), (d) WCSD1 ($\chi = 0.68$) and (e) SD1 ($\chi = 0.74$) when the reaction front is at 4 cm from the grate.

Presented in Fig. 6.27 is the predicted peak values of major combustible species concentration at fuel bed top for different fuel types during entire combustion time. It is important to determine the amount of volatiles that exit the top of the fuel bed as it indicates the extent to which they

are oxidized inside the bed. A secondary air supply is required for cases where a large amount of combustible volatile is exiting the top of the bed. The air is supplied at the freeboard region for complete oxidation of these volatiles. Alternatively, a proper mixing

Figure 6.27: Predicted peak values of major combustible species concentration at fuel bed top for different fuel types during entire combustion time.

of these volatiles and the air is required in the freeboard region for complete combustion. Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for different fuel types burning under oxy-fuel condition are presented in Table E.1-E.5 in Appendix E.1. The tables show that the amount of CH₄, H₂, CO and tar decrease as initial bed porosity is increased. The amount in the top of the fuel bed were in the range of 0.006–0.011, 0.045–0.069, 0.048–0.106 and 0.0167–0.0313 for CH₄, H₂, CO and tar, respectively. The decrease is high for CO while it is low for CH₄, H₂ and tar. CH₄, H₂ and tar are produced solely from devolatilization of dry wood while CO is a product of both

devolatilization, oxidation of tar through reaction R(9) and char gasification with CO_2 through reaction R(16). Therefore, the behaviour of the former three species in the bed are expected to follow a similar trend. As noted earlier, less porous bed operates under fuel-rich conditions and therefore have high amount of unburned hydrocarbons. On the other hand, a porous bed operates under fuel-lean condition and subsequently have low amount of unburnt volatiles. For the operation conditions presented in this study, a well-designed combustion chamber with a secondary air supply is required in order to complete the oxidation of unburnt hydrocarbon.

In this section, CFD-DEM model was used to comprehensively study the influence of particle packing density and bed porosity on wood conversion in the fixed bed in the entire possible operation range. The model was validated in the initial bed porosity range of 0.50-0.75. A good agreement was achieved between the model and experiment with most points having deviations which were less than 10%. It was established that porous bed shift combustion stoichiometry towards fuel-lean conditions, which is more in CO_2 environment than in N_2 environment. Less porous bed operates in fuel-rich conditions. Consequently, their conversion rates are slow. As a result, they have high ignition time, slow flame front propagation speed and thin reaction zone thickness. In addition, char amount is not oxidized during pyrolysis stage due to O_2 deficit. A substantial amount of char is oxidized in the char combustion stage leading to two peak temperature points. On the other hand, for very porous beds, char and volatiles are concurrently oxidized during pyrolysis stage due to excess O_2 . Therefore, they have a single peak temperature point with relatively higher values than those for the first peaks of the less porous bed. They also have fast conversion processes, which quicken ignition, increase flame front propagation and thicken reaction zones. Furthermore, it

was established that the operation range is narrower in CO₂ environment than in N₂ environment.

6.5 Chemical, Thermal and Dilution Effects of Carbon Dioxide

This section presents an experimental and numerical modeling of eucalyptus wood combustion under oxy-fuel conditions using a fixed bed reactor. The main objective was to isolate the role of various carbon dioxide effects on the burning rate. Wood combustion was numerically simulated under four different mixtures of O₂ and Ar/CO₂/N₂: 21% O₂/79% N₂; 21% O₂/22.5% CO₂/56.5% Ar; 40% O₂/60% CO₂; and 40% O₂/47% CO₂/13% Ar. The first three mixtures were designed to have the same peak temperatures in order to isolate chemical and dilution effects of CO₂. This was achieved by substituting some percentage of CO₂ with Ar in O₂/CO₂ mixture while maintaining a constant concentration of O₂. The fourth mixture had a higher peak temperature which was meant to isolate the thermal effect of CO₂. The accuracy of model data was good with deviation of most points from measured values being within 10%. It was found that ignition time in CO₂ environment decreases gradually as O₂ concentration is increased. On the other hand, burning rate and flame front speed increase as O₂ concentration is increased. Furthermore, it was established that dilution effect is the most influential parameter on the burning rate of wood combustion in an oxy-fuel system.

6.5.1 Overall Effect of CO₂ on Wood Conversion Processes

The overall contribution of the various effects of CO₂, namely, chemical, thermal and oxygen concentration are evaluated through CFD-DEM modeling. The model results are validated by comparing them with experimental values. Shown in Fig. 6.28 are measured and predicted temperature profiles at 5 cm from bed bottom for air-fuel and oxy-fuel environments both at 21%

O₂ concentration. The accuracy of model data was good with deviation of most points from measured values being within 10%.

Figure 6.28: Measured and predicted temperature profiles at 5 cm from the bed bottom for wood combustion in 21% O₂/79% N₂ and 21% O₂/79% CO₂ mixtures.

Figure 6.28 show that the temperature profile at any given height in both N₂ and CO₂ environments exhibit similar behavior. They all have two peaks. When the flame front reaches an ignition point, the temperature rises rapidly up to the first peak. Then it decreases gradually to another point and finally rises to the second peak. Combustible pyrolysis products such as CH₄, tar, H₂ and CO are oxidized through exothermic reactions which generate heat and subsequently increases the temperature. The exothermic reactions occur concurrently with pyrolysis and drying of wood particles which are endothermic reactions and cause decrease in temperature after the first peak. When pyrolysis and drying processes are completed, exothermic reactions dominate and temperature rises again to the second peak. After the second peak, the temperature gradually decreases until the end of combustion. During this phase, a wood particle has completely been

devolatilized leaving a pure char that undergo oxidation and gasification with H_2O and CO_2 . It is deduced that gasification process which is endothermic is more pronounced than exothermic process (oxidation), hence the temperature decrease.

Figure 6.28 also shows that at corresponding height, air-fuel peak temperature is higher than oxy-fuel temperature by about 200 K. This is as a result of combination of both chemical and thermal effect. Lower temperatures are seen in oxy-fuel environment because CO_2 has higher heat capacity than N_2 . Furthermore, chemical effect through endothermic reaction of CO_2 with char contribute in lowering the temperature of oxy-fuel environment.

Presented in Fig. 6.29 are predicted temperature profiles at 5 cm from the bed bottom for wood combustion in different combustion atmospheres. It is observed that peak temperature occurrence time comes much earlier in N_2 atmosphere than in CO_2 atmosphere. This is an indication that combustion rate is slower in CO_2 environment. For oxy-fuel combustion, peak temperature value is directly proportional to O_2 concentration. In addition, its occurrence time increases as O_2 concentration is decreased. Peak temperature of oxy-fuel atmosphere which is equivalent to that of standard air-fuel condition occur at about 40% O_2 concentration. However, its occurrence time is slightly earlier than in air-fuel condition. This is attributed to higher O_2 concentration which enhance oxidation reactions of volatiles that releases more heat and increases flame speed.

The time taken for the reaction front to start at the top surface of the fuel bed was defined as ignition time. Presented in Fig. 6.30 is ignition time for wood combustion in both oxy-fuel and air-fuel environments. The graph shows that at any given oxygen concentration, ignition time in oxy-fuel environment is almost twice that of corresponding air-fuel condition. Retarded ignition in CO_2 environment could be attributed to its high specific heat capacity and low O_2 diffusivity in it. In both cases, ignition time gradually decreases as oxygen concentration is increased.

Figure 6.29: Predicted temperature profiles at 5 cm from the bed bottom for wood combustion in different combustion atmospheres.

Figure 6.30: Measured and predicted ignition time for fixed bed combustion of wood in N₂ and CO₂ environments.

A comparison of burning rates for wood combustion in N₂ and CO₂ burning conditions are

presented in Fig. 6.31. At the same O_2 concentration, the burning rate in CO_2 burning atmosphere is less than in N_2 burning atmosphere. The burning rate of wood particles in oxy-fuel condition is lowered by the aforementioned CO_2 effects, which contribute differently as would be discussed later. Thermal diffusivity of CO_2 is less than that of N_2 by about 35% (Suda *et al.*, 2007). In addition, CO_2 absorbs radiative heat more than N_2 . The overall effects of these thermal properties of CO_2 is a decrease in burning rate as seen in Fig. 6.31. Furthermore, the burning rate in oxy-fuel environment is also decreased by chemical effect of CO_2 through Bourdoudard reaction R(16), which is endothermic. On the other hand, the role played by dilution is clearly demonstrated in Fig. 6.31. In both cases, burning rate is directly proportional to O_2 concentration. More O_2 concentration enhances oxidation of combustible pyrolysis products and char, hence releasing more heat and increasing the burning rates.

Figure 6.31: Measured and predicted burning rates for fixed bed combustion of wood in N_2 and CO_2 environments.

Figure 6.32: Measured and predicted flame front propagation speed for fixed bed combustion of wood in N₂ and CO₂ environments.

Illustrated in Fig. 6.32 is the flame front propagation speed for wood combustion in oxy-fuel and air-fuel burning atmospheres. It is observed that for all oxygen concentration, CO₂ burning atmosphere had lower propagation speed as compared to N₂ burning atmosphere. Furthermore, as oxygen concentration increases flame propagation speed also increases. Flame speed is directly linked to the burning rate. Therefore, the factors which reduce the burning rates in oxy-fuel environment as discussed in the preceding paragraph are also responsible for the reduced flame speed.

The species and temperature profiles along axial length of the fixed bed when the flame front is at 4 cm from the grate for 21% O₂/79% CO₂, 30% O₂/70% CO₂, 40% O₂/60% CO₂ and 50% O₂/50% CO₂ are presented in Figs 6.33 and 6.34. The flame structures are similar in profile but differ in magnitude. The flame front for the mixture with high O₂ concentration, 50%, reaches 4 cm plane at 191 s, which is earlier than those for 40%, 30% and 21% that reached the plane at 275 s, 360 s

and 482 s, respectively. This is because flame speed increases as O_2 concentration is increased. As shown in Figs 6.33, 6.34 and Table 6.1, the amount of tar and CH_4 are high at the reaction zone of 21% O_2 concentration mixture and decreases gradually for 30%, 40% and 50% O_2 concentration mixtures; comparison of species when the flame front is at 4 cm is shown in Figs E.13-E.15 in Appendix E.2. The same behavior is observed in the concentration of tar and CH_4 in

Figure 6.33: Species and temperature profiles along axial length of the bed when the flame front is at 4 cm from the grate for (a) 21% O_2 /79% CO_2 and (b) 30% O_2 /70% CO_2 .

these O_2/CO_2 mixtures when the reaction front is at 3 cm, 2 cm and 1 cm from the grate as illustrated in Figs E.16-E.24. The graphs show that the mixture with 21% O_2 concentration is operating under fuel rich conditions and does not have enough O_2 to oxidize these species through reactions R(7) and R(9). On the other hand, the graphs show that the mixtures with 30%, 40% and 50% O_2 concentration are operating under fuel lean conditions and have excess O_2 in their reaction zones. Thus reduced amount of tar and CH_4 are observed in these mixtures as compared to those of 21% O_2 concentration mixture. Consequently, since these reactions are exothermic, a high amount of heat is released as O_2 concentration is increased. This is seen in the peak temperatures attained by these mixtures, Fig. 6.29. The high amount of heat released increases the heating rates for the particles in the bed and explains the higher flame front propagation speed and burning rates

for high O_2 concentration mixtures. High heat energy also accelerates the ignition of the particles for mixtures with high O_2 concentration.

Figure 6.34: Species and temperature profiles along axial length of the bed when the flame front is at 4 cm from the grate for (a) 40% O_2 /60% CO_2 and (b) 50% O_2 /50% CO_2 .

Figures 6.33, 6.34 and Table 6.1 show that the amount of CO is highest in the reaction zone of the mixture with 30% O_2 concentration, comparison is shown in Appendix E.2. Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for wood combustion burning under oxy-fuel condition of different O_2/CO_2 mixtures are presented in Table E.6-E.9 in Appendix E.2. The mixtures with 21%, 40% and 50% O_2 concentration have almost the same amount of CO in their reaction zone. Unlike tar and CH_4 whose sole source is devolatilization of the wood particles, CO is produced from devolatilization process, oxidation of tar through reaction R(9) and char gasification with CO_2 through reaction R(16). CO is consumed by oxidation reaction R(6). For a mixture with high O_2 concentration, excess O_2 brings an antagonistic effect to the amount of CO where there is a tendency for high consumption through oxidation reaction R(6) and high production by oxidation of tar through reaction R(9) as compared to that of a mixture with low O_2 concentration. However, for mixtures with high O_2 concentration, the production of CO through

char gasification could be less than that of low O₂ concentration mixture because of low amount of CO₂. The overall effect of these reactions is that there is an increase in CO production as O₂ concentration is increased up to a peak point then it starts to decrease.

Burning rate, ignition of fuel particles and flame front propagation speed are all influenced by thermal behavior of the bed. Apart from heat of combustion through chemical reactions discussed in the preceding paragraphs, flame temperature at a given point is also determined by heat flux in the form of conduction, convection and radiation. Heat flux distribution in the fixed bed is mostly by radiation. H₂O and CO₂ are the main products of combustion that participate in radiation. The presence of high amount of CO₂ in an oxy-fuel environment makes it more emissive than air-fuel environment. As depicted by the flame temperatures in Figs. 6.29 and 6.34, a high amount of heat energy is released in the fuel bed with a high O₂ concentration mixture. In this study, the heat energy contribution from different sources have not been separated. Therefore, an increase in heat energy cannot be explicitly linked to a particular source. Though, in the region of intense combustion, heat contributed by combustion is more dominant; the contribution by radiation heat flux is only 10-15% (Lallemant *et al.*, 1996).

Table 6.1: Peak values of major combustible species and temperature profiles for wood combustion under oxy-fuel environment for different O₂/CO₂ mixtures when the flame front is at 4 cm from the grate.

Temperature/ species mole fraction (-)	O ₂ /CO ₂ mixture			
	21% O ₂	30% O ₂	40% O ₂	50% O ₂
Temperature (K)	1338	1406	1499	1605
Tar	0.02427	0.02164	0.01605	0.01837
CO	0.05839	0.06488	0.06013	0.06124
CH ₄	0.00819	0.00769	0.00542	0.00684

6.5.2 Isolation of CO₂ Effects on Wood Conversion Processes

Wood combustion in four different mixtures of O₂ and Ar/CO₂/N₂ were numerically simulated so as to separate the various effects of CO₂ on burning rate of wood. For all the cases, temperature profiles at 5 cm from fuel bed was considered. A method of adjusting the flame temperature using Ar, which was initially proposed by Du *et al.* (2009) and previously used by other researchers (Al-Qurashi *et al.* 2011; Zhou *et al.* 2016), was implemented in this study. The four mixtures are denoted by letters A, B, C and D and their composition were: 21% O₂/79% N₂; 21% O₂/22.5% CO₂/56.5% Ar; 40% O₂/60% CO₂; and 40% O₂/47% CO₂/13% Ar, respectively. Furthermore, other properties of the different mixtures such as mass fraction of the constituents, combined heat capacity and oxygen diffusion coefficient are provided in Table 6.2. These properties were evaluated and compared at room temperature (298 K), ignition temperature (500 K) and flame temperature (1400 K). Combustion of wood in mixtures A, B and C were designed to have the same peak temperatures, as shown in Fig. 6.35. A high amount of Ar in mixture B was to increase the peak temperature which is low when CO₂ alone is used as a diluent. As shown in Table 6.2, this mixture has a lower specific heat capacity. This enabled the mixture to have the same peak temperature as that of mixture A and C. The peak temperature of wood combustion in mixture D was higher than for the other three by 167 K.

The burning rates of wood combustion in the four mixtures were evaluated and presented in Fig. 6.36. Burning rate in mixture A was used as a datum. The difference in burning rates of combustion in mixture A and B is due to chemical effect because they have the same oxygen concentration and temperature values. Since temperature is the only similar parameter for combustion in mixture A and C, then the difference in their burning rate is due to a combination of oxygen concentration and chemical effect. Oxygen concentration effect is achieved when oxygen concentration is increased to 40% while maintaining the same temperature in CO₂ environment - combustion in

mixture B and C. Finally, the difference in burning rates for combustion in mixture C and D is due to thermal effect since they have the same oxygen concentration but different temperature values.

Table 6.2: Composition, combined heat capacity and O₂ diffusion coefficient of the four mixtures at different temperatures.

Properties		Gas mixtures			
		A	B	C	D
Mass fraction of the components [-]	Ar	0.000	0.576	0.000	0.134
	O ₂	0.233	0.171	0.327	0.331
	N ₂	0.767	0.000	0.000	0.000
	CO ₂	0.000	0.253	0.673	0.535
c _p for the mixture [kJ/kg K]	At 298 K	1.005	0.67	0.868	0.825
	At 500 K	1.03	0.725	1.006	0.939
	At 1400 K	1.209	0.826	1.255	1.147
O ₂ diffusion coefficient in the mixture (cm ² /s)	At 298 K	0.209	0.184	0.156	0.164
	At 500 K	0.513	0.462	0.398	0.415
	At 1400 K	2.888	2.642	2.31	2.401

Individual contribution of CO₂ effects on burning rates of wood combustion is presented in Fig. 6.37. It was established that chemical, thermal and oxygen concentration influenced burning rate of wood by 5%, 9% and 86%, respectively. It is evident that oxygen concentration is the most influential parameter on the burning rate. As oxygen concentration is increased, oxidation of char and combustible pyrolysis products are also enhanced. Therefore, more heat is generated and fuel burning rate is significantly improved. The influence of thermal and chemical are not very significant. Thermal effect is only 9% and translate to a temperature change of 167 K. Chemical effect on the burning rate is quite small because the rate of the chemical reactions involving CO₂ consumption (R(14) and R(16)) are far much less compared to the rate of (R(6) and R(13)).

Figure 6.35: Predicted temperature profiles at 5 cm from the bed bottom for wood combustion in four combustion environments.

Figure 6.36: Predicted separate effects of CO₂ on burning rates for wood combustion in four combustion environments.

Figure 6.37: Predicted contributions of separate effects of CO₂ on burning rates for wood combustion in four combustion environments.

The overall and separate effects of CO₂ burning atmosphere on the combustion properties of wood burning in a fixed bed were investigated through numerical modeling. Modeling was validated by comparison with measured data. It was established that the dilution effect is the most influential parameter on the burning rate of wood combustion in an oxy-fuel system. The influence of thermal and chemical are not very significant. The peak temperature of oxy-fuel atmosphere which is equivalent to that of standard air-fuel condition occur at a higher O₂ concentration. However, its occurrence time is slightly earlier than in air-fuel condition. At any given oxygen concentration, ignition time in oxy-fuel is almost twice that of corresponding air-fuel condition. In both cases, ignition time gradually decreases as oxygen concentration is increased. At the same oxygen concentration, burning rate and flame propagation speed in CO₂ combustion environment was less than in N₂ combustion environment.

CHAPTER SEVEN

CONCLUSIONS

7.1 Introduction

Presented in this chapter is a summary of the main findings of this study. The findings covered three major areas considered in this work; flame propagation speed under oxy-fuel conditions, particle packing density and separate effects of CO₂ in oxy-fuel combustion. In addition, conclusions arising out of the study are also discussed.

7.2 Summary

The main findings of this study is summarized as follows:

- CFD-DEM model agreed very well with experimental values for mass loss, propagation speed, flame front positions, burning rate and ignition time.
- Flame front propagation speed in oxy-fuel atmosphere reduced to 78% of that of the air-fuel condition with similar O₂ concentration.
- Under the same O₂ concentration, peak temperature and burning rate are reduced while ignition time is increased in an oxy-fuel environment as compared to air-fuel environment.
- For oxy-fuel combustion, peak temperature value, burning rate and propagation speed increases while ignition time reduces as O₂ concentration is increased.
- The packing density affects the combustion process in an oxy-fuel environment by changing the burning conditions and flammability limits. As bed porosity is increased, the combustion condition is shifted from fuel-rich to fuel-lean side and this increases the conversion rate, reduces the ignition time, increases the flame front propagation speed and thicken the reaction zones.

- There is an optimum packing density, $\chi = 0.71$, beyond which the efficiency falls off due to the onset of quenching in the spaces.
- Dilution effect of CO_2 is the most influential parameter on the burning rate of wood combustion in an oxy-fuel environment. The influence of thermal and chemical are not very significant.

7.3 Conclusions

Modeling and experimental work on oxy-fuel combustion of biomass in a laboratory fixed bed reactor has been investigated in this thesis. The focus was on flame propagation speed under oxy-fuel conditions, particle packing density and separate effects of CO_2 in oxy-fuel combustion. In all the cases, CFD-DEM approach was used to simulate wood conversion in a fixed bed and the results compared to experimental data. A good agreement between model and experimental results were achieved in all the cases studied.

First, the effect of CO_2 environment on flame propagation speed and flame structures were investigated. Computational results agree very well with experimental values except temperature which showed poor prediction at low O_2 concentration. The agreement of temperatures corrected for radiation losses with predicted values are better than those of uncorrected values. Hence, it was established that prediction accuracy of CFD-DEM is not the same in different O_2/CO_2 mixtures. Furthermore, it was observed that flame speed in oxy-fuel atmosphere reduced to 78% of that of the air-fuel condition with same O_2 concentration. This was determined both by experiment and through computation. Reduced flame speed was attributed to a higher heat capacity of CO_2 and lower O_2 diffusivity in CO_2 whose overall effect is reduction of temperature and heating rates of fuel particles. Low mass fraction of combustible volatiles predicted in the CO_2 environment also contribute to a reduced flame speed. Flame

structures have similar profiles but differ in value of temperature and species quantities. Temperatures in the CO₂ environments were lower than those in the N₂ environments. During initial stages of combustion, the amount of tar and steam is observed to be highest in 79% N₂ environment and lowest in 79% CO₂ environment. The amount of CO was almost equal in both environments during pyrolysis but high amount was predicted in oxy-fuel environments during char combustion stage.

Second, CFD-DEM model was used to comprehensively study the influence of particle packing density and bed porosity on wood conversion in the fixed bed in the entire possible operation range. The model was validated in the initial bed porosity range of 0.50-0.75. A good agreement was achieved between the model and experiment with most points having deviations which were less than 10%. It was established that the packing density affects the combustion process in an oxy-fuel environment by changing the burning conditions and flammability limits. As bed porosity is increased, the combustion condition is shifted from fuel-rich to fuel-lean side and this increases the conversion rate, reduces the ignition time, increases the flame front propagation speed and thicken the reaction zones. In addition, as bed porosity is increased, volatiles and char are concurrently oxidized during pyrolysis stage leading to a single temperature peak. On contrary, less porous bed has two distinct temperature peaks since volatiles and char are oxidized sequentially due to O₂ deficit. It was also found out that there is an optimum packing density, $\chi = 0.71$, beyond which the efficiency falls off due to the onset of quenching in the spaces. Furthermore, the operational range with respect to porosity was decreased in an oxy-fuel burning condition due to higher quenching effects of CO₂.

Finally, the overall and separate effect of CO₂ environment on the combustion properties of wood burning in a fixed bed were investigated through numerical modeling. It was established

that the peak temperature of oxy-fuel atmosphere which is equivalent to air-fuel at 21% O₂ concentration occur at about 40% O₂ concentration. Its occurrence time is slightly earlier than that of 21% O₂/79% N₂ atmosphere. At any given oxygen concentration, ignition time in oxy-fuel is almost twice that of corresponding air-fuel condition. In both cases, ignition time gradually decreases as oxygen concentration is increased. At the same oxygen concentration, burning rate and flame propagation speed in CO₂ combustion environment was less than in N₂ combustion environment. Chemical, thermal and oxygen concentration influenced burning rate of wood by 5%, 9% and 86%, respectively.

7.4 Significance of the Study

This study deals with experimental and numerical simulation of fixed bed combustion of wood under oxy-fuel environment. Oxy-fuel combustion considered in this research work is significant because it is a clean energy technology where CO₂ is captured through recycling of flue gas, and at the same time nitrogen oxides (NO_x) emissions are reduced. Fixed bed combustion technology that is also considered in this study is relevant in industrial application, particularly for power plants that generate up to 40 MW_{th}. The fixed bed technique is favourable because of its simplicity. The mechanisms through which CO₂ affects fundamental combustion properties of wood burning in a fixed bed are investigated in this research work. An understanding of these mechanisms is important because it helps in design of optimized oxy-fuel burners. Furthermore, the combustion properties investigated in this study, viz., temperature profiles, ignition time, burning rate, flame propagation speed and species evolution in the bed are the main parameters to consider when designing a new burner. Therefore, the findings from this work are important and may be useful when designing burners which operate under oxy-fuel combustion conditions. The study revealed that the packing density affects

combustion process in an oxy-fuel environment by changing the burning conditions and flammability limits. The study also revealed that there is an optimum packing density beyond which the efficiency falls due to the onset of quenching in the spaces. These findings are meaningful, relevant and appealing to audience in energy sector, biomass conversion, fuel sector, power plant and scientific community at large.

CHAPTER EIGHT

OUTLOOK FOR FUTURE WORK

In practice, shrinking or local collapse is a possible problem during combustion of biomass fuels. In this thesis, the experimental set up did not have a provision for measuring, monitoring and visualizing the volume change in bed layers. Combustion chamber was not made of a transparent material. Therefore, it was not possible to observe or measure shrinkage. A shrinkage model from literature was implemented in our computational work. Hence, there is need to carry out an experimental study which consider shrinkage in the fuel bed. In this study, particle packing density was analyzed by considering initial arrangement of particles in the bed. However, in practice, the packing density and porosity changes as combustion proceeds. Channeling in the bed could also arise as combustion takes place. These were not considered in this work. Hence, there is also need to consider them in a future study.

In this study, CFD-DEM model slightly over predicted temperature of wood combustion under oxy-fuel conditions at low O_2 concentration. This could be attributed mainly to the kinetic model and the heat transfer model that were implemented in this study. Chemical kinetic model for gas-phase used in this study is a skeletal mechanism that had a few reactions as presented in Table 3.4. The model consisted of oxidation reactions of the products of devolatilization, i.e., H_2 , CH_4 , tar and CO. Furthermore, it had dominant reaction pathway R(10), which is important in an oxy-fuel environment. The skeletal mechanism used in this thesis was necessary due to high demand for computation power required in three dimensional modelling. Though there was a good agreement between the model results and experimental data, better prediction could be achieved by incorporating a full chemical kinetic mechanism for hydrocarbon combustion. Combustion properties of the fixed bed such as burning rate, ignition of fuel particles and flame front propagation speed are all influenced by thermal behavior of the bed. Flame temperature

at a given point is determined by heat of combustion through chemical reactions and heat flux distribution in the bed which is mostly by radiation. The presence of high amount of CO_2 in an oxy-fuel environment makes it more emissive than air-fuel environment. A radiation model which take into consideration this fact should be implemented when modeling wood combustion in an oxy-fuel environment. In this work unmodified WSGGM was used to account for heat transfer by radiation. This model was initially developed for air-fuel environment. There are studies which show that the impact of modifying WSGGM for application in oxy-fuel condition is negligible in small scale reactors. While it has been noted that modified WSGGM model has significant improvement on the accuracy when considering large scale reactors, the effect on small scale reactors is minimal. This is because evaluation of gaseous radiative properties using non-gray method employed in modified WSGGM has an inherent potential of improving the accuracy of oxy-fuel combustion models but the degree of improvement depends on the scale or the beam length of the furnace under study. For small scale reactors operating under oxy-fuel conditions, unmodified WSGGM can be used to predict combustion with good accuracy. The reactor used in this study is small, therefore, unmodified WSGGM was implemented with an expectation that it would not significantly affects the results. Other radiation models could be implemented to test their suitability in modeling oxy-fuel environment in small combustion devices. Furthermore, in this study, the heat energy contribution from different sources have not been separated. A detail analysis of heat transfer in the bed could be investigated in a future study.

In this thesis, ash inhibition model was not considered. During the late stage of char combustion ash is produced as one of the products. Mineral matter present in ash act as catalyst in char consumption. This effect is significant at low temperatures. However, at high temperatures

where heat and mass transfer is significant, ash inhibit char consumption. Ash inhibit char combustion by forming an outer inorganic layer which prevent O_2 from reaching the reacting surface. In addition, the effective surface area is reduced since some part of the particle volume is occupied by ash. Consequently, char oxidation and gasification given by reactions R(15) to R(17) are not accurately predicted as their reaction rates are expressed in terms of external area. All these ash effects have not been considered in the model used in this study. Therefore, there is a need for consideration of these effects in a future study in order to improve the accuracy of the model.

Validity of the model was checked by comparing mass loss history and temperatures obtained from simulations to corresponding experimental data. Other combustion properties such as flame speed, ignition time, burning rates were determined using mass loss and temperature measurement. The model was used to quantify combustion properties through analysis of wood conversion into char and volatiles and their consumption rates in the bed under different oxidizer concentration and initial bed porosity. The model flame structures in terms of distribution of main gas species along the axial length of the reactor at a given time were used to analyze oxy-fuel combustion conditions. Furthermore, their time histories were also used. The volatiles that were considered in the model used in this work include CO, H_2 , CH_4 , tar, H_2O and CO_2 . These volatiles are generated from drying and pyrolysis of wood. These are endothermic reactions which absorb heat and reduce bed temperature. On the other hand, combustible pyrolysis product such as CH_4 , tar, H_2 and CO are oxidized through exothermic reaction which generate heat and subsequently increases the temperature. Thus, a well predicted temperature indicates that the amount of volatiles released in the bed are also correctly

approximated by the model. Despite this assumption, there is need for measurement of the volatiles in order to ensure the validity of the model.

Finally, the presence of CO_2 in oxidizer alters gas properties such as density, heat capacity, diffusivity and gas emissivity with consequences on fuel reactivity, flame temperature and emissions. As a result, particulate matter and soot formation in an oxy-fuel environment are not the same as in air-fuel environment. Furthermore, since N_2 is replaced by CO_2 , formation of nitrogen oxides (NO_x) is expected to be minimal in an oxy-fuel environment. Indeed, in such environment, NO_x is only formed through fuel-bound route. Pollutant formation in a fixed bed combustion under oxy-fuel environment is an important aspect which need to be addressed in a future study.

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APPENDIX A

ROSIN-RAMMLER DISTRIBUTION FUNCTION

Rosin-Rammler distribution function, Eq. (A.1), was originally developed for characterization of powdered coal (Williams *et al.*, 2016). However, it has found application in many materials, (Djamarani & Clark, 1997) including biomass particles (Bitra *et al.*, 2009; Gil *et al.*, 2012b). It is a good method for particles obtained through comminution; various types of crushing, grinding and milling.

$$R_R(d) = 100 \left(\exp \left(-\frac{d}{\bar{d}} \right)^{n_R} \right). \quad (A.1)$$

where d is the particle diameter or mesh size, $\bar{d}$ is the characteristic size, n_R is the parameter of Rosin-Rammler distribution and R_R is the percentage of accumulated oversize mass. n_R was determined according to Brezání and Zelenák (2010).

Even though parameter n_R and $\bar{d}$ can be obtained using an equation fitting software, it is alternatively obtained using linear regression of data plotted in Rosin-Rammler diagram (Brezání & Zelenák, 2010). The later was implemented in this thesis.

Logarithm of Eq (A.1) is taken twice and rearranged to give the following expression:

$$\log \left(\log \left(\frac{100}{R_R(d)} \right) \right) = n_R \cdot \log d - n_R \cdot \log \bar{d} + \log(\log e). \quad (A.2)$$

For any material, parameter n_R and $\bar{d}$ are constant, therefore from Eq. (A.2),

$$\log(\log e) - n_R \cdot \log \bar{d} = \text{const.} \quad (A.3)$$

Hence, Eq. (A.2) may be expressed as follows:

$$\log \left(\log \left(\frac{100}{R_R(d)} \right) \right) = n_R \cdot \log d + \text{const.} \quad (\text{A. 4})$$

A plot of $\log \left(\log \left(\frac{100}{R_R(d)} \right) \right)$ against $\log d$ is a straight line, and is refers to Rosin-Rammler (RR) diagram, Peleg (1996).

Characteristic size, $\bar{d}$, of a give material is obtained by classifying it on a mesh $d = \bar{d}$. Using this in Eq. (A.1), then the percentage of oversize material is given as $R_R(d) = 36.79 \%$. Consequently, characteristic size is obtained as follows:

$$\bar{d} = 10^{\frac{\log_{10}(\log_{10}(100/36.79)) - \text{const}}{n}}. \quad (\text{A. 5})$$

And n is the gradient of the plotted line given as follows:

$$n_R = \frac{\log \left(\log \frac{100}{R_R(d_2)} \right) - \log \left(\log \frac{100}{R_R(d_1)} \right)}{\log d_2 - \log d_1}, \quad (\text{A. 6})$$

where $[d_1, R_R(d_1)]$ and $[d_2, R_R(d_2)]$ are random data points on the best fitted line.

Table A.1: Particle size distribution of wood particles samples.

Sawdust 1 (SD1)		Sawdust 2 (SD2)		Wood chips (WC)	
Mesh size	Mass	Mesh size	Mass	Mesh size	Mass
(mm)	Retained (%)	(mm)	Retained (%)	(mm)	Retained (%)
0.5	95	2.2	92	4.5	65
0.71	80	2.5	81	5	45
1	65	2.8	72	5.6	32
1.25	42	3.15	35	6.3	20
1.4	15	3.55	12	7.1	7

Presented on Table A.1 are data for the particles size distribution of the wood used in this study. The size distribution was obtained using Fritsch vibratory sieve shaker. The RR diagram for fuel sample SD1 is shown in Fig. A.1. From this graph, parameter n_R and $\bar{d}$ were calculated as

3.212 and 1.23 mm, respectively. Similarly, these parameters were calculated for all the fuel samples and presented in Table A.2.

Figure A.1: RR diagram for fuel sample SD1.

Table A.2: Characteristic size of different fuel samples.

Parameter	Sawdust 1 (SD1)	Sawdust 2 (SD2)	Wood chips (WC)
$\bar{d}$	1.227	3.183	5.474
n	3.212	6.801	3.789
R^2	0.974	0.988	0.985

APPENDIX B

TEMPERATURE MEASUREMENT APPARATUS

Temperature of combustion zone were measured using type K class 2 thermocouple (range of -200 to +1372 °C) which were coupled to a data acquisition system comprising of MAX31850 cold-junction compensated, 1-wire thermocouple-to-digital converter, Arduino program code and a computer, as shown in Fig. B.1.

Figure B.1: Temperature data acquisition system.

The uncertainty analysis of the whole system was estimated using model Eq. (B.1). In this analysis, main errors were only considered.

$$T_D = T_M + \delta E_S + \delta E_C + C_S \delta T_R + \delta E_{VC} + \delta E_P + \delta E_A, \quad (B.1)$$

where T_D is the display temperature, T_M is the temperature at measuring point, δE_S is the deviation of the sensor, δE_C is the error due to insufficient temperature conditioning, C_S is the sensor sensitivity, δT_R is the reference point temperature change, δE_{VC} is the voltage change due to compensation cable, δE_P is the error due to processing and linearization in electronic device and δE_A is the error due to component aging (long term drift).

B.1 Determination of Individual Uncertainty Components

Individual uncertainty components were estimated using European standards and/or manufacturers datasheet.

1. Deviation of the sensor (δE_S) – Specified according to European standards DIN EN 60584. For type K class 2 thermocouple, DIN EN 60584 requires that $\delta E_S = 0.0075 \cdot |t|$
2. Error due to insufficient temperature conditioning (δE_C) – It was assumed that measurement was stable. Therefore, this uncertainty was neglected.
3. Error due to reference point temperature change ($C_S \delta T_R$) – Cold junction accuracy according to the datasheet of MAX31850 thermocouple converter is given as $\pm 2^\circ\text{C}$
4. Voltage change due to compensation cable (δE_{VC}) – Compensation cable had a tolerance of $\pm 2.5^\circ\text{C}$.
5. Error due to processing and linearization in electronic device (δE_P) – According to the datasheet of MAX31850 thermocouple converter, this error was specified as follows:
 - a. $\delta E_P = \pm 2^\circ\text{C}$ for temperature range -200 to $+700^\circ\text{C}$
 - b. $\delta E_P = \pm 4^\circ\text{C}$ for temperature range $+700$ to $+1372^\circ\text{C}$
6. Error due to component aging (δE_A) - According to the datasheet of MAX31850 thermocouple converter, this error was specified as $\pm 0.24^\circ\text{C}$.

A simple measurement uncertainty (68.3% confidence interval), δ_{SU} was first calculated. This was achieved by dividing individual uncertainty components by $\sqrt{3}$ (assuming a rectangle distribution) and then added geometrically as shown by Eq. (B.2).

$$\delta_{SU} = \sqrt{\left(\frac{\delta E_S}{\sqrt{3}}\right)^2 + \left(\frac{C_S \delta T_R}{\sqrt{3}}\right)^2 + \left(\frac{\delta E_{VC}}{\sqrt{3}}\right)^2 + \left(\frac{\delta E_P}{\sqrt{3}}\right)^2 + \left(\frac{\delta E_A}{\sqrt{3}}\right)^2}, \quad (B.2)$$

Total measurement uncertainty, δ_{TU} with a confidence interval of 95% was calculated by multiplying simple measurement uncertainty by 2 ($\delta_{TU} = 2 \times \delta_{SU}$). The results for the whole thermocouple measurement range are tabulated in Table B.1.

Table B.1: Uncertainty analysis of temperature measurement apparatus.

Temperature (°C)	Individual Uncertainty Contribution (°C)					Simple measurement uncertainty (°C)	Total measurement uncertainty (°C)
	$\frac{\delta E_S}{\sqrt{3}}$	$\frac{C_S \delta T_R}{\sqrt{3}}$	$\frac{\delta E_{VC}}{\sqrt{3}}$	$\frac{\delta E_P}{\sqrt{3}}$	$\frac{\delta E_A}{\sqrt{3}}$		
0	0.000	1.155	1.443	1.155	0.139	2.184	4.368
10	0.043	1.155	1.443	1.155	0.139	2.184	4.369
20	0.087	1.155	1.443	1.155	0.139	2.186	4.371
30	0.130	1.155	1.443	1.155	0.139	2.188	4.375
40	0.173	1.155	1.443	1.155	0.139	2.191	4.381
50	0.217	1.155	1.443	1.155	0.139	2.195	4.389
60	0.260	1.155	1.443	1.155	0.139	2.199	4.398
70	0.303	1.155	1.443	1.155	0.139	2.205	4.410
80	0.346	1.155	1.443	1.155	0.139	2.211	4.422
90	0.390	1.155	1.443	1.155	0.139	2.218	4.437
100	0.433	1.155	1.443	1.155	0.139	2.226	4.453
110	0.476	1.155	1.443	1.155	0.139	2.235	4.470
120	0.520	1.155	1.443	1.155	0.139	2.245	4.490
130	0.563	1.155	1.443	1.155	0.139	2.255	4.510
140	0.606	1.155	1.443	1.155	0.139	2.266	4.533
150	0.650	1.155	1.443	1.155	0.139	2.278	4.557
160	0.693	1.155	1.443	1.155	0.139	2.291	4.582
170	0.736	1.155	1.443	1.155	0.139	2.305	4.609
180	0.779	1.155	1.443	1.155	0.139	2.319	4.638
190	0.823	1.155	1.443	1.155	0.139	2.334	4.667
200	0.866	1.155	1.443	1.155	0.139	2.349	4.699
210	0.909	1.155	1.443	1.155	0.139	2.366	4.731
220	0.953	1.155	1.443	1.155	0.139	2.383	4.765
230	0.996	1.155	1.443	1.155	0.139	2.400	4.800
240	1.039	1.155	1.443	1.155	0.139	2.419	4.837
250	1.083	1.155	1.443	1.155	0.139	2.437	4.875
260	1.126	1.155	1.443	1.155	0.139	2.457	4.914
270	1.169	1.155	1.443	1.155	0.139	2.477	4.954

280	1.212	1.155	1.443	1.155	0.139	2.498	4.996
290	1.256	1.155	1.443	1.155	0.139	2.519	5.038
300	1.299	1.155	1.443	1.155	0.139	2.541	5.082
310	1.342	1.155	1.443	1.155	0.139	2.563	5.127
320	1.386	1.155	1.443	1.155	0.139	2.586	5.173
330	1.429	1.155	1.443	1.155	0.139	2.610	5.220
340	1.472	1.155	1.443	1.155	0.139	2.634	5.268
350	1.516	1.155	1.443	1.155	0.139	2.658	5.316
360	1.559	1.155	1.443	1.155	0.139	2.683	5.366
370	1.602	1.155	1.443	1.155	0.139	2.709	5.417
380	1.645	1.155	1.443	1.155	0.139	2.734	5.469
390	1.689	1.155	1.443	1.155	0.139	2.761	5.521
400	1.732	1.155	1.443	1.155	0.139	2.787	5.575
410	1.775	1.155	1.443	1.155	0.139	2.814	5.629
420	1.819	1.155	1.443	1.155	0.139	2.842	5.684
430	1.862	1.155	1.443	1.155	0.139	2.870	5.740
440	1.905	1.155	1.443	1.155	0.139	2.898	5.796
450	1.949	1.155	1.443	1.155	0.139	2.927	5.854
460	1.992	1.155	1.443	1.155	0.139	2.956	5.912
470	2.035	1.155	1.443	1.155	0.139	2.985	5.970
480	2.078	1.155	1.443	1.155	0.139	3.015	6.030
490	2.122	1.155	1.443	1.155	0.139	3.045	6.090
500	2.165	1.155	1.443	1.155	0.139	3.075	6.150
510	2.208	1.155	1.443	1.155	0.139	3.106	6.212
520	2.252	1.155	1.443	1.155	0.139	3.137	6.273
530	2.295	1.155	1.443	1.155	0.139	3.168	6.336
540	2.338	1.155	1.443	1.155	0.139	3.199	6.399
550	2.382	1.155	1.443	1.155	0.139	3.231	6.463
560	2.425	1.155	1.443	1.155	0.139	3.263	6.527
570	2.468	1.155	1.443	1.155	0.139	3.296	6.591
580	2.511	1.155	1.443	1.155	0.139	3.328	6.656
590	2.555	1.155	1.443	1.155	0.139	3.361	6.722
600	2.598	1.155	1.443	1.155	0.139	3.394	6.788
610	2.641	1.155	1.443	1.155	0.139	3.427	6.855
620	2.685	1.155	1.443	1.155	0.139	3.461	6.921
630	2.728	1.155	1.443	1.155	0.139	3.494	6.989
640	2.771	1.155	1.443	1.155	0.139	3.528	7.057
650	2.815	1.155	1.443	1.155	0.139	3.562	7.125
660	2.858	1.155	1.443	1.155	0.139	3.597	7.194
670	2.901	1.155	1.443	1.155	0.139	3.631	7.263
680	2.944	1.155	1.443	1.155	0.139	3.666	7.332

690	2.988	1.155	1.443	1.155	0.139	3.701	7.402
700	3.031	1.155	1.443	1.155	0.139	3.736	7.472
710	3.074	1.155	1.443	2.309	0.139	4.269	8.537
720	3.118	1.155	1.443	2.309	0.139	4.300	8.600
730	3.161	1.155	1.443	2.309	0.139	4.331	8.663
740	3.204	1.155	1.443	2.309	0.139	4.363	8.726
750	3.248	1.155	1.443	2.309	0.139	4.395	8.790
760	3.291	1.155	1.443	2.309	0.139	4.427	8.854
770	3.334	1.155	1.443	2.309	0.139	4.459	8.919
780	3.377	1.155	1.443	2.309	0.139	4.492	8.984
790	3.421	1.155	1.443	2.309	0.139	4.524	9.049
800	3.464	1.155	1.443	2.309	0.139	4.557	9.115
810	3.507	1.155	1.443	2.309	0.139	4.590	9.181
820	3.551	1.155	1.443	2.309	0.139	4.623	9.247
830	3.594	1.155	1.443	2.309	0.139	4.657	9.314
840	3.637	1.155	1.443	2.309	0.139	4.690	9.381
850	3.681	1.155	1.443	2.309	0.139	4.724	9.448
860	3.724	1.155	1.443	2.309	0.139	4.758	9.516
870	3.767	1.155	1.443	2.309	0.139	4.792	9.584
880	3.811	1.155	1.443	2.309	0.139	4.826	9.652
890	3.854	1.155	1.443	2.309	0.139	4.860	9.720
900	3.897	1.155	1.443	2.309	0.139	4.895	9.789
910	3.940	1.155	1.443	2.309	0.139	4.929	9.858
920	3.984	1.155	1.443	2.309	0.139	4.964	9.928
930	4.027	1.155	1.443	2.309	0.139	4.999	9.997
940	4.070	1.155	1.443	2.309	0.139	5.034	10.067
950	4.114	1.155	1.443	2.309	0.139	5.069	10.137
960	4.157	1.155	1.443	2.309	0.139	5.104	10.208
970	4.200	1.155	1.443	2.309	0.139	5.139	10.278
980	4.244	1.155	1.443	2.309	0.139	5.175	10.349
990	4.287	1.155	1.443	2.309	0.139	5.210	10.420
1000	4.330	1.155	1.443	2.309	0.139	5.246	10.492
1010	4.373	1.155	1.443	2.309	0.139	5.282	10.563
1020	4.417	1.155	1.443	2.309	0.139	5.318	10.635
1030	4.460	1.155	1.443	2.309	0.139	5.354	10.707
1040	4.503	1.155	1.443	2.309	0.139	5.390	10.779
1050	4.547	1.155	1.443	2.309	0.139	5.426	10.852
1060	4.590	1.155	1.443	2.309	0.139	5.462	10.925
1070	4.633	1.155	1.443	2.309	0.139	5.499	10.997
1080	4.677	1.155	1.443	2.309	0.139	5.535	11.071
1090	4.720	1.155	1.443	2.309	0.139	5.572	11.144

1100	4.763	1.155	1.443	2.309	0.139	5.609	11.217
1110	4.806	1.155	1.443	2.309	0.139	5.645	11.291
1120	4.850	1.155	1.443	2.309	0.139	5.682	11.365
1130	4.893	1.155	1.443	2.309	0.139	5.719	11.439
1140	4.936	1.155	1.443	2.309	0.139	5.756	11.513
1150	4.980	1.155	1.443	2.309	0.139	5.794	11.587
1160	5.023	1.155	1.443	2.309	0.139	5.831	11.662
1170	5.066	1.155	1.443	2.309	0.139	5.868	11.736
1180	5.110	1.155	1.443	2.309	0.139	5.906	11.811
1190	5.153	1.155	1.443	2.309	0.139	5.943	11.886
1200	5.196	1.155	1.443	2.309	0.139	5.981	11.961
1210	5.239	1.155	1.443	2.309	0.139	6.018	12.037
1220	5.283	1.155	1.443	2.309	0.139	6.056	12.112
1230	5.326	1.155	1.443	2.309	0.139	6.094	12.188
1240	5.369	1.155	1.443	2.309	0.139	6.132	12.264
1250	5.413	1.155	1.443	2.309	0.139	6.170	12.340
1260	5.456	1.155	1.443	2.309	0.139	6.208	12.416
1270	5.499	1.155	1.443	2.309	0.139	6.246	12.492
1280	5.543	1.155	1.443	2.309	0.139	6.284	12.568
1290	5.586	1.155	1.443	2.309	0.139	6.322	12.645
1300	5.629	1.155	1.443	2.309	0.139	6.361	12.721
1310	5.672	1.155	1.443	2.309	0.139	6.399	12.798
1320	5.716	1.155	1.443	2.309	0.139	6.437	12.875
1330	5.759	1.155	1.443	2.309	0.139	6.476	12.952
1340	5.802	1.155	1.443	2.309	0.139	6.514	13.029
1350	5.846	1.155	1.443	2.309	0.139	6.553	13.106
1360	5.889	1.155	1.443	2.309	0.139	6.592	13.183
1370	5.932	1.155	1.443	2.309	0.139	6.630	13.261

B.2 Calibration of Thermocouple Data Acquisition System

The total measurement uncertainty estimated and provided in Table B.1 was checked by calibrating thermocouple data acquisition system at 22 °C in a water bath thermostat. Measurements for each thermocouple was repeated 40 times under the same conditions. Calibration data is provided in Table B.2. Standard deviation for both the estimated uncertainty and calibration data are within the same range.

Table B.2: Calibration of thermocouple data acquisition system.

Tests	Reference Temperature (°C)	Thermocouple 1 (°C)	Thermocouple 2 (°C)	Thermocouple 3 (°C)	Thermocouple 4 (°C)	Thermocouple 5 (°C)
1	22.00	23.25	25.25	22.75	24.25	24.75
2	22.00	23.00	24.75	21.50	26.25	26.00
3	22.00	24.50	24.25	21.75	27.00	26.25
4	22.00	26.75	18.25	24.75	23.00	27.00
5	22.00	22.50	23.00	27.25	23.25	24.50
6	22.00	20.25	23.75	26.50	24.50	21.00
7	22.00	25.75	20.75	24.50	21.25	20.00
8	22.00	20.00	21.75	20.25	20.25	22.75
9	22.00	19.50	21.75	21.75	24.25	19.75
10	22.00	22.75	26.50	20.25	19.25	20.75
11	22.00	23.25	24.50	25.75	18.25	20.50
12	22.00	22.75	25.75	19.25	20.75	21.50
13	22.00	21.75	22.00	22.75	21.50	22.00
14	22.00	21.75	22.50	20.75	22.00	20.50
15	22.00	22.25	23.00	25.25	23.75	24.50
16	22.00	18.75	25.50	23.75	24.50	23.50
17	22.00	24.50	26.00	24.75	20.50	24.50
18	22.00	24.75	19.25	21.75	26.50	21.75
19	22.00	21.75	20.00	22.50	22.50	20.50
20	22.00	25.00	21.75	20.75	22.75	22.75
21	22.00	23.75	20.75	20.00	24.50	25.50
22	22.00	20.75	21.25	24.00	24.75	25.75
23	22.00	20.50	23.75	25.50	20.25	26.50
24	22.00	27.25	24.50	22.00	23.50	27.50
25	22.00	25.25	22.75	26.75	23.00	20.25
26	22.00	20.50	24.75	25.75	24.75	23.50
27	22.00	24.25	20.25	25.25	25.50	24.50
28	22.00	25.75	25.75	20.50	26.75	24.75
29	22.00	23.25	24.50	21.75	25.50	25.75
30	22.00	22.75	22.25	24.50	25.75	25.75
31	22.00	23.00	20.50	25.50	20.25	21.75
32	22.00	24.50	26.25	26.00	21.50	24.75
33	22.00	26.75	25.50	24.75	22.75	25.50
34	22.00	21.75	25.25	22.00	21.75	23.25
35	22.00	21.50	23.25	23.75	25.50	22.75
36	22.00	26.00	19.75	25.50	20.75	23.50
37	22.00	20.50	21.75	26.25	23.00	20.75

38	22.00	22.75	24.25	25.25	26.25	24.75
39	22.00	23.50	26.75	25.75	25.75	24.25
40	22.00	23.50	24.75	26.00	24.75	23.75
Mean		23.06	23.22	23.63	23.32	23.49
Std.dev		2.074	2.198	2.207	2.233	2.148

APPENDIX C

RADIATION LOSS CORRECTION

Temperature measured by thermocouple may differ significantly from the true gas temperature because of radiation heat loss from the thermocouple surface to the cooler surrounding walls. Error due to radiation loss was corrected according to the methodology developed by Blevins & Pitts (1999) and have been applied by other researchers (Brohez *et al.*, 2004; Rashidian *et al.*, 2017; Roberts *et al.*, 2013). In this method, maximum and minimum measurement error which occur when using bare bead and single shielded aspirated thermocouple (TC), respectively, are used to estimate the error in sheathed thermocouple with the same bead size. A description of model equations for bare-bead and single-shielded thermocouple are given in the following subsections.

C.1 Model Equations for Bare-Bead Thermocouple

A representation of the heat transfers in a bare-bead thermocouple is shown in Fig. C.1 (Blevins & Pitts, 1999). Heat transfers are through radiation and convection. The energy balance on the bead is given by the following expression:

$$h_{bg}(T_g - T_b) = \varepsilon_b \sigma (T_b^4 - T_\infty^4), \quad (C.1)$$

where h_{bg} is the heat transfer coefficient between external gas flow and bare thermocouple bead, T_b , T_g , and T_∞ are thermocouple bead temperature, gas temperature and average effective temperature of surrounding, respectively, ε_b is the thermocouple bead emissivity and σ is the Stefan-Boltzmann constant.

h_{bg} is evaluated from the following correlation:

$$h_{bg} = Nu_d \frac{\lambda_g}{D_b}, \quad (C.2)$$

where D_b is the bead diameter, λ_g is gas thermal conductivity and Nu_d is Nusselt number. Nu_d is estimated using Whitaker's correlation for external flow over a sphere (Whitaker, 1972) given by Eq. (C.3).

Figure C.1: Heat transfers in a bare-bead thermocouple.

$$Nu_d = 2 + (0.4Re^{0.5} + 0.06Re^{2/3})Pr^{0.4} \quad 3.5 \leq Re \leq 7.6 \times 10^4 \quad (C.3)$$

and

$$\lambda_g = \frac{\mu_g c_p}{Pr}, \quad (C.4)$$

where Re is Reynolds number, Pr is Prandtl number, c_p specific heat capacity and μ_g is dynamic viscosity of gas.

Therefore, in order to correct a temperature measured by bare-bead thermocouple for radiation loss, raw temperature (measured) and surrounding temperature are required.

C.2 Model Equations for Single-Shielded Thermocouple

A representation of the heat transfers in a single-shielded aspirated thermocouple is shown in Fig. C.2 (Blevins & Pitts, 1999). Heat transfers are also through radiation and convection. The energy balance on the bead is given as follows:

Figure C.2: Heat transfers in a single-shielded aspirated thermocouple.

$$h_{ab}(T_g - T_b) = \varepsilon_b \sigma (T_b^4 - T_o^4), \quad (C.5)$$

and on the shield

$$h_{as}(T_g - T_0) + h_{gs}(T_g - T_0) = -\varepsilon_b \sigma \left(\frac{A_b}{A_0} \right) (T_b^4 - T_0^4) + \varepsilon_0 \sigma (T_0^4 - T_\infty^4), \quad (C.6)$$

where A_b and A_0 are the surface area of thermocouple bead and outermost shield, respectively, h_{ab} is the heat transfer coefficient between aspirating gas flow and bare thermocouple bead, h_{as} is the heat transfer coefficient between aspirating gas flow and shield, h_{gs} is the heat transfer coefficient between external gas flow and shield, T_0 is the outermost shield temperature and ε_0 is the outermost shield emissivity.

h_{ab} is calculated in the same way as for bare-bead thermocouple using Eqs. (C.2-C.4). h_{as} and h_{gs} are calculated using correlation for a cylinder in crossflow (Rashidian *et al.*, 2017), as shown in the following expressions:

$$Nu_d = 0.989 Re^{0.330} Pr^{1/3} \quad 0.4 \leq Re \leq 4 \quad (C.7)$$

$$Nu_d = 0.911 Re^{0.385} Pr^{1/3} \quad 4 \leq Re \leq 40 \quad (C.8)$$

$$Nu_d = 0.683 Re^{0.466} Pr^{1/3} \quad 40 \leq Re \leq 4000 \quad (C.9)$$

$$Nu_d = 0.193 Re^{0.618} Pr^{1/3} \quad 4000 \leq Re \leq 40000 \quad (C.10)$$

Thus, in order to correct a temperature measured by single-shielded aspirated thermocouple for radiation loss, raw temperature (measured) and surrounding temperature are also required.

APPENDIX D

NUMERICAL MODELLING TECHNIQUES

D.1 Radiation Model Formulation

When radiation passes through a medium, the intervening material absorbs and increments its radiant intensity I in the Ω direction. This process is governed by Radiative Transfer Equation (RTE). For a specific wavelength, λ , the equation is expressed as follows (Fiveland, 1988; Incropera *et al.*, 2006):

$$\frac{dI_\lambda}{ds} = -\beta_\lambda I_\lambda + k_{a\lambda} I_{b\lambda} + \frac{k_{s\lambda}}{4\pi} \int_{4\pi} I_\lambda(\Omega) d\Omega + k_{pa\lambda} I_{pb\lambda} + \frac{k_{ps\lambda}}{4\pi} \int_{4\pi} I_\lambda(\Omega) d\Omega, \quad (D.1)$$

where I_λ is the radiative intensity at wavelength λ , β_λ is the extinction coefficient, which is defined as follows:

$$\beta_\lambda = k_{a\lambda} + k_{s\lambda} + k_{pa\lambda} + k_{ps\lambda}, \quad (D.2)$$

$k_{a\lambda}$ is the absorption coefficient at wavelength λ , $k_{s\lambda}$ scattering coefficient at wavelength λ , $k_{pa\lambda}$ particle absorption coefficient at wavelength λ , $k_{ps\lambda}$ particle scattering coefficient at wavelength λ , $I_{b\lambda}$ is the black body intensity at wavelength λ , Ω is the solid angle and s is the distance in Ω direction. The black body intensity at wavelength λ is expressed by Eq. (D.3):

$$I_{b\lambda} = \frac{2C_R}{n^2 \lambda^5 (\exp(C_{R2}/n\lambda T) - 1)}, \quad (D.3)$$

and $C_R = 0.595522 \times 10^{-16} \text{ W m}^2/\text{s}$ and $C_{R2} = 0.01439 \text{ m K}$. The in-scattering component is assumed to be isotropic. When the medium has several components, the absorption coefficient $k_{a\lambda}$ is expressed by Eq. (D.4):

$$k_{a\lambda} = \sum_i k_{a\lambda i}, \quad (D.4)$$

where i represent the participating media, such as, fuel particles, CO₂, H₂O, or soot.

A gray gas medium is the one whose optical properties such as absorptivity, reflectivity, scattering coefficient and refractive index do not depend on wavelength. For a gray medium, Eq. (3.29) is integrated over entire spectrum to produce a wavelength independent equation.

The particle radiation is valid for both gray and multiband radiation for continuous media. However, for the case of multiband radiation, the particle properties are still gray. The surface and continuum properties can be spectral, but the particle properties are gray. Particle scattering is isotropic.

The boundary condition that is applied to the RTE Eq. (D.1) for each wavelength λ is expressed by Eq. (D.5):

$$I_\lambda(\mathbf{s}) = \epsilon_{w\lambda} I_{b\lambda} + \frac{\rho_{w\lambda}^d}{\pi_{eff}} \int_{\mathbf{n} \cdot \mathbf{s}' < 0} I_\lambda(s') |\mathbf{n} \cdot \mathbf{s}'| d\Omega + \rho_{w\lambda}^s I_\lambda(\mathbf{s}^s) + \tau_{w\lambda}(\mathbf{s}^i) I_\lambda(\mathbf{s}^i), \quad (D.5)$$

where $\epsilon_{w\lambda}$ is the diffuse emissivity, $\rho_{w\lambda}^d$ is the diffuse reflectivity, $\pi_{eff} = \sum_{\mathbf{s}_i \cdot \mathbf{n}_i} w_i (\mathbf{s}_i \cdot \mathbf{n}_i)$ is the half moment for the ordinate set chosen, $\rho_{w\lambda}^s$ is the specular reflectivity, $\tau_{w\lambda}$ is the transmissivity. Only interfaces can be partially transmissive; all other external boundaries are modeled as opaque. $\mathbf{s}^s = \mathbf{s} - 2(\mathbf{s} \cdot \mathbf{n})\mathbf{n}$, $\mathbf{s}^i$ is the incoming ray direction as determined by the laws of refraction or Snell's law, $\mathbf{n}$ is the surface normal.

The radiant heat flux for a particular direction, q_r is obtained by integrating Eq. (D.5) for all the solid angles and the entire spectrum as follows:

$$q_r(r) = \int_0^\infty \int_{4\pi} I_\lambda(s) s d\Omega d\lambda. \quad (D.6)$$

Equation (D.6) enables energy to be exchanged between radiant energy field and fluid. This is achieved by incorporating the divergence of heat flux Eq. (D.6) into gas phase energy equation. The divergence of Eq. (D.6) is evaluated as follows (CD-Adapco, 2017; Incropera *et al.*, 2006):

$$\nabla \cdot q_r = \int_0^\infty k_{a\lambda} \left(4\pi I_{b\lambda} - \int_{4\pi} I_\lambda d\Omega \right) d\lambda, \quad (D.7)$$

Similarly, the divergence of the heat flux for particle is expressed as follows:

$$\nabla \cdot q_{pr} = \int_0^\infty k_{pa\lambda} \left(4\pi I_{pb\lambda} - \int_{4\pi} I_\lambda d\Omega \right) d\lambda, \quad (D.8)$$

DOM solves RTE equation for a given direction. The radiation field is divided into discrete solid angles, which are measured in steradian [sr], as shown in Fig. D.1. One steradian is a solid angle whose area at the sphere surface is equal to the square of radius and subtended at spheres' centre. Therefore, a whole sphere has a solid angle of 4π sr.

Figure D.1: Illustration of a discrete solid angle used for DOM solution.

DOM requires specification of the number of solid angles or ordinates into which the sphere surrounding any given point is divided. The accuracy of the solution is improved by using a large number of solid angles or ordinates. More details about this method can be found in

Fiveland (1984) and Klason *et al.* (2008). Based on this method, Eq. (D.1) is discretized as follows:

$$s_i \cdot \nabla I_{i\Delta\lambda} = -\beta_{\Delta\lambda} I_{i\Delta\lambda} + k_{a\Delta\lambda} I_{b\Delta\lambda} + \frac{k_{s\Delta\lambda}}{4\pi} \sum_{j=1}^n w_j I_{j\Delta\lambda} + \bar{k}_{pa\Delta\lambda} I_{pb\Delta\lambda} + \frac{\bar{k}_{ps\Delta\lambda}}{4\pi} \sum_{j=1}^n w_j I_{j\Delta\lambda}, \quad (D.9)$$

where $\Delta\lambda$ is a wavelength band from λ_m to λ_n , w_j is the quadrature weights that is a function of the chosen ordinates, n is the number of ordinates, $\bar{k}_{pa\Delta\lambda}$ and $\bar{k}_{ps\Delta\lambda}$ are equivalent particle absorption and scattering coefficients, respectively.

The black body emission in the wavelength band λ_m to λ_n is expressed by Eq. (D.10):

$$I_{b\Delta\lambda} = \int_0^{\lambda_n} I_{b\lambda} d\lambda - \int_0^{\lambda_m} I_{b\lambda} d\lambda. \quad (D.10)$$

The equivalent particle absorption and scattering coefficients are expressed by Eqs. (D.11) and (D.12), respectively.

$$\bar{k}_{pa\Delta\lambda} = \sum_i Q_{a,i} N_i \frac{\pi d_i^2}{4}, \quad (D.11)$$

$$\bar{k}_{ps\Delta\lambda} = \sum_i Q_{s,i} N_i \frac{\pi d_i^2}{4}, \quad (D.12)$$

where i indicates the parcel index number, N_i is the particle number density, $Q_{a,i}$ is the particle absorption efficiency and $Q_{s,i}$ is the particle scattering efficiency.

RTE equation is set and solved for each direction. Therefore, for a radiation field, the number of equations to be computed is equal to the number of ordinates. The resulting algebraic equations are solved using appropriate techniques as applied in other transport equations. It is

important to evaluate boundary conditions at the wall. Thus, after angular discretization, the boundary conditions given by Eq. (D.5) take the following form:

$$I_{i\Delta\lambda,w} = \epsilon_{w\Delta\lambda} I_{b\Delta\lambda} + \frac{\rho_{w\Delta\lambda}^d}{\pi_{eff}} \sum_{\mathbf{n} \cdot \mathbf{s}'_j < 0} I_{j\Delta\lambda} |\mathbf{n} \cdot \mathbf{s}'_j|_w + f \rho_{w\Delta\lambda}^s I_{\Delta\lambda}(\mathbf{s}^s) + \tau_{w\Delta\lambda} I_{i\Delta\lambda}, \quad (D.13)$$

Beside the other symbols defined before, f is the correction factor that is used when the direction of specular reflection is not aligned with any discrete ordinate direction. The diffuse reflection term represents summation over incident ordinate directions.

Convergence of solution is determined using the usual way of the normalized difference in the incident energy from successive space-angle sweeps. This is set by specifying an appropriate convergence tolerance on the solver.

Radiation energy is exchanged with fluid medium through a source term in the gas phase energy Eq. (4.5). The coupling is through Eq. (D.7) whose discretized form for a particular cell is expressed by Eq. (D.14):

$$-\nabla \cdot q_r = \sum_{\lambda} k_{a\Delta\lambda} \left(\sum_{j=1}^n w_j I_{j\Delta\lambda} - 4\pi I_{b\Delta\lambda} \right), \quad (D.14)$$

The net absorption rate of radiative energy by all particles within a given cell is expressed by Eq. (D.15):

$$-\nabla \cdot q_{pr} = \sum_{\lambda} \bar{k}_{pa\Delta\lambda} \left(\sum_{j=1}^n w_j I_{j\Delta\lambda} - 4\pi I_{pb\Delta\lambda} \right), \quad (D.15)$$

At convergence, Eqs. (D.15) exactly balances the net radiative energy that all particles absorb.

D.2 Finite Volume Discretization for Continuous Phase

In this technique, the computation domain is divided into a finite number of small control volumes which are equivalent to the cell in a computational grid. Integral transport equations in their discrete form are applied at each control volume, V .

The integral form of a general transport equation of a scalar quantity, ϕ , in a continuum is given by Eq. (D.16):

$$\frac{d}{dt} \int_V \rho \chi \phi dV + \int_A \rho \phi (\mathbf{v} - \mathbf{v}_{gg}) \cdot d\mathbf{a} = \int_A \Gamma \nabla \phi \cdot d\mathbf{a} + \int_V S_\phi dV, \quad (D.16)$$

The discrete form of Eq. (D.16) applied to a cell-centered control volume for cell-0 is expressed by Eq. (D.17):

$$\frac{d}{dt} (\rho \chi \phi V)_0 + \sum_f [\rho \phi (\mathbf{v} \cdot \mathbf{a} - G)]_f = \sum_f (\Gamma \nabla \phi \cdot \mathbf{a})_f + (S_\phi V)_0, \quad (D.17)$$

where, $\mathbf{a}$ is the face area vector, A is the face area, subscript f is the face quantity, G is the grid flux, $\mathbf{v}$ is the velocity $\mathbf{v}_{gg}$ is the grid velocity, subscript 0 is the cell-0 quantity and Γ is the diffusion coefficient. G is computed from the mesh motion as $G_f = \mathbf{v}_{gg} \cdot \mathbf{a}_f$.

The different terms in Eq. (D.17), namely, transient term, convective flux, diffusion flux and source term are discretized using different techniques.

The transient term is discretized using first-order or second-order temporal discretization scheme. The first-order scheme is Euler implicit scheme which consider the current time level $(n + 1)$ and the previous time level n , expressed by Eq. (D.18):

$$\frac{d}{dt} (\rho \chi \phi V)_0 = \frac{(\rho \chi \phi V)_0^{n+1} - (\rho \chi \phi V)_0^n}{\Delta t}. \quad (D.18)$$

The second order temporal scheme uses solutions at three time levels; current time level ($n + 1$) and two previous time levels, n and $(n-1)$. It is expressed by Eq. (D.19):

$$\frac{d}{dt}(\rho\chi\phi V)_0 = \frac{(\gamma^2 - 1)[(\rho\chi\phi V)_0^{n+1} - (\rho\chi\phi V)_0^n] + [(\rho\chi\phi V)_0^{n-1} - (\rho\chi\phi V)_0^n]}{\gamma(\gamma - 1)\Delta t^{n+1}}. \quad (D.19)$$

and

$$\gamma = 1 + \frac{\Delta t^{n+1}}{\Delta t^n}, \quad \Delta t^{n+1} = t^{n+1} - t^n, \quad \Delta t^n = t^n - t^{n-1}. \quad (D.20)$$

On the first time step of a second order temporal scheme, a first order discretization scheme is used since only two time levels are available.

The convective flux at a face is discretized as follows:

$$[\rho\phi(\mathbf{v} \cdot \mathbf{a} - G)]_f = (\dot{m}\phi)_f = \dot{m}_f\phi_f. \quad (D.21)$$

where $\dot{m}_f$ is the mass flow rate at the face. In STAR CCM+, the face value of the scalar ϕ_f is computed from cell value using different schemes. In this work first-order upwind, second order upwind and central differencing scheme have been applied for different scenarios.

In case of first-order upwind scheme, the convective flux is calculated as follows:

$$(\dot{m}\phi)_f = \begin{cases} \dot{m}_f\phi_0 & \text{for } \dot{m}_f \geq 0 \\ \dot{m}_f\phi_1 & \text{for } \dot{m}_f < 0 \end{cases} \quad (D.22)$$

This scheme is less accurate because it introduces a dissipative error which help the solution in convergence. It is used to obtain initial solution before switching to more accurate schemes.

In case of second-order upwind scheme, the convective flux is calculated as follows:

$$(\dot{m}\phi)_f = \begin{cases} \dot{m}_f \phi_{f,0} & \text{for } \dot{m}_f \geq 0 \\ \dot{m}_f \phi_{f,1} & \text{for } \dot{m}_f < 0 \end{cases} \quad (D.23)$$

where the face values $\phi_{f,0}$ and $\phi_{f,1}$ are linearly interpolated from the cell values on either side of the face as expressed by Eqs. (D.24) and (D.25), respectively.

$$\phi_{f,0} = \phi_0 + \mathbf{s}_0 \cdot (\Delta\phi)_{r,0}, \quad (D.24)$$

$$\phi_{f,1} = \phi_1 + \mathbf{s}_1 \cdot (\Delta\phi)_{r,1}, \quad (D.25)$$

where $\mathbf{s}$ is the vector between cell face and cell centroid, $\mathbf{x}$ is the position vector and $\mathbf{s}_0 = \mathbf{x}_f - \mathbf{x}_0$, $\mathbf{s}_1 = \mathbf{x}_f - \mathbf{x}_1$ while $(\Delta\phi)_{r,0}$ and $(\Delta\phi)_{r,1}$ are the limited reconstruction gradients in cells 0 and 1, respectively. This scheme has a second-order accuracy. Despite introduction of dissipation errors through reconstruction gradients, it is still more accurate than first-order scheme. However, it has a poorer convergence.

And in case of central differencing scheme, the convective flux is calculated as follows:

$$(\dot{m}\phi)_f = \dot{m}_f (\omega_f \phi_0 + (1 - \omega_f) \phi_1). \quad (D.26)$$

where ω_f is the geometric weighting factor related to mesh stretching. For uniform mesh ω_f would have a value of 0.5. It is second-order accurate. However, it is prone to dispersive error which is problematic to positive definite quantities such as temperature and turbulent kinetic energy.

In diffusion term, the interior face gradient $(\nabla\phi_f)$ is computed from cell values ϕ_0 and ϕ_1 through the following expression:

$$\nabla\phi_f = (\phi_1 - \phi_0)\vec{\alpha} + \overline{\nabla\phi} - (\overline{\nabla\phi} \cdot \mathbf{ds})\vec{\alpha}, \quad (D.27)$$

where

$$\vec{\alpha} = \frac{\mathbf{a}}{\mathbf{a} \cdot \mathbf{ds}}, \quad \mathbf{ds} = \mathbf{x}_1 - \mathbf{x}_0 \text{ and } \overline{\nabla\phi} = \frac{\nabla\phi_0 + \nabla\phi_1}{2}.$$

The second-order accurate expression for diffusion flux at an interior face, D_f is subsequently represented by Eq. (D.28):

$$D_f = \Gamma_f \nabla\phi_f \cdot \mathbf{a} = \Gamma_f (\phi_1 - \phi_0) \vec{\alpha} \cdot \mathbf{a} + \overline{\nabla\phi} \cdot \mathbf{a} - (\overline{\nabla\phi} \cdot \mathbf{ds}) \vec{\alpha} \cdot \mathbf{a}, \quad (D.28)$$

where Γ_f is a suitable average value of the cell values.

The second and third terms in Eq. (D.28) represent the secondary gradient contribution. They are essential for maintaining accuracy on non-orthogonal meshes. The formulation of the diffusion flux at the face assumes that the centroids of cells 0 and 1 lie on opposing sides of the face, as illustrated by Fig. D.2. It is further assumed that their location is consistent with the convention that the face area vector points out of cell 0. None-physical solutions are avoided by using mesh for which the angle between $\mathbf{a}$ and $\mathbf{ds}$ should be less than 90 degrees. In STAR CCM+ software, this is ensured by checking mesh skewness angle which is computed and stored in the adjacent cell. The value that is stored in each cell represents the largest skewness angle for each face of the cell.

Figure D.2: Discretization of diffusion flux at an interior face.

Similarly, the second-order accurate expression for diffusion flux at a boundary face, D_f is subsequently represented by Eq. (D.29):

$$D_f = \Gamma_f \nabla \phi_f \cdot \mathbf{a} = \Gamma_f (\phi_f - \phi_0) \tilde{\alpha} \cdot \mathbf{a} + \nabla \phi \cdot \mathbf{a} - (\nabla \phi \cdot \mathbf{ds}) \tilde{\alpha} \cdot \mathbf{a}, \quad (D.29)$$

where $\mathbf{ds} = \mathbf{x}_f - \mathbf{x}_0$.

D.3 Lagrange Phase Formulation

Solid-phase was modeled through Lagrangian multiphase approach. The Lagrangian multiphase model enables solution of any number of different phases with each being modelled in Lagrangian framework. In this framework, parcels which represent particles are tracked in the continuum. A parcel represents a localized group of dispersed phases having the same properties. A given number of particles are grouped together in a single parcel. Thus a parcel is analogous to a cell used in discretization of a continuous fluid domain. To improve prediction accuracy and a better representation of the entire population of particles, a large number of parcels should be used.

The position of each parcel, $r_p(t)$ with respect to the frame of reference, is tracked using equation of motion:

$$\frac{dr_p}{dt} = \mathbf{v}_p - \mathbf{v}_g, \quad (D.30)$$

where $\mathbf{v}_g(\mathbf{x}, t)$ is the grid velocity which is evaluated at parcel mean centroid and $\mathbf{v}_p(t)$ is the absolute velocity of the parcel.

The solution of equations in a Lagrangian framework implies the time-marching of ordinary differential equations (ODEs). An ODE for the position of each parcel, Eq. (D.30) is formulated in order to solve the governing equation for Lagrangian phase equations.

The conversion of wood particles in the fixed bed is unsteady. A time-step in an unsteady simulation advances the solution from time t to time $t + \Delta t$. In STAR CCM+ software, a single iteration of the unsteady solver for the Lagrangian Multiphase model involves:

1. Recovering the Lagrangian Multiphase solution at time t .
2. Advancing the Lagrangian Multiphase solution to time $t + \Delta t$ by time-marching. A local time-step is used for each parcel. The time-step is adjusted dynamically according to the time-step controls in force.

These two steps are executed in each iteration of the unsteady solver, before the flow solver. Through two way coupling model, source terms that the Lagrangian phase models compute are stored for subsequent application in their respective transport equations in continuous phase.

APPENDIX E

SPECIES GENERATION AND DEPLETION IN FUEL BED

E.1 Particle Packing Density

Figures E.1 – E.12 show comparison of species generation and depletion in the fuel bed at different bed heights for wood combustion in a fixed bed under oxy-fuel conditions and different particles packing density. Comparisons are done when the flame front is passing through 4 cm, 3 cm, 2 cm and 1 cm from fuel bed bottom, respectively.

Figure E.1: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 4 cm from the grate: (a) Tar mole fraction (b) CO mole fraction.

Figure E.2: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 4 cm from the grate: (a) CH₄ mole fraction (b) H₂ mole fraction.

Figure E.3: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 4 cm from the grate: (a) O₂ mole fraction (b) H₂O mole fraction.

(a)

(b)

Figure E.4: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 3 cm from the grate: (a) Tar mole fraction (b) CO mole fraction.

(a)

(b)

Figure E.5: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 3 cm from the grate: (a) CH₄ mole fraction (b) H₂ mole fraction.

Figure E.6: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 3 cm from the grate: (a) O_2 mole fraction (b) H_2O mole fraction.

Figure E.7: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 2 cm from the grate: (a) Tar mole fraction (b) CO mole fraction.

(a)

(b)

Figure E.8: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 2 cm from the grate: (a) CH₄ mole fraction (b) H₂ mole fraction.

(a)

(b)

Figure E.9: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 2 cm from the grate: (a) O₂ mole fraction (b) H₂O mole fraction.

(a)

(b)

Figure E.10: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 1 cm from the grate: (a) Tar mole fraction (b) CO mole fraction.

(a)

(b)

Figure E.11: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 1 cm from the grate: (a) CH₄ mole fraction (b) H₂ mole fraction.

Figure E.12: Comparison of species concentration profiles along axial length of the bed for different fuel types burning under oxy-fuel condition when reaction front is at 1 cm from the grate: (a) O₂ mole fraction (b) H₂O mole fraction.

Tables E.1 – E.5 show the peak values for the major combustible species mole fraction and temperature along axial length of the bed for combustion of different types of wood in a fixed bed under oxy-fuel conditions. The tables present values for position 1 cm to 10 cm of the fixed bed measured from fuel bed bottom.

Table E.1: Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for fuel type SD1 burning under oxy-fuel condition.

Temperature/ species mole fraction (-)	Peak values along axial length of the bed (Measure from the grate)									
	1 cm	2 cm	3 cm	4 cm	5 cm	6 cm	7 cm	8 cm	9 cm	10 cm
Temperature (K)	1156	1274	1307	1157	1027	1096	1115	1027	913	678
Tar	0.0131	0.0156	0.0153	0.0168	0.0159	0.0166	0.0100	0.0023	0.0001	0.0000
CO	0.0313	0.0330	0.0386	0.0305	0.0409	0.0478	0.0371	0.0110	0.0013	0.0002
CH ₄	0.0043	0.0045	0.0054	0.0058	0.0058	0.0058	0.0022	0.0004	0.0000	0.0000
H ₂	0.0429	0.0475	0.0494	0.0460	0.0446	0.0468	0.0364	0.0100	0.0011	0.0002

Table E.2: Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for fuel type WC + SD1 burning under oxy-fuel condition.

Temperature/ species mole fraction (-)	Peak values along axial length of the bed (Measure from the grate)									
	1 cm	2 cm	3 cm	4 cm	5 cm	6 cm	7 cm	8 cm	9 cm	10 cm
Temperature (K)	1048	1235	1314	1319	1263	1299	1200	922	801	656
Tar	0.0144	0.0168	0.0158	0.0176	0.0165	0.0212	0.0118	0.0006	0.0001	0.0000
CO	0.0270	0.0386	0.0366	0.0377	0.0410	0.0617	0.0404	0.0040	0.0013	0.0002
CH ₄	0.0050	0.0050	0.0046	0.0055	0.0060	0.0072	0.0026	0.0001	0.0000	0.0000
H ₂	0.0396	0.0551	0.0516	0.0507	0.0504	0.0541	0.0391	0.0036	0.0012	0.0003

Table E.3: Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for fuel type SD2 burning under oxy-fuel condition.

Temperature/ species mole fraction (-)	Peak values along axial length of the bed (Measure from the grate)									
	1 cm	2 cm	3 cm	4 cm	5 cm	6 cm	7 cm	8 cm	9 cm	10 cm
Temperature (K)	1236	1409	1381	1331	1246	1275	1196	1189	1082	978
Tar	0.0205	0.0266	0.0256	0.0242	0.0259	0.0253	0.0200	0.0113	0.0016	0.0001
CO	0.0843	0.0842	0.0822	0.0818	0.0801	0.0827	0.0526	0.0283	0.0073	0.0009
CH ₄	0.0067	0.0088	0.0085	0.0083	0.0092	0.0086	0.0055	0.0030	0.0003	0.0000
H ₂	0.0503	0.0633	0.0607	0.0679	0.0634	0.0604	0.0497	0.0267	0.0061	0.0008

Table E.4: Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for fuel type WC + SD2 burning under oxy-fuel condition.

Temperature/ species mole fraction (-)	Peak values along axial length of the bed (Measure from the grate)									
	1 cm	2 cm	3 cm	4 cm	5 cm	6 cm	7 cm	8 cm	9 cm	10 cm
Temperature (K)	1370	1380	1362	1227	1267	1280	1199	1157	1042	1444
Tar	0.0243	0.0220	0.0208	0.0212	0.0213	0.0270	0.0233	0.0100	0.0056	0.0027
CO	0.0947	0.0951	0.0946	0.0956	0.0953	0.0960	0.0621	0.0402	0.0187	0.0052
CH ₄	0.0078	0.0073	0.0072	0.0073	0.0075	0.0090	0.0074	0.0027	0.0011	0.0003
H ₂	0.0589	0.0527	0.0517	0.0598	0.0579	0.0648	0.0546	0.0546	0.0296	0.0161

Table E.5: Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for fuel type WC burning under oxy-fuel condition.

Temperature/ species mole fraction (-)	Peak values along axial length of the bed (Measure from the grate)									
	1 cm	2 cm	3 cm	4 cm	5 cm	6 cm	7 cm	8 cm	9 cm	10 cm
Temperature (K)	1385	1379	1364	1366	1330	1325	1298	1265	1134	1105
Tar	0.0259	0.0261	0.0227	0.0248	0.0226	0.0313	0.0260	0.0185	0.0174	0.0161
CO	0.1053	0.1047	0.1047	0.1057	0.1063	0.1062	0.0568	0.0543	0.0513	0.0481
CH ₄	0.0086	0.0085	0.0078	0.0084	0.0077	0.0110	0.0087	0.0048	0.0044	0.0039
H ₂	0.0603	0.0551	0.0554	0.0649	0.0616	0.0692	0.0564	0.0564	0.0541	0.0508

E.2 Wood Combustion in a Fixed Bed under Oxy-fuel Condition

Figures E.13 – E.24 show comparison of species generation and depletion in the fuel bed at different bed heights for wood combustion in a fixed bed under oxy-fuel conditions for different O₂/CO₂ mixtures. Comparisons are done when the flame front is passing through 4 cm, 3 cm, 2 cm and 1 cm from fuel bed bottom, respectively.

(a)

(b)

Figure E.13: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 4 cm from the grate: (a) Tar mole fraction (b) CO mole fraction.

(a)

(b)

Figure E.14: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 4 cm from the grate: (a) CH₄ mole fraction (b) H₂ mole fraction.

Figure E. 15: Comparison of species concentration profiles along axial length of the burning under oxy-fuel condition for different O_2/CO_2 mixtures when reaction front is at 4 cm from the grate: (a) O_2 mole fraction (b) H_2O mole fraction.

Figure E.16: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O_2/CO_2 mixtures when reaction front is at 3 cm from the grate: (a) Tar mole fraction (b) CO mole fraction.

Figure E.17: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 3 cm from the grate: (a) CH₄ mole fraction (b) H₂ mole fraction.

Figure E.18: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 3 cm from the grate: (a) O₂ mole fraction (b) H₂O mole fraction.

Figure E.19: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 2 cm from the grate: (a) Tar mole fraction (b) CO mole fraction.

Figure E.20: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 2 cm from the grate: (a) CH₄ mole fraction (b) H₂ mole fraction.

Figure E.21: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 2 cm from the grate: (a) O₂ mole fraction (b) H₂O mole fraction.

Figure E.22: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 1 cm from the grate: (a) Tar mole fraction (b) CO mole fraction.

Figure E.23: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 1 cm from the grate: (a) CH₄ mole fraction (b) H₂ mole fraction.

Figure E.24: Comparison of species concentration profiles along axial length of the bed burning under oxy-fuel condition for different O₂/CO₂ mixtures when reaction front is at 1 cm from the grate: (a) O₂ mole fraction (b) H₂O mole fraction.

Tables E.6 – E.9 show the peak values for the major combustible species mole fraction and temperature along axial length of the bed for combustion of wood in a fixed bed under oxy-fuel conditions for different O₂/CO₂ mixtures. The tables present values for position 1cm to 10 cm of the fixed bed measured from fuel bed bottom.

Table E.6: Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for wood combustion burning under oxy-fuel condition of 21% O₂/79% CO₂.

Temperature/ species mole fraction (-)	Peak values along axial length of the bed (Measure from the grate)									
	1 cm	2 cm	3 cm	4 cm	5 cm	6 cm	7 cm	8 cm	9 cm	10 cm
Temperature (K)	1375	1365	1346	1367	1368	1369	1388	1289	1190	907
Tar	0.0205	0.0266	0.0257	0.0242	0.0260	0.0254	0.0201	0.0113	0.0016	0.0001
CO	0.0444	0.0544	0.0523	0.0619	0.0603	0.0629	0.0527	0.0284	0.0073	0.0009
CH ₄	0.0067	0.0088	0.0085	0.0083	0.0092	0.0086	0.0055	0.0030	0.0003	0.0000
H ₂	0.0505	0.0635	0.0609	0.0681	0.0636	0.0606	0.0499	0.0268	0.0062	0.0008

Table E.7: Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for wood combustion burning under oxy-fuel condition of 30% O₂/70% CO₂.

Temperature/ species mole fraction (-)	Peak values along axial length of the bed (Measure from the grate)									
	1 cm	2 cm	3 cm	4 cm	5 cm	6 cm	7 cm	8 cm	9 cm	10 cm
Temperature (K)	1493	1493	1492	1493	1493	1493	1493	1493	1458	1446
Tar	0.0138	0.0217	0.0275	0.0244	0.0273	0.0238	0.0160	0.0083	0.0028	0.0003
CO	0.0706	0.0955	0.1018	0.1077	0.1018	0.0996	0.0844	0.0289	0.0162	0.0031
CH ₄	0.0033	0.0076	0.0100	0.0087	0.0104	0.0084	0.0038	0.0017	0.0002	0.0000
H ₂	0.0481	0.0606	0.0785	0.0732	0.0700	0.0639	0.0503	0.0274	0.0150	0.0028

Table E.8: Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for wood combustion burning under oxy-fuel condition of 40% O₂/60% CO₂.

Temperature/ species mole fraction (-)	Peak values along axial length of the bed (Measure from the grate)									
	1 cm	2 cm	3 cm	4 cm	5 cm	6 cm	7 cm	8 cm	9 cm	10 cm
Temperature (K)	1035	1414	1541	1541	1541	1541	1541	1499	1295	1251
Tar	0.0099	0.0117	0.0131	0.0201	0.0179	0.0179	0.0044	0.0032	0.0002	0.0000
CO	0.0189	0.0197	0.0388	0.0528	0.0578	0.0616	0.0342	0.0296	0.0024	0.0001
CH ₄	0.0032	0.0036	0.0044	0.0068	0.0063	0.0066	0.0010	0.0004	0.0000	0.0000
H ₂	0.0099	0.0117	0.0131	0.0201	0.0179	0.0179	0.0044	0.0032	0.0002	0.0000

Table E.9: Peak values of temperature and the major combustible species mole fraction along the axial length of the fixed bed for wood combustion burning under oxy-fuel condition of 50% O₂/50% CO₂.

Temperature/ species mole fraction (-)	Peak values along axial length of the bed (Measure from the grate)									
	1 cm	2 cm	3 cm	4 cm	5 cm	6 cm	7 cm	8 cm	9 cm	10 cm
Temperature (K)	1605	1596	1605	1605	1605	1605	1605	1605	1557	1296
Tar	0.0172	0.0206	0.0167	0.0176	0.0184	0.0189	0.0036	0.0013	0.0002	0.0000
CO	0.0521	0.0595	0.0529	0.0458	0.0495	0.0631	0.0238	0.0117	0.0022	0.0003
CH ₄	0.0063	0.0072	0.0057	0.0063	0.0068	0.0068	0.0007	0.0001	0.0000	0.0000
H ₂	0.0575	0.0669	0.0585	0.0529	0.0535	0.0606	0.0218	0.0105	0.0020	0.0003

APPENDIX F

LIST OF PUBLICATIONS FROM THIS THESIS

Journal Publications

1. 1. Tanui J. K., Kioni P. N., Mirre T. and Nowitzki M. (2018). The effect of carbon dioxide on flame propagation speed of wood combustion in a fixed bed under oxy-fuel conditions. *Fuel Processing Technology*, 179, 285-295.
<https://www.sciencedirect.com/science/article/pii/S0378382018304867>
2. Tanui J. K., Kioni P. N., Mirre T. and Nowitzki M. (2019). Chemical, thermal and dilution effects of carbon dioxide in oxy-fuel combustion of wood in a fixed bed. *Journal of Mechanical Science and Technology*, 33(12), 6063-6073.
<http://link.springer.com/article/10.1007/s12206-019-1150-z>
3. Tanui J. K., Kioni P. N., Mirre T. and Nowitzki M. (2019). Application of CFD-DEM method in modelling of wood combustion in a fixed bed. *Submitted to Bulgarian Chemical Communication*.
4. Tanui J. K., Kioni P. N., Mirre T., Nowitzki M. and Karuri N. W. (2020). The influence of particle packing density on wood combustion in a fixed bed under oxy-fuel conditions. *Energy*, 194.
<https://www.sciencedirect.com/science/article/abs/pii/S0360544219325587>

Conference Papers

1. Tanui J. K., Kioni P. N., Mirre T. and Nowitzki M. (2018). Cooperation with Kenya – PhD research on numerical simulation of wood combustion in a laboratory fixed bed using CFD-DEM Approach. **poster in Forschung in Wildau – innovativ und praxisnah, 2018.**
2. Tanui J. K., Kioni P. N., Mirre T., Nowitzki M. and Karuri N. W. (2019). A Numerical study of volatile matter generation from wood combustion in a fixed bed under O₂/CO₂ environment. *5TH Dekut International Conference on Science, Technology, Innovation and Entrepreneurship (STI&E), 2019.*

Research article

The effect of carbon dioxide on flame propagation speed of wood combustion in a fixed bed under oxy-fuel conditions

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ARTICLE INFO

Keywords:

Oxy-fuel
Flame front
Propagation speed
Fixed bed
Wood combustion
CFD-DEM

ABSTRACT

This paper presents an investigation of wood combustion in a laboratory-scale fixed bed with an aim of establishing the effect of CO₂ environment on flame propagation speed and flame structures. Different oxy-fuel combustion atmospheres in which the composition of O₂ in CO₂ was varied from 21% to 50% by volume were tested and compared to air-fuel condition. Euler-Lagrange (Computational Fluid Dynamics - Discrete Element Method, CFD-DEM) approach which captures information of individual particle processes is used to model wood conversion in a packed bed. Results show that flame front propagation speed in oxy-fuel atmosphere reduced to 78% of that of the air-fuel condition with similar O₂ concentration. For oxy-fuel conditions, propagation speed increased with increase in O₂ concentration. The CFD-DEM model agrees very well with experimental values for mass loss, propagation speed and flame front positions. However, peak temperatures are poorly predicted at lower oxygen concentrations. The accuracy of temperature prediction improves at higher oxygen concentrations. During initial and devolatilization stage, mass fraction of tar predicted in CO₂ environment are smaller than in N₂ environment, while the amount of CO predicted is almost equal in both environments. However, during char combustion stage a high amount of CO is observed in oxy-fuel conditions.

1. Introduction

Biomass fuel is still the major source of energy for a significant proportion of the world population. Conventionally, biomass is burned in combustors that use air as oxidizer. The need for efficiency and reduced emissions has led to development of clean combustion technologies such as oxy-fuel combustion. In this technique, fuel is burnt in condition in which CO₂ replaces N₂ as the inert gas. CO₂ is obtained from recycling of exhaust gas. It is a strategy of reducing or capturing CO₂. This technique is applied to both gaseous, Marsh et al. [1], and solid fuels, Bhunia et al. [2] and Álvarez et al. [3]. It has been identified as the most competitive carbon capture technology for retrofitting of the existing power plants, Scheffknecht et al. [4].

Previous works on oxy-fuel combustion range from laboratory research to actual test of the power plants. Tests have been carried out in pilot scale, industrial scale and full scale power plant [4]. Large scale oxy-fuel power plants of sizes between 30 and 300 MW_{th} have been established and installed worldwide [4]. Most of these power plants are coal-fired, but a few others use biomass or are co-fired [5, 6]. Thus there is need for better understanding of oxy-fuel combustion in a CO₂ rich environment. Shan et al. [7] study of single biomass pellet reported

that CO₂ environment increases ignition delay time. A similar behavior has been observed for oxy-coal combustion [8, 9]. This was attributed to a decrease in particle surface heating rate due to decreased co-flow temperature associated with the higher specific heat capacity of CO₂ than N₂ and low oxygen diffusion rate in CO₂. According to Molina et al. [8], other possible reasons for increased ignition delay time are suppression of radical formation by CO₂ chemical effects and thermal decomposition of CO₂. It has been observed that internal ignition temperature of the pellet decreases with increase in O₂ concentration [7]. However, Shan et al. [7] concluded that the effect of oxidation temperature on internal ignition temperature is more than the effect of oxygen concentration.

Another observation [7, 10] is that volatile combustion time increases while combustion temperature decreases [10] when N₂ is replaced with CO₂ (21% oxygen). Riaza et al. [10] noted that the intensity of combustion of a single biomass particle is reduced in CO₂ environment with 21% O₂. As O₂ is increased, combustion intensity also increases.

Oxy-fuel combustion of biomass co-firing with coal has also been studied [11–13]. Biomass and coal blends are preferred because it results in reduction of CO₂, NO_x and SO_x emission when compared to a

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Nomenclature			
A_s	Particle surface area [m ²]	θ	Particle porosity [–]
C_1	Permeability [m ²]	λ	Thermal conductivity [W m ^{−1} K ^{−1}]
C_2	Inertia loss coefficient [m ^{−1}]	μ	Viscosity [kg m ^{−1} s ^{−1}]
c_p	Specific heat [J kg ^{−1} K ^{−1}]	ρ	Density [kg m ^{−3}]
D	Diffusivity [m ² s ^{−1}]	σ	Stefan-Boltzmann constant [W m ^{−2} K ^{−4}]
d_p	Particle diameter [m]	τ	Shear stress tensor [Pa]
G	Incident radiative heat flux [W m ^{−2}]	χ	Region porosity [–]
g	Gravity [m s ^{−2}]	Subscripts	
H_i	Enthalpy of formation of species i [J kg ^{−1}]	0	Initial state of the particle
h	Enthalpy [J kg ^{−1}]	e	Effective
J	Diffusion mass flux [kg m ^{−2} s ^{−1}]	g	Gas
m_p	Particle mass [kg]	i, g	Gaseous species
N_g	Number of gas species [–]	i, s	Solid-phase species
p	Pressure [Pa]	s	Solid
$Q_{a,p}$	Particle absorption coefficient [–]	Superscripts	
q_R	Radiative heat flux [W m ^{−2}]	g	Heterogeneous reaction
S_E	Energy source term [J m ^{−3} s ^{−1}]	Operators	
S_m	Momentum source term [kg m ^{−2} s ^{−2}]	∇	Gradient operator
T	Temperature [K]	∇	Divergence operator
t	Time [s]		
v	Velocity [m s ^{−1}]		
w_i	Rate of production of species i [kg m ^{−3} s ^{−1}]		
Y	Mass fraction [–]		
Greek symbols			
α	Exponent factor [–]		

pure coal plant. In addition, alkali metals present in biomass fuel provides catalytic effects on oxidation and gasification reactions. Indeed, the catalytic effect has been found to be more pronounced under oxy-fuel combustion conditions [11]. Irfan et al. [14] observed that there were improved ignition properties for coal/biomass blends in both oxy-fuel and air-fuel conditions.

Pohlmann et al. [15] has studied the effects of O₂/CO₂ and O₂/N₂ environment on char reactivity and burnout of pulverized torrefied and carbonized biomass burned in a drop tube furnace. CO₂ environment increases the burnout of biomass fuel. In addition, CO₂ environment increases char surface area [16, 17]. Char from CO₂ devolatilization environment is small in size and has low reactivity [18, 19]. Improved char burnout in CO₂ has been attributed to contribution from CO₂ gasification [15, 18, 20]. Even though the burnout time is high, the release of volatile is low under the fast heating conditions in a drop tube furnace operated under oxy-fuel environment [15].

Even though different aspects of oxy-fuel combustion of biomass have been investigated, the mechanism through which CO₂ environment affects fundamental combustion phenomena such as flame propagation speed and flame structures in a fixed bed reactor have not been reported. Flame propagation speed is one of the main parameters to consider when designing a new burner.

Flame propagation rate in biomass fixed bed gasifiers has been investigated under different operating conditions [21–26] although not in oxy-fuel environment. It is affected by various factors such as biomass fuel type, density, size, ultimate and proximate analysis and superficial velocity. Based on superficial velocity, operation regimes have been classified either as two-regime [21] or three-regime [27]. In the two-regime classification, propagation speed increases in the fuel rich regime and decreases in the fuel lean regime. On the other hand, three-regime classification has fuel rich regime, fuel lean regime and convective cooling regime where propagation speed increases rapidly, gradually and decreases rapidly, respectively. Furthermore, the role of ash in flame propagation speed has been assessed [28]. Ash affects

radiative heat transfer to the unburnt biomass, hence affecting the flame propagation. Although numerous works on flame propagation rate of biomass combustion in fixed bed have been done, none addresses an oxy-fuel environment.

The main aim of this work is to comprehensively investigate the effects of CO₂ environment on flame propagation speed and flame structures. A commercial CFD software CD-Adapco (STAR CCM+ version 11.04) [29] is used to simulate thermal conversion of wood in oxy-fuel environments. Euler-Lagrange approach which captures detailed information of individual particle processes is used to model wood conversion in a packed bed. Furthermore, measurements were done in a laboratory-scaled fixed bed reactor operated under oxy-fuel conditions. CFD simulations were validated by comparing them with measured data in a laboratory set-up.

2. Experimental set-up

A schematic diagram and a photo of the combustion test rig used in this work are shown in the Fig. 1a and b, respectively. It is a laboratory-scale fixed bed, which has provision for regulating the flow of O₂, CO₂ and N₂. Its internal and external radius are 20 mm and 40 mm, respectively and the height is 200 mm. It has provisions for thermocouple insertions located at 10 mm intervals. Internal and external parts are made of stainless steel and between them is a 20 mm thick refractory cement for insulation. Thermal conductivity of refractory cement is 0.34 W/m·K [30]. Critical insulation radius for this material, considering typical values of convective heat transfer coefficient for air in natural convection as 10–20 W/m²·K [31], lies between 17 and 34 mm. An external radius of 40 mm used in this reactor is, therefore, sufficient for heat insulation. Fuel bed is held by a stainless steel grate.

The reactor was operated in counter-current flame propagation mode. Top fuel was ignited initially and the flame front propagates downward into the virgin fuel. Oxidizer was supplied from the bottom. For this arrangement, there is no fuel bed movement. The fuel bed was

Fig. 1. A schematic diagram and a photo of the combustion test rig.

Fig. 2. A photo of processed wood fuel samples.

ignited using methane gas flame with a flow rate of $0.051 \text{ m}^3/\text{h}$. Ignition time was about 10 s. The amount of methane used in ignition was estimated to be 94 mg and released a total amount of heat of 4719 J. It was expected that this amount of heat ignites a top layer of wood of about 2.26 g, therefore, wood temperature during ignition was raised to about 1182°C .

Oxidizer was a mixture of pure O_2 and N_2 or CO_2 in various composition. The different gas components were supplied independently through a perforated bottom plate of a 100 mm long mixing chamber made of brass. The chamber was filled with 8 mm long hollow glass with internal diameter of 4 mm for settling and generating a relatively uniform flow. A constant mass flow rate of $0.1 \text{ kg}/\text{m}^2/\text{s}$ was used for all the tests carried out. Gas flow rates were measured using variable area flowmeters (rotameters) in-built in Atlas LOI equipment with a tolerance of $\pm 2\%$. During combustion, the reactor was placed on a weighing balance in order to obtain mass loss history. The weighing balance has an accuracy of $\pm 0.01 \text{ g}$. Temperature in the fuel bed was monitored by five Type K thermocouples. Uncertainty of thermocouple data acquisition system is dependent on combustion zone temperature. For the whole range of thermocouple measurement, it is between $\pm 2.184^\circ\text{C}$ and $\pm 6.630^\circ\text{C}$. In addition, temperature measured by thermocouple may differ significantly from the true gas temperature because of radiation heat loss from the thermocouple surface to the cooler surrounding walls. Error due to radiation loss was corrected according to the methodology developed by Blevins and Pitts [32] and

has been applied by other researchers [33]. In this method, maximum and minimum measurement error which occurs when using bare bead and single shielded aspirated thermocouple (TC), respectively, are used to estimate the error in sheathed thermocouple with the same bead size.

Measurement was made for different O_2/CO_2 mixtures which varied in composition of O_2 in CO_2 from 21% to 50% by volume. For comparison purposes, measurements were made for air-fuel condition. The gaseous mixtures were supplied at room temperature (295 K). Each test was done in three replicate to check repeatability.

In this work, eucalyptus wood was combusted in the reactor. The reactor was filled with spherical wood of 5 mm diameter to a height of 60 mm. A photo of processed wood fuel samples is presented in Fig. 2, while their proximate and ultimate analysis is presented in Table 1.

3. Numerical modeling

3.1. Gas and solid phase dynamics

A packed bed of solid fuel consists of particles which interact with one another in terms of heat exchange by conduction and radiation. They also interact with gas phase surrounding them in the void spaces. In addition, they undergo conversion through several processes, that is, drying, pyrolysis and char oxidation. All these processes must be accounted for in the modeling of particle combustion in a fuel bed.

In this work, all numerical simulations were carried out using a commercial CFD software CD-Adapco (STAR CCM+ version 11.04) [29]. Euler-Lagrange (CFD-DEM) approach was used to model biomass

Table 1
Proximate and ultimate analysis of fuel sample.

Proximate analysis	(wt%)	Standards
Moisture	10.3	CEN-TS 14774-2:2009
Volatile matter (wt% dry basis)	84.9	CEN-TS 15148:2009
Fixed carbon (wt% dry basis) - by difference	14.9	–
Ash (wt% dry basis)	0.2	CEN-TS 14775:2009
Ultimate analysis	(wt% dry basis)	Standards
C	50.87	CEN-TS 15104:2011
H	5.73	CEN-TS 15104:2011
N	0.3	CEN-TS 15104:2011
O (by difference)	43.1	–
Gross calorific value (MJ/kg)	19.3	CEN-TS 14918:2009

Table 2
Physical properties of wood [34].

Particle diameter, d_p (m)	0.005
Eucalyptus wood	
Density, ρ (kg/m ³)	1220
Porosity, θ	0.64
Specific heat, c_p (J/kgK)	$1500 + T_s$
Conductivity, λ_a (W/mK)	0.2
Char	
Density, ρ (kg/m ³)	250
Porosity, θ	0.85
Specific heat, c_p (J/kgK)	$420 + 2.09T_s - 6.85 \times 10^{-4} T_s^2$
Conductivity, λ_a (W/mK)	0.1

conversion in a packed bed. Solid particles and their conversion were modeled using DEM while fluid phase was modeled as a continuous phase using CFD. Detailed description of the governing equations for combustion is provided in CD-Adapco user guide [29]. Here we only discuss details of user-defined and specific sub-models subject to the following assumptions:

1. Wood fuel is considered as spherical particles which are modeled as thermally thin. Therefore, the particle is assumed to be internally homogeneous with a low Biot number. The physical properties of the wood and char used in simulations are presented in Table 2.
2. Fuel bed is considered as a porous media where the pressure loss is accounted for by Ergun equation [34]. This is incorporated as a source term in gas-phase momentum equation.
3. Gas flow in the bed is assumed to be turbulent.
4. Gas phase and solid phase interact by exchanging mass, species and energy. Heat is exchanged between solid-phase and gas-phase by convection and radiation while within solid phase is by conduction and radiation.
5. Porosity of the particle, θ is assumed to vary during bed thermal conversion as a result of local consumption of solid phase. Therefore, the particle diameter slightly shrinks producing a slight change in the bed size during entire combustion period. The porosity is modeled [29] according to Eqs. (1) and (2):

$$\frac{d_p}{d_{p,0}} = \left(\frac{m_p}{m_{p,0}} \right)^{\alpha/3} \quad (1)$$

$$\theta = 1 - \left(\frac{m_p}{m_{p,0}} \right)^{1-\alpha} \quad (2)$$

where d_p is the particle diameter, m_p is the particle mass, α is the exponent factor ($0 \leq \alpha \leq 1$) and θ is the initial state of the particle.

Based on these assumptions, governing equations are presented on Table 3 (gas-phase) and Table 4 (solid-phase) [29].

In this work, flow in bed and free board regions have been assumed to be turbulent based on previous research on comparable systems [35, 36]. Turbulence was accounted by standard $k-\epsilon$ model. Two-way

Table 3
Gas-phase conservation equations.

$\frac{\partial}{\partial t}(\rho g) + \nabla \cdot (\rho_g \mathbf{v}_g) = \sum_{i,g} w_{i,g}^{gs}$
$\frac{\partial}{\partial t}(\rho_g \mathbf{v}_g) + \nabla \cdot (\rho_g \mathbf{v}_g \mathbf{v}_g) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho_g \mathbf{g} + S_m$
$\frac{\partial}{\partial t}(\rho_g h_g) + \nabla \cdot (\rho_g \mathbf{v}_g h_g) = \frac{\partial}{\partial t}(\chi p) + \nabla \cdot (\lambda_{g,e} \nabla T_g - \sum_{i=1}^{N_g} h_{i,g} J_{i,g}) + \nabla \cdot (\mathbf{v}_g p)$ $- \nabla \cdot (\mathbf{r} \cdot \mathbf{v}_g) + S_E$
$\frac{\partial}{\partial t}(\rho_g Y_{i,g}) + \nabla \cdot (\rho_g \mathbf{v}_g Y_{i,g}) = \nabla \cdot (\rho_g D \nabla Y_{i,g}) + w_{i,g}^{gs}$
$S_m = -\left(\frac{\rho}{C_1} \mathbf{v}_g + C_2 \rho_g \mathbf{v}_g \mathbf{v}_g\right)$
$S_E = A_s h_c (T_s - T_g) - \epsilon \lambda_{g,e} w_{i,g}^{gs} H_{i,g} + q_R$

Table 4
Solid-phase conservation equations.

$\frac{\partial}{\partial t}((1-\chi)\rho_s) = \sum_{i,s} w_{i,s}^{gs}$
$\frac{\partial}{\partial t}((1-\chi)\rho_s Y_{i,s}) = w_{i,s}^{gs}$
$\rho_s c_{ps} (1-\chi) \frac{\partial T_p}{\partial t} = \nabla \cdot (\lambda_{s,e} \nabla T_p) + A_s h_c (T_g - T_p) + \frac{A_s}{4} Q_{\alpha,p} (G - 4\sigma T_p^4) + \sum_{i,s} w_{i,s}^{gs} H_{i,s}$

coupling model allow solid-phase to exchange mass, species and energy with the continuous phase. The interaction between solid-phase and gas-phase in terms of convective heat transfer is enabled by a source term added to solid phase energy equation, Table 4, and subtracted in gas-phase energy equation, Table 3. Heat transfer coefficient is estimated from Nusselt number which is calculated from Wakao et al. [37] correlation. Similarly, mass and species exchanged between the two phases are coupled by source terms which have same magnitude but opposite in sign; $\sum_{i,g} w_{i,g}^{gs} = -\sum_{i,s} w_{i,s}^{gs}$ and $w_{i,g}^{gs} = -w_{i,s}^{gs}$ for mass and species, respectively.

The presence of high concentration of H₂O and CO₂ gases in an oxy-fuel combustion environment alters radiative gas properties. The choice of the property model affects the accuracy of the overall radiation model. Some models use oversimplified approach, for example, gray gas model, while others use comprehensive approach, for example, wavelength dependent property models. A widely used model is Weighted-Sum-of-Gray-Gas-Model (WSGGM) which works well in an air-fuel combustion environment, Smith et al. [38]. There have been some efforts, for instance Yin et al. [39], to modify WSGGM so as to improve its accuracy in predicting radiation in an oxy-fuel combustion environment. It has been noted that modified WSGGM model has significant improvement on the accuracy when considering large scale reactors [12, 40]. A minimal change of < 1% on temperature was noted when applied on a small scale reactor [12]. The reactor used in this study is small, therefore, unmodified WSGGM was implemented with an expectation that it would not significantly affects the results.

3.2. Chemical kinetic model

Biomass conversion was modeled by four sub-models, namely, drying, pyrolysis, gas-phase reactions and char oxidation models. The overall kinetic model used in this work is presented in Table 5. Drying of the wet wood was modeled by a first-order kinetic rate model, shown in reaction R(1) [41].

Dry wood decomposed into primary components char, tar and gas through pyrolysis process. The kinetics of dry wood conversion into tar, char and gas is given by reactions R(2)–R(4) while the tar cracking is reaction R(5). The mass fractions for gas species from wood pyrolysis in reaction R(2) were specified according to Mahmoudi et al. [42] and Di Blasi [43]. The components of tar cracking reaction R(5) are inert tar, CO, CO₂, H₂ and CH₄ whose mass fractions amounts are 0.22, 0.564, 0.111, 0.017 and 0.088, respectively [44, 45].

Gas species considered in homogenous gas-phase reactions R(6)–R(14) are those generated from drying (H₂O), devolatilization (CO₂, H₂O, CO, H₂, CH₄, tar), tar cracking and char heterogeneous reactions. Oxidation of CO, CH₄, H₂ and tar are represented by reactions R(6)–R(9). For the purpose of checking the chemical effect in oxy-fuel environment reaction R(10), which has been identified as dominant reaction pathway [46, 47], is incorporated into the mechanism. Important chain-branching steps of H₂(R(11), R(12)) relevant to this reaction are included. Furthermore, the forward and reverse reactions R(13) and R(14) for H₂O and CO have been considered [35, 41].

Char consumption is represented by heterogeneous reactions R(15)–R(17). Char oxidation is given by reaction R(15) while its gasification by CO₂ and H₂O is by reactions R(16) and R(17), respectively. The parameter Ω in reaction R(15) control the ratio of CO₂ to CO emitted when char is burning. It is expressed as a function of char surface

Table 5
Biomass kinetic model.

Drying		Rate expression		Source
R(1)	Wet wood $\rightarrow$ dry wood + H ₂ O (g)	$R_{dry} = Y_{mPh,wet} 1.6 \times 10^{27} \exp. (-25,000/T_s)$		[41]
Pyrolysis reactions		Rate expression	Kinetics	Source
		$K_i = A_i T^n \exp. (-E_i/RT)$	$A \text{ (s}^{-1}\text{)}, E \text{ (kJ/mol)}$	
R(2)	Dry wood $\rightarrow$ gas	$w'_b = K_2 \rho_{b,dry}$	$A_2 = 111 \times 10^9$, $E_2 = 177$	[49]
R(3)	Dry wood $\rightarrow$ tar	$w'_b = K_3 \rho_{b,dry}$	$A_3 = 9.28 \times 10^9$, $E_3 = 149$	[49]
R(4)	Dry wood $\rightarrow$ char	$w'_b = K_4 \rho_{b,dry}$	$A_4 = 30.5 \times 10^9$, $E_4 = 125$	[49]
R(5)	Tar $\rightarrow \gamma_t$ Tar _{naert} + γ_{CO} CO + γ_{CO_2} CO ₂ + γ_{H_2} H ₂ + γ_{CH_4} CH ₄	$w'_{Tar} = K_5 \rho_{Tar}$	$A_5 = 9.55 \times 10^4$, $E_5 = 93.37$	[44, 50]
Homogeneous gas-phase reactions		Rate expression	Kinetics	Source
		$K_i = A_i T^n \exp. (-E_i/RT)$	$A \text{ (s}^{-1}\text{)}, E \text{ (kJ/mol)}$	
R(6)	2CO + O ₂ $\rightarrow$ 2CO ₂	$R_{CO} = K_6 [CO] [O_2]^{0.25} [H_2O]^{0.5}$	$A_6 = 2.24 \times 10^{12}$, $n = 0$, $E_6 = 167.36$	[44, 50]
R(7)	CH ₄ + 2O ₂ $\rightarrow$ CO ₂ + 2H ₂ O	$R_{CH_4} = K_7 [CH_4]^{0.7} [O_2]^{0.8}$	$A_7 = 11.58 \times 10^{13}$, $n = 0$, $E_7 = 202.5$	[44, 50]
R(8)	2H ₂ + O ₂ $\rightarrow$ 2H ₂ O	$R_{H_2} = K_8 [H_2] [O_2]$	$A_8 = 2.19 \times 10^9$, $n = 0$, $E_8 = 109.2$	[44, 50]
R(9)	Tar + 2.9O ₂ $\rightarrow$ 6CO + 3.1H ₂	$R_{Tar} = K_9 [Tar]^{0.5} [O_2]$	$A_9 = 9.2 \times 10^6$, $n = 0$, $E_9 = 80.2$	[44, 50]
R(10)	CO + OH $\rightarrow$ CO ₂ + H	$R_{CO} = K_{10} [CO] [OH]$	$A_{10} = 4.76 \times 10^7$, $n = 1.3$, $E_{10} = 0.293$	[51]
R(11)	H + O ₂ $\rightarrow$ O + OH	$R_H = K_{11} [O] [OH]$	$A_{11} = 2.65 \times 10^{16}$, $n = -0.671$, $E_{11} = 71.347$	[51]
R(12)	H ₂ + O ₂ $\rightarrow$ OH + OH	$R_{H_2} = K_{12} [H_2] [O_2]$	$A_{12} = 2.51 \times 10^{12}$, $n = 0$, $E_{12} = 163.075$	[52]
R(13)	H ₂ O + CO $\rightarrow$ CO ₂ + H ₂	$R_{H_2O} = K_{13} [H_2O] [CO]$	$A_{13} = 2.78$, $n = 0$, $E_{13} = 12.55$	[41, 49]
R(14)	CO ₂ + H ₂ $\rightarrow$ H ₂ O + CO	$R_{CO_2} = K_{14} [CO_2] [H_2]$	$A_{14} = 93.69$, $n = 0$, $E_{14} = 46.594$	[41, 49]
Heterogeneous reactions		Rate expression	Kinetics	Source
		$K_i = A_i T^n \exp. (-E_i/RT)$	$A \text{ (s}^{-1}\text{)}, E \text{ (kJ/mol)}$	
R(15)	Ω C + O ₂ $\rightarrow$ 2($\Omega - 1$) CO (2 - Ω) CO ₂	$w'_{char,O_2} = K_{15} P_{O_2} S_{a,char}$	$A_{15} = 2.54 \times 10^{-3}$, $E_{15} = 74.8$	[44, 50]
R(16)	C + CO ₂ $\rightarrow$ 2CO	$w'_{char,CO_2} = K_{16} P_{CO_2} S_{a,char}$	$A_{16} = 1.81 \times 10^{-2}$, $E_{16} = 130$	[44, 50]
R(17)	C + H ₂ O $\rightarrow$ CO + H ₂	$w'_{char,H_2O} = K_{17} P_{H_2O} S_{a,char}$	$A_{17} = 1.81 \times 10^{-2}$, $E_{17} = 130$	[44, 50]

temperature [41, 48]:

$$\Omega = \frac{2(1 + 4.3 \exp[-3390/T_{particle}])}{2 + 4.3 \exp[-3390/T_{particle}]} \quad (3)$$

3.3. Mesh and boundary conditions

Computational domain representing the burner was meshed into highly-refined unstructured grids which ensured grid independent solutions. The burner was considered to have double symmetry. Therefore, a quarter of the burner with the dimensions described in section 2 was used in all simulated cases. Mesh independent test was carried out to determine appropriate number of cells. Approximately 200,000 cells made of polyhedral elements and prismatic layers near the wall were used.

Cold mixture of O₂/N₂ or CO₂ at 295 K enters the computational domain at the inlet boundary. For all the tests, the mass flux at the inlet

was 0.1 kg/m²/s while mass fraction of O₂ and N₂ or CO₂ was specified according to the case tested. Combustion products exited at the domain at the top which was modeled as outflow boundary with zero temperature and species gradients. The wall was considered stationary with no slip condition. Thermal boundary conditions at the wall were modeled as a mixture of convective and radiation heat transfer. Convective heat flux at the wall was selected with an adopted heat transfer coefficient of 10 W/m²·K. An emissivity of 0.8 was adopted because the wall was made from stainless steel [31].

4. Results and discussions

The accuracy of the simulation solutions was ensured by running mesh independence tests. The prediction of temperature profiles along axial length of the reactor for oxy-fuel environment at two different times applying different computational mesh sizes are shown in Fig. 3a and b. In both cases, there was a significant change in results when mesh size was increased from 100,000 cells to 200,000 cells. But the

Fig. 3. Comparison of temperatures profiles along axial length of the reactor for wood combustion in O_2/CO_2 mixtures at two different times applying different computational mesh sizes.

Fig. 4. Mass loss history for wood combustion in fixed bed at 21% O_2 /79% N_2 and 21% O_2 /79% CO_2 mixtures.

predictions using 200,000 cells, 300,000 cells and 400,000 cells did not have much differences. Therefore, a computational mesh with 200,000 cells was selected for all the cases computed.

Validity of the model is checked by comparing mass loss history, peak temperatures and flame propagation speed obtained from simulations to corresponding experimental data. Shown in Fig. 4 is the mass loss history for wood combustion in 21% O_2 concentration under both N_2 and CO_2 . The model agrees very well with experimental values. The curve for oxy-fuel condition is less steep with a longer devolatilization stage when compared with N_2 atmosphere. A slightly long char stage is also observed in CO_2 atmosphere. In overall, combustion of the same amount of wood takes a longer time for oxy-fuel condition than for air-fuel condition. This suggests a slow fuel consumption and burning rate in CO_2 atmosphere.

Presented in Figs. 5, 6 and 7 are temperature maps in the fuel bed at different times for different combustion atmospheres. The simulated and measured peak temperatures attained in the bed are compared in Fig. 8. Temperatures are poorly predicted at lower oxygen concentrations. The accuracy of prediction improves at higher oxygen concentrations. Temperatures corrected for radiation losses are also plotted in Fig. 8. Indeed, their agreement with predicted values is better than those of uncorrected values. Consequently, this emphasizes the importance of considering radiation losses when validating a model.

It is important to note that after ignition, different conversion processes such as drying, devolatilization, char combustion and homogenous reactions takes place simultaneously at various height of

the bed. Since some processes are endothermic and others are exothermic, the temperatures at various regions are strongly dependent on the dominant process as discussed further below. In the model used in this study, gaseous species release from biomass, depending on availability of oxidative species either react within fuel bed or are transported to freeboard region where they continue reacting and produce heat. For all the cases studied, it is observed that during initial stages of combustion, freeboard temperatures are almost equal to bed temperatures. For 21% O_2 concentration, the period extended up to 300 s, Fig. 5, and 450 s, Fig. 6, for N_2 and CO_2 environments, respectively. As O_2 concentration is increased in oxy-fuel condition, the period reduces from 450 s to 300 s, Fig. 7. During this stage, heat release by homogeneous reactions is absorbed by downstream particles which are still undergoing devolatilization. At the same time, immediate upstream particles take up heat for drying.

As combustion progresses downward which is clearly depicted by propagation of reaction front, e.g. between 400 and 750 s in Figs. 5, 7 and 600–950 s in Fig. 6, more volatiles are released. During this period, freeboard temperatures are higher than bed temperatures. At this time, particles adjacent to freeboard probably have completed endothermic processes (drying and devolatilization). In addition, these particles are in char combustion stage which releases more heat. Heat released from homogeneous reaction and char combustion is transported from bed to freeboard by convection of combustion products which are dominated by H_2O and CO_2 .

After some time, reaction front reaches the bottom of the reactor and all volatiles have been released. After this point, combustion in the bed is dominated by char combustion, e.g. at 1000 s of Figs. 5, 7 and 1100 s in Fig. 6. Freeboard temperatures decrease during this period. This is because homogeneous reactions which release intense heat are almost complete.

Even though the temperature distribution in fuel bed under both conditions exhibits the same behavior, the magnitudes are different. At 21% O_2 concentration, air-fuel has a peak temperature of 1497 K while oxy-fuel has 1388 K. As shown in Fig. 8, as O_2 concentration is increased, temperature also increases. A value of temperature close to that of 21% O_2 /79% N_2 mixture is achieved at around 30% O_2 /70% CO_2 mixture. Low values of temperatures in oxy-fuel conditions are associated with higher specific heat capacity of CO_2 gas than that of N_2 gas. This applies for all the temperatures above 650 K where specific heat capacity of CO_2 gas is higher than that of N_2 gas.

The flame front propagation speed is estimated from distance and time data of temperature measuring points, Sakthivadivel and Iniyan [22]. For both experiment and model, flame front passes through a point when there is an abrupt increase in temperature from ambient value to a peak value, Ryu et al. [23]. The exact position of predicted and measured reaction front for wood combustion in 21% O_2

Fig. 5. Temperature distribution in the wood fuel bed burning at 21% O_2 /79% N_2 at different times.

concentration under both N_2 and CO_2 is shown in Fig. 9. For air-fuel conditions at 21% O_2 concentration, a higher value of flame speed is observed. In general, propagation speed for air-fuel condition reported in literature [25, 26] is higher than those observed in oxy-fuel conditions of the current study. However direct comparison cannot be done because flame front propagation speed is dependent on several factors such as air mass flux, fuel properties, particles size, reactor operation mode, et cetera. Flame front speed have been shown [22–25] to increase with increase in air mass flux up to a peak point where it starts to decrease. Mahapatra et al. [24] reported a peak value of 0.089 mm/s for air flow rate of 0.132 $kg/m^2/s$ and casuarina wood as fuel. While studying char combustion in a packed bed, Dasappa and Paul [25] reported a peak value of 0.30 mm/s for air mass flux of 0.1 $kg/m^2/s$. Yang et al. [26] showed that flame speed decreased from 0.24 mm/s for 10 mm sized particles to 0.21 mm/s for 35 mm sized particles. In a

recent study, Sakthivadivel and Iniyan [22] obtained a flame speed of about 0.05–0.07 mm/s for different fuels tested in air-fuel environment.

In order to have a proper comparison, investigation of flame propagation speed for the same wood fuel with the same particle size burning in air-fuel conditions was conducted. Fig. 9 shows that the gradient (propagation speed) is steeper in N_2 environment than in CO_2 environment. Indeed, it is observed that flame speed in oxy-fuel atmosphere reduced to 76% (model) and 78% (experiment) of that of the air-fuel condition with similar O_2 concentration. It is also noted that ignition delay is longer in CO_2 environment. Reduction in speed could be attributed to transport and thermodynamic properties of CO_2 gas and chemical effects associated with it. The chemical reactions involving consumption of CO_2 include reverse water gas shift reaction R(14) and Bourdoudard reaction R(16). The reaction rates of both reactions are several orders of magnitude smaller than those of homogeneous

Fig. 6. Temperature distribution in the wood fuel bed burning at 21% O_2 /79% CO_2 at different times.

Fig. 7. Temperature distribution in the wood fuel bed burning at 30%O₂/70%CO₂ at different times.

Fig. 8. Predicted and measured peak temperatures in the wood fuel bed burning at different CO₂ atmospheres.

Fig. 9. Predicted and measured flame front position for wood combustion in fixed bed at 21%O₂/79%N₂ and 21%O₂/79%CO₂ mixtures. Fuel bed top is taken as datum.

reactions R(6)–R(13). Therefore, their contribution to flame speed is quite small. On the other hand, CO₂ gas has a higher heat capacity than N₂ gas (1.5 times higher than that of N₂). In addition, CO₂ is a heavy gas and O₂ diffusivity in it is lower. Consequently, the overall effect is reduction of temperature and heating rates of fuel particles. Thus a reduced flame speed is observed in CO₂ environment. It is also noted that mass fraction of combustible volatiles released in CO₂ environment are smaller. This also contributes to reduction in flame speed and is discussed in subsequent paragraphs.

Shown in Fig. 10 are plots of flame front propagation speed in fuel bed operated at different oxy-fuel conditions. The curves show good agreement between the predicted and measured values. Flame speed increased from 0.06 mm/s at 21%O₂/79%CO₂ to 0.21 mm/s at 50%O₂/50%CO₂. As O₂ concentration is increased, gas mixture properties also change. This means a reduced portion of CO₂ in which O₂ diffusivity is improved. As a result, an increase in temperature is seen (Fig. 8) and also heating rates of particles is increased. Hence, the flame speed also increases.

Presented in Figs. 11–14 are the flames structures of wood

Fig. 10. Predicted and measured flame front propagation speed in the wood fuel bed burning at different CO₂ atmospheres.

(a) 79% N₂ at 200 s(b) 79% CO₂ at 300 s(c) 70% CO₂ at 200 s

Fig. 11. Species and temperatures profiles along axial length of the reactor for wood combustion in O₂/N₂ and O₂/CO₂ mixtures when reaction front is at 5 cm from fuel bottom.

(a) 79% N₂ at 300 s(b) 79% CO₂ at 450 s(c) 70% CO₂ at 300 s

Fig. 12. Species and temperatures profiles along axial length of the reactor for wood combustion in O₂/N₂ and O₂/CO₂ mixtures when reaction front is at 4 cm from fuel bottom.

(a) 79% N₂ at 400 s(b) 79% CO₂ at 600 s(c) 70% CO₂ at 400 s

Fig. 13. Species and temperatures profiles along axial length of the reactor for wood combustion in O₂/N₂ and O₂/CO₂ mixtures when reaction front is at 3 cm from fuel bottom.

combustion in both environments at different combustion stages. The main species mass fraction and temperature profiles at a given time are plotted against axial length of the reactor. Fig. 11 illustrates flame structures in oxy-fuel and air-fuel conditions when reaction front is at 5 cm from the bottom of reactor. Because each case has a different flame speed it occurs at different times; at 200 s in 79% N₂, Fig. 11a, and 70% CO₂, Fig. 11c, and at 300 s in 79% CO₂, Fig. 11b. In all the cases, reaction zone covers a region of depth between 4 cm to 7 cm. The particles within this region are mainly undergoing drying and pyrolysis. Homogeneous reactions of pyrolysis products, tar, CO, CH₄, H₂, with O₂

are exothermic. It is observed that gaseous species react within the fuel bed and are also transported to freeboard region. Some of the heat released is absorbed by particles because pyrolysis is an endothermic reaction while the remaining amount is convected to freeboard region. Although the flame structures depict similar profiles, the magnitude of species and temperature are different. Highest amounts of tar and steam are observed in 79% N₂ environment while lowest amounts of these species are seen in 79% CO₂ environment. The amount of CO is almost equal in all the 3 cases. The high amount of tar and steam in 79% N₂ environment is attributed to high temperature which enhances

Fig. 14. Species and temperatures profiles along axial length of the reactor for wood combustion in O_2/N_2 and O_2/CO_2 mixtures during char combustion stage.

pyrolysis process. Low amount of tar in oxy-fuel condition affirms the influence on flame propagation speed.

As the flame front propagates downward, the positions of the peak values of species also change, Figs. 12 and 13. The position where peak temperatures occur, however, remain just approximately at the fixed bed top. This is because particles in this region have completed pyrolysis process and no longer absorb heat released by homogeneous reactions. Furthermore, at this stage, the heat transfer through convection is high enough to raise the exit temperature. Very low amounts of tar and CO and high amounts of CO_2 and H_2O in this region reflect an increase in consumption rate of volatiles. For oxy-fuel cases, the amount of CO_2 from combustion adds to the supplied amount and hence dominates the combustion products, Fig. 12b and c. Just like in the initial stage, flame front in CO_2 environment arrives at 4 cm, Fig. 12b, and 3 cm, Fig. 13b, later than in air-fuel condition. For the flow condition tested, tar and CO are completely consumed within the fuel bed. As seen in the figures, O_2 is sufficient for complete oxidation of these species. The amount of tar and CO at reaction front decreases as it moves downward, Fig. 13. As shown in Fig. 13a–c, the mass fraction of these species are almost equal in the three cases.

After the flame front reaches the bottom of the bed, the fuel bed is completely in char combustion stage. Major species generation and temperature profiles during this stage, for each of the three cases, are shown in Fig. 14. Absence of tar indicates that devolatilization stage has ended. As in the previous combustion stages, it is also noted that this stage occurs at a later time in CO_2 environment than in N_2 environment. Temperatures in the bed are relatively lower than in the previous combustion stages. As expected, temperatures in oxy-fuel conditions, Fig. 14b and c, are lower than that in air-fuel case, Fig. 14a. Low temperatures in all cases are attributed to absence of homogeneous reactions of volatiles which reduces rate of heat release. The only heat release is in char and CO oxidation. In addition, char gasification with CO_2 and H_2O is an endothermic reaction. Moreover, heat is lost by convective heat transfer to freeboard region. Because of cold air inlet, cooling effect results in relatively low temperatures in the grate. For char combustion stage, char is converted to CO and CO_2 . A high amount of CO is observed in oxy-fuel condition which is as a result of gasification of char in the CO_2 environment.

5. Conclusion

A comprehensive study of the effect of CO_2 combustion atmosphere on flame propagation speed and flame structures in wood combustion in a laboratory-scaled fixed bed operated under counter-current mode was presented in this paper. CFD-DEM approach was used to simulate wood conversion in a packed bed and the results compared to experimental data. Computational results agree very well with experimental values except temperature which showed poor prediction at low O_2

concentration. The agreement of temperatures corrected for radiation losses with predicted values are better than those of uncorrected values. Hence, it was established that prediction accuracy of CFD-DEM is not the same in different O_2/CO_2 mixtures. Furthermore, it was observed that flame speed in oxy-fuel atmosphere reduced to 78% of that of the air-fuel condition with same O_2 concentration. This was determined both by experiment and through computation. Reduced flame speed was attributed to a higher heat capacity of CO_2 and lower O_2 diffusivity in CO_2 whose overall effect is reduction of temperature and heating rates of fuel particles. Low mass fraction of combustible volatiles predicted in the CO_2 environment also contributes to a reduced flame speed. Flame structures have similar profiles but differ in value of temperature and species quantities. As expected, temperatures in the CO_2 environments were lower than those in the N_2 environments. During initial stages of combustion, the amount of tar and steam is observed to be highest in 79% N_2 environment and lowest in 79% CO_2 environment. The amount of CO was almost equal in both environments during pyrolysis but high amount was predicted in oxy-fuel environments during char combustion stage.

Acknowledgement

This work was financially supported by both Dedan Kimathi University of Technology, Kenya and Technische Hochschule Wildau, Germany. The first author would like to thank the German Academic Exchange Service (DAAD) for granting him stipend while undertaking this work at Technische Hochschule Wildau, Germany.

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Chemical, thermal and dilution effects of carbon dioxide in oxy-fuel combustion of wood in a fixed bed[†]

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(Manuscript Received February 18, 2019; Revised September 20, 2019; Accepted October 10, 2019)

Abstract

Experimental and numerical modeling was performed on eucalyptus wood combustion under oxy-fuel conditions using a fixed bed reactor in order to isolate the role of various carbon dioxide effects on the burning rate. Wood combustion was investigated under four different mixtures of O₂ and Ar/CO₂/N₂: 21 % O₂/79 % N₂; 21 % O₂/22.5 % CO₂/56.5 % Ar; 40 % O₂/60 % CO₂; and 40 % O₂/47 % CO₂/13 % Ar. The first three mixtures were designed to have the same peak temperatures in order to isolate chemical and dilution effects of CO₂. This was achieved by substituting some percentage of CO₂ with Ar in O₂/CO₂ mixture while maintaining a constant concentration of O₂. The fourth mixture was meant to isolate the thermal effect of CO₂. The results were obtained from both the experimental rig and numerical simulation for a fixed bed configuration. Wood combustion in the fixed bed was modeled using Lagrange-Euler method, where gas-phase was calculated using computational fluid dynamics (CFD), that is Euler phase, while solid-phase was tracked in Lagrange phase using discrete element method (DEM). The results show that ignition time in CO₂ environment decreases gradually as O₂ concentration is increased. On the other hand, burning rate and flame front speed increase as O₂ concentration is increased. It was established that dilution effect is the most influential parameter on the burning rate of wood combustion in an oxy-fuel system.

Keywords: Burning rate; CO₂ effect; Fixed bed; Oxy-fuel combustion; Wood combustion

1. Introduction

The demand for biomass fuel has increased due to ever increasing energy need that cannot be fully satisfied by other energy sources, such as coal. Biomass is an attractive energy source as compared to coal as it is renewable. Most of the energy scenarios indicate that biomass will be increasingly used to meet increasing energy demand in future [1].

For a long time, biomass has been converted to energy using burners which operate under air-fuel conditions. However, in the last two decades, there has been increasing use of combustion of biomass in power generation [2, 3]. Oxy-fuel combustion is a technique of capturing CO₂ by recirculating exhaust gas. It is applicable to solid fuels [4], liquid fuels [5] and gaseous fuels [6]. The technique was introduced in power plants the first time in 1982 [7]. Since then, a lot of research, for instance [8–10], have been done to understand the combustion phenomenon.

The studies on fundamental combustion phenomena - transport, chemical and thermodynamics processes - occurring in

oxy-fuel combustion are based on models and experiments on laboratory-scale devices. These include studies on ignition delay time in coal [11], ignition temperature, burnout and NO_x emission in biomass and coal blends [12], and gaseous emissions from biomass/coal co-firing [13]. Such studies provide insights into combustion phenomena in practical oxy-fuel environment [12, 13]. The presence of CO₂ in oxidizer alters physical and thermal properties of the gas mixture, which has impact on fuel reactivity, flame temperature and emissions. Unlike inert species such as argon and nitrogen which have only thermal and dilution effects on combustion processes, addition of reactive species such as CO₂ introduces a chemical effect [14, 15]. Dilution effect is the reduction of concentration of oxidizer caused by addition of CO₂, thermal effect is the decrease in temperature caused by addition of CO₂ and chemical effect is the direct active participation in the chemical reactions.

The three roles played by CO₂ addition can be separated by adjusting the flame temperature to a value corresponding to a reference condition without change in oxidizer and fuel relative concentrations [15, 16]. This technique has been applied to study the effects of CO₂ on soot formation, but it can also be applied to study the effects on other combustion properties [17].

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Fig. 1. Schematic diagram of experimental set-up.

Most previous studies focused on the overall effects of CO₂ burning environment on ignition time [18], ignition and combustion temperature [19], burnout [20], combustion intensity [19] and thermal reactivity [21]. The individual effects in terms of chemical, thermal and dilution on the combustion properties are still not clear. An understanding of these basic mechanisms through which CO₂ affects combustion processes is important because it helps in the design of optimized oxy-fuel burners.

The main objective of this work was to isolate the role of chemical, thermal and dilution effects of CO₂ on wood burning rate through numerical modeling. Four different mixtures of O₂ and Ar/CO₂/N₂ were designed to separate CO₂ effects on wood combustion. Temperature in O₂/CO₂ combustion environment was adjusted to be equal to that of O₂/N₂ environment by adding an appropriate amount of Ar while O₂ amount remained the same. The model was validated by comparing temperature profiles with experimental values. Experiments were done on a laboratory-scale fixed bed.

2. Methodology

2.1 Experimental set-up

A schematic diagram of the experimental set-up used in this work is shown in the Fig. 1. It is a cylindrical burner made of stainless steel which is insulated with refractory cement. A detailed description of the set-up has been given in our previous paper [22].

For all the tests, the burner was filled with wood up to a height of 6 cm. Five type K thermocouples are located at an equidistant of 10 mm from one another. They are connected to a data acquisition system that records temperature every second. Temperature measurement and data acquisition using type K thermocouples were done in accordance to ASTM MNL12 [23]. Combined measurement uncertainty for thermocouple and data acquisition system depends on measured temperature and for the entire range was determined to be

between ± 2.2 °C and ± 6.6 °C. The burner was operated in a batch mode; fuel was fed once while oxidizer was supplied continuously.

2.2 Numerical modeling

Numerical simulations of combustion of wood in the fixed bed were carried out using a commercial software CD-Adapco (STAR CCM+ version 11.04) [24]. Wood burning in a fixed bed was simulated using Lagrange-Euler method, where gas-phase was calculated using computational fluid dynamics, that is, the Euler phase, while solid-phase was tracked in Lagrange phase, using discrete element method. The governing equations of the model are given by Eqs. (1)–(9) and fully described in Ref. [22, 24]:

- Mass conservation equation for gas-phase, Eq. (1) and solid-phase, Eq. (2):

$$\frac{\partial}{\partial t}(\chi \rho_g) + \nabla \cdot (\rho_g \mathbf{v}_g) = \sum_{i,g} w_{i,g}^{sp} \quad (1)$$

$$\frac{\partial}{\partial t}((1-\chi)\rho_s) = \sum_{i,s} w_{i,s}^{sp} \quad (2)$$

- Momentum conservation equation for gas-phase, Eq. (3):

$$\frac{\partial}{\partial t}(\chi \rho_g \mathbf{v}_g) + \nabla \cdot (\rho_g \mathbf{v}_g \mathbf{v}_g) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho_g \mathbf{g} + \mathbf{S}_m \quad (3)$$

where $\mathbf{S}_m$ is momentum source term given as;

$$\mathbf{S}_m = -\left(\frac{\mu}{c_1} \mathbf{v}_g + C_2 \rho_g |\mathbf{v}_g| \mathbf{v}_g \right) \quad (4)$$

- Energy conservation equation for gas-phase, Eqs. (5) and (6) and solid-phase, Eq. (7):

$$\begin{aligned} & \frac{\partial}{\partial t}(\chi \rho_g h_g) + \nabla \cdot (\rho_g \mathbf{v}_g h_g) \\ &= \frac{\partial}{\partial t}(\chi \rho_p) + \nabla \cdot (\lambda_{g,s} \nabla T_g - \sum_{i,g} h_{i,g} J_{i,g}) + \nabla \cdot (\mathbf{v}_g p) - \nabla \cdot (\mathbf{r} \cdot \mathbf{v}_g) + S_E \end{aligned} \quad (5)$$

where S_E energy source term given as;

$$S_E = A_s h_c (T_s - T_g) - \sum_{i,g} w_{i,g}^{sp} H_{i,g} + q_R \quad (6)$$

$$\begin{aligned} \rho_s c_p (1-\chi) \frac{\partial T_s}{\partial t} &= \nabla \cdot (\lambda_{s,s} \nabla T_s) + A_s h_c (T_g - T_s) + \\ & \quad \frac{A_s}{4} Q_{a,p} (G - 4\sigma T_s^4) + \sum_{i,s} w_{i,s}^{sp} H_{i,s} \end{aligned} \quad (7)$$

- Species conservation equation for gas-phase species i,g , Eq. (8) and solid-phase species i,s , Eq. (9)

$$\frac{\partial}{\partial t}(\chi \rho_g Y_{i,g}) + \nabla \cdot (\rho_g \mathbf{v}_g Y_{i,g}) = \nabla \cdot (\rho_g D \nabla Y_{i,g}) + w_{i,g}^{sp} \quad (8)$$

Table 1. Proximate and ultimate analyses of fuel sample.

Proximate analysis (wt%)	
Moisture	10.3
Volatile matter (wt% dry basis)	84.9
Fixed carbon (wt% dry basis)	14.9
Ash (wt% dry basis)	0.2
Ultimate analysis (wt% dry basis)	
C	50.87
H	5.73
N	0.3
O (by difference)	43.1
Gross calorific value (MJ/kg)	19.3

Table 2. Physical properties of wood.

Particle size, d_p (m)	0.005
Eucalyptus wood	
Density, ρ (kg/m ³)	1220
Porosity, θ	0.64
Specific heat, c_p (J/kgK)	$1500 + T_s$
Conductivity, λ_s (W/mK)	0.2
Char	
Density, ρ (kg/m ³)	250
Porosity, θ	0.85
Specific heat, c_p (J/kgK)	$420 + 2.09T_s - 6.85 \times 10^{-4}T_s^2$
Conductivity, λ_s (W/mK)	0.1

$$\frac{\partial}{\partial t}((1-\chi)\rho_s Y_{i,s}) = w_{i,s}^{gr} \quad (9)$$

The symbols are defined in Nomenclature. Exchange of species, mass and energy between the two phases was enabled by a two-way coupling model [22, 24].

Turbulence in both freeboard and bed region was accounted for using standard $k-\epsilon$ model. Interaction between turbulence and chemistry was solved using eddy dissipation concept. Weighted-sum-of-gray-gas-model (WSGGM) [25], was used as a property model for the radiating gases.

Proximate and ultimate analyses for the samples investigated in this study are presented in Table 1 and physical properties in Table 2. The latter are based on the Mehrabian et al. [26] work.

Chemical kinetics of wood conversion in the bed was simulated using different sub-models, which consisted of drying model, pyrolysis model, homogeneous reaction model and heterogeneous reaction model. Kinetics data of these sub-models are given in Table 3. The rate expressions for these reactions are presented in Table 4. These models were adopted from previous research on wood combustion [27–32]. However, in this work oxy-fuel combustion was accounted for by incorporating a reaction involving CO₂ (R(10)) and its associated chain-branching reactions (R(11) and R(12)) in the ho-

mogeneous reaction sub-model. Char combustion rate was evaluated based on partial pressure of O₂, CO₂ and H₂O available at its surface [33]. The stoichiometric ratio of CO₂ to CO from char combustion is dependent on particle surface temperature [27]:

$$\Omega = \frac{2(1 + 4.3 \exp[-3390 / T_{particle}])}{2 + 4.3 \exp[-3390 / T_{particle}]} \quad (10)$$

Grid independent solutions were achieved by meshing computational domain into highly-refined unstructured grid as shown in Fig. 2. A quarter of the burner was used for computation since it has a double symmetry. The choice of mesh size was based on a mesh independent test whose results are shown in Fig. 3. The predicted temperature profile at 5 cm from bed bottom under oxy-fuel condition is significantly different when using a mesh that consists of 100000 cells as compared to that of 200000 cells. The difference in temperature profiles is negligible for mesh that consists of 200000, 300000 and 400000 cells, respectively. Therefore, a mesh with 200000 cells was used for all the cases computed.

Oxidizer enters the domain through inlet boundary located at the bottom. The concentration of oxygen and N₂/CO₂/Ar was set in accordance to the required predesigned conditions. In the first set of experiments, O₂ concentration by volume was varied between 21 % and 50 % with diluent as either N₂ or CO₂. In addition, four mixtures were designed to separate the effects of CO₂ environment. The four mixtures were denoted by letters A, B, C and D and their composition by volume was 21 % O₂/79 % N₂; 21 % O₂/22.5 % CO₂/56.5 % Ar; 40 % O₂/60 % CO₂; and 40 % O₂/47 % CO₂/13 % Ar, respectively. The inlet mass flux for the mixture for all the tests was 0.1 kg/m²/s. The temperature for each of the mixture at the inlet was 295 K. Top boundary was the outlet boundary with temperature and gases concentration gradient set to zero using Neumann boundary condition. A stationary wall with no-slip conditions was considered; the tangential velocity at the wall was explicitly set to zero. The model includes terms to account for heat transfer by radiation and convection at the wall. Emissivity of the surface and coefficient of heat transfer were 0.8 and 10 W/m².K, respectively.

3. Results and discussion

Measured temperature profiles at various distances from bed bottom for wood combustion in 21 % oxygen in N₂ and CO₂ are presented in Figs. 4(a) and (b), respectively. The graphs show that the temperature profile at any given height in both environments exhibits similar behavior. They all have two peaks. When the flame front reaches an ignition point, the temperature rises rapidly to the first peak. Then it decreases gradually to another point and finally rises to the second peak.

Combustible pyrolysis products such as CH₄, tar, H₂ and CO are oxidized through exothermic reactions which generate heat, subsequently increasing the temperature. The exothermic

Table 3. Biomass kinetic model.

Drying	Rate expression			Source
R(1) Wet wood $\rightarrow$ Dry wood + H ₂ O (g)	$R_{dy} = Y_d \rho_{d, wet} 1.610^{27} \exp(-25000 / T_s)$			[27]
Pyrolysis				
Reaction	$K_i = A_i T^n \exp(-E_i / RT)$			Source
	A_i (s ⁻¹)	E_i (kJ/mol)	n	
R(2) Dry wood $\rightarrow$ Gas	111×10^9	177	0	[28]
R(3) Dry wood $\rightarrow$ Tar	9.28×10^9	149	0	[28]
R(4) Dry wood $\rightarrow$ Char	30.5×10^9	125	0	[28]
R(5) Tar $\rightarrow \gamma_i \text{Tar}_{gas} + \gamma_{CO} \text{CO} + \gamma_{CO_2} \text{CO}_2 + \gamma_{H_2} \text{H}_2 + \gamma_{CH_4} \text{CH}_4$	9.55×10^4	93.37	0	[29, 30]
Homogeneous gas-phase reactions				
Reaction	$K_i = A_i T^n \exp(-E_i / RT)$			Source
	A_i (s ⁻¹)	E_i (kJ/mol)	n	
R(6) 2CO + O ₂ $\rightarrow$ 2CO ₂	2.24×10^{12}	167.36	0	[29, 30]
R(7) CH ₄ + 2O ₂ $\rightarrow$ CO ₂ + 2H ₂ O	11.6×10^{13}	202.5	0	[29, 30]
R(8) 2H ₂ + O ₂ $\rightarrow$ 2H ₂ O	2.19×10^9	109.2	0	[29, 30]
R(9) Tar + 2.9O ₂ $\rightarrow$ 6CO + 3.1H ₂	9.2×10^6	80.2	0	[29, 30]
R(10) CO + OH $\rightarrow$ CO ₂ + H	4.76×10^7	0.293	1.3	[31]
R(11) H + O ₂ $\rightarrow$ O + OH	2.65×10^{16}	71.347	-0.7	[31]
R(12) H ₂ + O ₂ $\rightarrow$ OH + OH	2.51×10^{12}	163.075	0	[32]
R(13) H ₂ O + CO $\rightarrow$ CO ₂ + H ₂	2.78	12.55	0	[27, 28]
R(14) CO ₂ + H ₂ $\rightarrow$ H ₂ O + CO	93.69	46.594	0	[27, 28]
Heterogeneous reactions				
Reaction	$K_i = A_i T^n \exp(-E_i / RT)$			Source
	A_i (s ⁻¹)	E_i (kJ/mol)	n	
R(15) $\Omega \text{C} + \text{O}_2 \rightarrow 2(\Omega - 1)\text{CO} + (2 - \Omega)\text{CO}_2$	2.54×10^8	74.8	0	[29, 30]
R(16) C + CO ₂ $\rightarrow$ 2CO	1.81×10^2	130	0	[29, 30]
R(17) C + H ₂ O $\rightarrow$ CO + H ₂	1.81×10^2	130	0	[29, 30]

Table 4. Rate expression for the reactions.

Reaction	Rate expression	Reaction	Rate expression
R(2)	$w_b = K_2 \rho_{b, dry}$	R(10)	$R_{CO} = K_{10} [\text{CO}] [\text{OH}]$
R(3)	$w_b = K_3 \rho_{b, dry}$	R(11)	$R_{H_2} = K_{11} [\text{O}] [\text{OH}]$
R(4)	$w_b = K_4 \rho_{b, dry}$	R(12)	$R_{H_2O} = K_{12} [\text{H}_2] [\text{O}_2]$
R(5)	$w_{tar} = K_5 \rho_{tar}$	R(13)	$R_{H_2O} = K_{13} [\text{H}_2\text{O}] [\text{CO}]$
R(6)	$R_{CO} = K_6 [\text{CO}] [\text{O}_2]^{0.25} [\text{H}_2\text{O}]^{0.5}$	R(14)	$R_{CO_2} = K_{14} [\text{CO}_2] [\text{H}_2]$
R(7)	$R_{CH_4} = K_7 [\text{CH}_4]^{0.7} [\text{O}_2]^{0.8}$	R(15)	$w_{char, CO_2} = K_{15} P_{CO_2} S_{a, char}$
R(8)	$R_{H_2} = K_8 [\text{H}_2] [\text{O}_2]$	R(16)	$w_{char, CO_2} = K_{16} P_{CO_2} S_{a, char}$
R(9)	$R_{tar} = K_9 [\text{Tar}]^{0.5} [\text{O}_2]$	R(17)	$w_{char, H_2O} = K_{17} P_{H_2O} S_{a, char}$

reactions occur concurrently with pyrolysis and drying of wood particles, which are endothermic reactions and cause decrease in temperature after the first peak. When pyrolysis and drying processes are completed, exothermic reactions dominate and temperature rises again to the second peak. After the second peak, the temperature gradually decreases until the end of combustion. During this phase, a wood particle has completely been devolatilized, leaving a pure char that under-

goes oxidation and gasification with H₂O and CO₂. It is deduced that gasification, which is endothermic, is more pronounced than exothermic process (oxidation), hence the temperature decrease.

Figs. 4(a) and (b) also show that at corresponding height, air-fuel peak temperature is higher than oxy-fuel temperature by about 200 K. This is a result of the combination of both chemical and thermal effects. Lower temperatures are seen in

Fig. 2. Computational mesh for the fixed bed: (a) Highly refined mesh in fuel bed and grate; (b) prismatic layers near the wall.

Fig. 3. Predicted temperature profiles at 5 cm from the bed bottom for wood combustion in 21 % O₂/79 % CO₂ mixture for different mesh sizes.

oxy-fuel environment because CO₂ has higher heat capacity than N₂. Furthermore, chemical effect through endothermic reaction of CO₂ with char contributes in lowering the temperature of oxy-fuel environment.

The individual contribution of various effects of CO₂, namely, chemical, thermal and oxygen concentration effects are evaluated through CFD-DEM modeling. The model results are validated by comparing them with experimental values. Shown in Fig. 5 are measured and predicted temperature profiles at 5 cm from bed bottom for air-fuel and oxy-fuel environments both at 21 % O₂ concentration. The accuracy of model data was good with deviation of most points from measured values being within 10 %.

Presented in Fig. 6 are predicted temperature profiles at 5 cm from the bed bottom for wood combustion in different combustion atmospheres. It is observed that peak temperature occurrence time comes much earlier in N₂ atmosphere than in CO₂ atmosphere. This is an indication that combustion rate is slower in CO₂ environment. For oxy-fuel combustion, peak temperature value is directly proportional to O₂ concentration. In addition, its occurrence time increases as O₂ concentration is decreased. Peak temperature of oxy-fuel atmosphere, which is equivalent to that of standard air-fuel condition, occurs at about 40 % O₂ concentration. However, its occurrence time is

(a) 21 % O₂/79 % N₂ mixture

(b) 21 % O₂/79 % CO₂ mixture

Fig. 4. Measured temperature profiles at various distances from the bed bottom for wood combustion in different combustion atmospheres.

Fig. 5. Measured and predicted temperature profiles at 5 cm from the bed bottom for wood combustion in 21 % O₂/79 % N₂ and 21 % O₂/79 % CO₂ mixtures. Error bars are the standard deviations.

Fig. 6. Predicted temperature profiles at 5 cm from the bed bottom for wood combustion in different combustion atmospheres.

Fig. 8. Measured and predicted burning rates for fuel bed of wood combustion in N_2 and CO_2 environments. Error bars are the standard deviations.

Fig. 7. Measured and predicted ignition time for fuel bed of wood combustion in N_2 and CO_2 environments. Error bars are the standard deviations.

Fig. 9. Measured and predicted flame front propagation speed for fuel bed of wood combustion in N_2 and CO_2 environments. Error bars are the standard deviations.

slightly earlier than in air-fuel condition.

The time taken for the reaction front to start at the top surface of the fuel bed was defined as ignition time. Presented in Fig. 7 is ignition time for wood combustion in both oxy-fuel and air-fuel environments. The graph shows that at any given oxygen concentration, ignition time in oxy-fuel environment is almost twice that of corresponding air-fuel condition. Retarded ignition in CO_2 environment could be attributed to its high specific heat capacity and low O_2 diffusivity in it. In both cases, ignition time gradually decreases as oxygen concentration is increased.

A comparison of burning rates for wood combustion in N_2 and CO_2 burning conditions is presented in Fig. 8. At the same O_2 concentration, the burning rate in CO_2 burning atmosphere is less than in N_2 burning atmosphere. The burning rate of wood particles in oxy-fuel condition is lowered by the aforementioned CO_2 effects, which contribute differently as will be discussed later. Thermal diffusivity of CO_2 is less than that of

N_2 by about 35 % [34]. In addition, CO_2 absorbs radiative heat more than N_2 . The overall effect of these thermal properties of CO_2 is a decrease in burning rate as seen in Fig. 8. Furthermore, the burning rate in oxy-fuel environment is also decreased by chemical effect of CO_2 through Boudouard reaction R(16), which is endothermic. On the other hand, the role played by dilution is clearly demonstrated in Fig. 8. In both cases, burning rate is directly proportional to O_2 concentration. More O_2 concentration enhances oxidation of combustible pyrolysis products and char, hence releasing more heat and increases the burning rates.

Illustrated in Fig. 9 is the flame front propagation speed for wood combustion in oxy-fuel and air-fuel burning atmospheres. For all oxygen concentrations, CO_2 burning atmosphere had lower propagation speed as compared to N_2 burning atmosphere. Furthermore, as oxygen concentration increased flame propagation speed also increased. Flame speed is directly linked to the burning rate. Therefore, the factors which

reduce the burning rates in oxy-fuel environment as discussed in the preceding paragraph are also responsible for the reduced flame speed.

The species and temperature profiles along axial length of the fixed bed when the flame front is at 4 cm from the grate for 21 % $O_2/79\%$ CO_2 , 30 % $O_2/70\%$ CO_2 , 40 % $O_2/60\%$ CO_2 and 50 % $O_2/50\%$ CO_2 are presented in Figs. 10(a)-(d). The flame structures are similar in profile but differ in magnitude. The flame front for the mixture with high O_2 concentration, 50 %, reaches 4 cm plane at 191 s, which is earlier than those for 40 %, 30 % and 21 % that reached the plane at 275 s, 360 s and 482 s, respectively. This is because flame speed increases as O_2 concentration is increased. As shown in Figs. 10(a)-(d) and Table 5, the amount of tar and CH_4 is high at the reaction zone of 21 % O_2 concentration mixture and decreases gradually for 30 %, 40 % and 50 % O_2 concentration mixtures. The graphs show that the mixture with 21 % O_2 concentration is operating under fuel rich conditions and does not have enough O_2 to oxidize these species through reactions R(7) and R(9). On the other hand, the graphs show that the mixtures with 30 %, 40 % and 50 % O_2 concentration are operating under fuel lean conditions and have excess O_2 in their reaction zones. Thus, reduced amount of tar and CH_4 are observed in these mixtures as compared to those of 21 % O_2 concentration mixture. Consequently, since these reactions are exothermic, a high amount of heat is released as O_2 concentration is increased. This is seen in the peak temperatures attained by these mixtures, Fig. 6. The high amount of heat released increases the heating rates for the particles in the bed and explains the higher flame front propagation speed and burning rates for high O_2 concentration mixtures. High heat energy also accelerates the ignition of the particles for mixtures with high O_2 concentration.

Figs. 10(a)-(d) and Table 5 show that the amount of CO is highest in the reaction zone of the mixture with 30 % O_2 concentration. The mixtures with 21 %, 40 % and 50 % O_2 concentration have almost the same amount of CO in their reaction zone. Unlike tar and CH_4 whose sole source is devolatilization of the wood particles, CO is produced from devolatilization process, oxidation of tar through reaction R(9) and char gasification with CO_2 through reaction R(16). CO is consumed by oxidation reaction R(6). For a mixture with high O_2 concentration, excess O_2 brings an antagonistic effect to the amount of CO where there is a tendency for high consumption through oxidation reaction R(6) and high production by oxidation of tar through reaction R(9) as compared to that of a mixture with low O_2 concentration. However, for mixtures with high O_2 concentration, the production of CO through char gasification could be less than that of low O_2 concentration mixture because of low amount of CO_2 . The overall effect of these reactions is that there is an increase in CO production as O_2 concentration is increased up to a peak point, then it starts to decrease.

Burning rate, ignition of fuel particles and flame front propagation speed are all influenced by thermal behavior of

Fig. 10. Species and temperature profiles along axial length of the bed for different O_2/CO_2 mixtures when the flame front is at 4 cm from the grate.

the bed. Apart from heat of combustion through chemical reactions discussed in the preceding paragraphs, flame temperature at a given point is also determined by heat flux distribution in the bed, which is mostly by radiation. H_2O and CO_2 are the main products of combustion that participate in radia-

Table 5. Peak values of major combustible species and temperature profiles for wood combustion in different O₂/CO₂ mixtures.

Temperature/ species mole fraction (-)	O ₂ /CO ₂ mixture			
	21 % O ₂	30 % O ₂	40 % O ₂	50 % O ₂
Temperature (K)	1338	1406	1499	1605
Tar	0.02427	0.02164	0.01605	0.01837
CO	0.05839	0.06488	0.06013	0.06124
CH ₄	0.00819	0.00769	0.00542	0.00684

tion. The presence of high amount of CO₂ in an oxy-fuel environment makes it more emissive than air-fuel environment. As depicted by the flame temperatures in Figs. 6 and 10, a large amount of heat energy is released in the fuel bed with a high O₂ concentration mixture. In this study, the heat energy contribution from different sources has not been separated. Therefore, an increase in heat energy cannot be explicitly linked to a particular source. Though, in the region of intense combustion, heat contributed by combustion is more dominant; the contribution by radiation heat flux is only 10–15 % [35].

Wood combustion in four different mixtures of O₂ and Ar/CO₂/N₂ was numerically simulated so as to separate the various effects of CO₂ on burning rate of wood. For all the cases, temperature profiles at 5 cm from fuel bed were considered. A method of adjusting the flame temperature using Ar, which was initially proposed by Du et al. [15] and previously used by other researchers [14, 16, 17], was implemented in this study. The compositions of the four mixtures are specified in Sec. 2.2. Furthermore, other properties of the different mixtures such as mass fraction of the constituents, combined heat capacity and oxygen diffusion coefficient are provided in Table 6. These properties were evaluated and compared at room temperature (298 K), ignition temperature (500 K) and flame temperature (1400 K). Combustion of wood in mixtures A, B and C was designed to have the same peak temperatures, as shown in Fig. 11. A large amount of Ar in mixture B was to increase the peak temperature, which is low when CO₂ alone is used as a diluent. As shown in Table 6, this mixture has a lower specific heat capacity. This enabled the mixture to have the same peak temperature as that of mixture A and C. The peak temperature of wood combustion in mixture D was higher than for the other three by 167 K.

The burning rates of wood combustion in the four mixtures were evaluated and presented in Fig. 12. Burning rate in mixture A was used as a datum. The difference in burning rates of combustion in mixture A and B is due to chemical effect because they have the same oxygen concentration and temperature values. Since temperature is the only similar parameter for combustion in mixture A and C, then the difference in their burning rate is due to a combination of oxygen concentration and chemical effect. Oxygen concentration effect is achieved when oxygen concentration is increased to 40 % while maintaining the same temperature in CO₂ environment (combustion

Table 6. Composition, combined heat capacity and O₂ diffusion coefficient of the four mixtures at different temperatures.

Properties		Gas mixtures			
		A	B	C	D
Mass fraction of components (-)	O ₂	0.233	0.171	0.327	0.331
	CO ₂	0.000	0.253	0.673	0.535
	N ₂	0.767	0.000	0.000	0.000
	Ar	0.000	0.576	0.000	0.134
c _p for the mixture (kJ/kg K)	At 298 K	1.005	0.670	0.868	0.825
	At 500 K	1.030	0.725	1.006	0.939
	At 1400 K	1.209	0.826	1.255	1.147
O ₂ diffusion coefficient in the mixture (cm ² /s)	At 298 K	0.209	0.184	0.156	0.164
	At 500 K	0.513	0.462	0.398	0.415
	At 1400 K	2.888	2.642	2.310	2.401

Fig. 11. Predicted temperature profiles at 5 cm from the bed bottom for wood combustion in four combustion environments.

Fig. 12. Predicted separate effects of CO₂ on burning rates for wood combustion in four combustion environments.

tion in mixture B and C). Finally, the difference in burning rates for combustion in mixture C and D is due to thermal effect since they have the same oxygen concentration but different temperature values.

The individual contribution of CO_2 effects on burning rates of wood combustion is evaluated from Fig. 12. It was established that chemical, thermal and oxygen concentration influenced burning rate of wood by 5 %, 9 % and 86 %, respectively. It is evident that oxygen concentration is the most influential parameter in the burning rate. As oxygen concentration is increased, oxidation of char and combustible pyrolysis products is also enhanced. Therefore, more heat is generated and fuel burning rate is significantly improved. The influence of thermal and chemical is not very significant. Thermal effect is only 9 % and translate to a temperature change of 167 K. Chemical effect on the burning rate is quite small because the rate of the chemical reactions involving CO_2 consumption (R(14) and R(16)) is far much less compared to the rate of (R(6) and R(13)).

4. Conclusions

The overall and separate effects of CO_2 burning atmosphere on the combustion properties of wood burning in a fixed bed were investigated through numerical modeling. Modeling was validated by comparison with measured data. The following are the key findings:

- The dilution effect is the most influential parameter on the burning rate of wood combustion in an oxy-fuel system. The influence of thermal and chemical is not very significant.
- Peak temperature of oxy-fuel atmosphere, which is equivalent to that of standard air-fuel condition, occurs at a higher O_2 concentration. However, its occurrence time is slightly earlier than in air-fuel condition.
- At any given oxygen concentration, ignition time in oxy-fuel is almost twice that of corresponding air-fuel condition. In both cases, ignition time gradually decreases as oxygen concentration is increased.
- At the same oxygen concentration, burning rate and flame propagation speed in CO_2 combustion environment was less than in N_2 combustion environment.

Acknowledgments

This work was financially supported by both Dedan Kimathi University of Technology, Kenya and Technische Hochschule Wildau, Germany. The first Author would like to thank German Academic Exchange Service (DAAD) for the financial support for his stay in Technische Hochschule Wildau, Germany.

Nomenclature

A : Arrhenius pre-exponent factor [$\text{s}^{-1} (\text{mol m}^{-3})$]

A_s	: Particle surface area [m^2]
c_p	: Specific heat [$\text{J kg}^{-1} \text{K}^{-1}$]
C_l	: Permeability [m^2]
C_2	: Inertia loss coefficient [m^{-1}]
CFD	: Computation fluid dynamics
d	: Particle diameter [m]
D	: Diffusivity [$\text{m}^2 \text{s}^{-1}$]
DEM	: Discrete element method
E	: Activation energy [J mol^{-1}]
g	: Gravity [m s^{-2}]
G	: Incident radiative heat flux [W m^{-2}]
h	: Enthalpy [J kg^{-1}]
h_c	: Convective heat transfer coefficient [$\text{W m}^{-2} \text{K}^{-1}$]
H_i	: Enthalpy of formation of species i [J kg^{-1}]
J	: Diffusion mass flux [$\text{kg m}^{-2} \text{s}^{-1}$]
K	: Rate constant [$\text{s}^{-1} (\text{mol m}^{-3})$]
N_g	: Number of gas species [-]
p	: Pressure [Pa]
q_R	: Radiative heat flux [W m^{-2}]
$Q_{a,p}$	: Particle absorption coefficient [-]
R	: Universal gas constant [$\text{J mol}^{-1} \text{K}^{-1}$]
S_a	: Specific surface area [m^{-1}]
S_E	: Energy source term [$\text{J m}^{-3} \text{s}^{-1}$]
S_M	: Momentum source term [$\text{kg m}^{-2} \text{s}^{-2}$]
t	: Time [s]
T	: Temperature [K]
v	: Velocity [m s^{-1}]
w_i	: Rate of production of species i [$\text{kg m}^{-3} \text{s}^{-1}$]
WSGGM	: Weighted-sum-of-gray-gas-model
Y	: Mass fraction [-]

Greek symbols

ε	: Turbulent dissipation rate [$\text{J kg}^{-1} \text{s}^{-1}$]
θ	: Particle porosity [-]
κ	: Turbulent kinetic energy [$\text{J kg}^{-1} \text{s}^{-1}$]
λ	: Thermal conductivity [$\text{W m}^{-1} \text{K}^{-1}$]
μ	: Viscosity [$\text{kg m}^{-1} \text{s}^{-1}$]
ρ	: Density [kg m^{-3}]
σ	: Stefan-Boltzmann constant [$\text{W m}^{-2} \text{K}^{-4}$]
τ	: Shear stress tensor [Pa]
χ	: Region porosity [-]
Ω	: Stoichiometric coefficient [-]

Subscripts

b	: Biomass
e	: Effective
g	: Gas
i	: i^{th} reaction
i,g	: Gaseous species
i,s	: Solid-phase species
p	: Particle
s	: Solid

Superscript

- gs : Heterogeneous reaction
 n : Exponent

Operators

- ∇ : Gradient operator
 $\nabla \cdot$: Divergence operator

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The influence of particle packing density on wood combustion in a fixed bed under oxy-fuel conditions

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ARTICLE INFO

Article history:

Received 4 November 2019

Received in revised form

20 December 2019

Accepted 26 December 2019

Available online 27 December 2019

Keywords:

Oxy-fuel combustion

Bed porosity

Packing density

Wood combustion

Fixed bed

ABSTRACT

Presented in this paper is a study of the influence of particle packing density on fixed bed combustion of wood in an oxy-fuel burning environment. The packing density, which determines the region porosity, is influenced by fuels' geometry. Size and shape were determined directly from fuel particles and used to evaluate the particle sphericity which is an input in the computational model. Euler-Lagrange method was used to model conversion of wood in a fixed bed. The computational model was validated by performing experiments in a fixed bed using wood of different shapes and sizes which formed a wide range of bed porosity. It was established that the packing density affects combustion process by changing the burning conditions and flammability limits. The combustion condition is shifted from fuel-rich to fuel-lean side as bed porosity is increased. Consequently, the flame front propagation speed and conversion rates increase while the ignition time reduces. The operational range with respect to porosity was decreased in an oxy-fuel burning condition due to higher quenching effects of CO₂. Furthermore, the study revealed that there is an optimum packing density, $\chi = 0.71$, beyond which the efficiency falls due to the onset of quenching in the spaces.

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1. Introduction

Wood is a source of energy for both domestic and industrial application in most parts of the world. In industrial application, particularly for power plants that generate up to 40 MW_{th}, Hermansson and Thunman [1], the chemical energy bound in wood is converted into thermal energy using fixed bed combustion in a grate furnace. The fixed bed technique is favourable because of its simplicity. Consequently, this technique has been applied in most biomass power plant all over the world [1]. This has generated research interests in approaches for increasing combustion efficiency and reduction of emissions, Costa et al. [2], Guo et al. [3] and Yahaya et al. [4]. In practice, wood particles burned in the furnace are of different shapes and sizes. Packing of these particles affects their arrangement in the bed and thus the bed porosity. Bed porosity is a complex parameter which besides being affected by the particles' physical properties also changes as combustion progresses due to bed shrinkage, Porteiro et al. [5] and Khodaei et al. [6].

Various types of biomass and their conversion processes have been studied in fixed beds operated in O₂/N₂ mixtures, Abrego et al. [7], Chen et al. [8], Meng et al. [9] and Plis & Wilk [10]. Lately, there is a lot of interests in utilization of wood in an oxy-fuel burner for thermal energy generation. This is a technology where biomass is burned in a O₂/CO₂ mixture instead of a O₂/N₂ mixture. This is a clean energy technology where the CO₂ is captured through recycling of flue gas, and at the same time nitrogen oxides (NO_x) emissions are reduced, Scheffknecht et al. [11]. Most of the previous research on combustion of biomass under an oxy-fuel environment were done for entrained flow reactor, Riaza et al. [12] and Gil et al. [13], drop tube furnace, Heuer et al. [14] and Pohlmann et al. [15], single particle investigations, Shan et al. [16] and thermogravimetric analysis (TGA) method, Gil et al. [17]. Even though oxy-fuel combustion is a clean combustion technology, it has been established that it reduces flame temperature [15], increases ignition delay time [16] and reduces combustion rate, Riaza et al. [18].

Fixed bed combustion of wood is influenced by its shape and size amongst other factors. The influence of shape is through the following four ways: Particle overlapping; grain direction; geometry and packing in the bed. Particles with flat and concave surfaces can overlap when arranged in a chamber whereas those with

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convex surfaces such as spherical shapes, do not overlap. Overlapping of surfaces reduces effective surface area for fluid flow and chemical reactions. The influence of particle overlapping is analyzed by defining a particle surface availability, Trudel and Hallet [19]. Alternatively, its effect is determined using a shape factor that is included in heat and mass transfer correlations, Glaser and Thodos [20].

Biomass fuels are made of fibres which are normally aligned with one another. It has been shown that pyrolysis rate is faster along the fibres than across them, Larfeldt et al. [21]. Volatiles also flow faster along the fibres as compared to movement across them, Henriksen et al. [22]. Char produced through pyrolysis under low heating rates has fibre arrangement similar to that of raw biomass, Trudel et al. [23]. Consequently, porosity is high across the fibres. This leads to a higher gas permeability along the grain [21]. In addition, conversion rate for char is increased on the surface normal to the fibres [23]. Thus, aspect ratio plays an important role in wood and char gasification, Pattanotai et al. [24].

The geometry of the particle affects biomass conversion through surface area. Most biomass particles utilized in power plants have a wide range of irregular shapes which can impact on its conversion. The shape of a particle is defined in terms of sphericity. It has been shown that sphericity of particles has a correlation with ignition rate and bed porosity, Hörttnäinen et al. [25]. Particles with high sphericity have decreased surface area, which impacts negatively on burning times, Huff [26].

The shape and the size of fuel particles also have significant influence on the packing density. Thus, hydrodynamics of flow and thermal properties of the bed are affected. In fact, a number of correlations for pressure loss were developed on the basis of hydraulic diameter of the bed, Comiti and Renaud [27]. The size of fuel particles affects wood conversion in a packed bed through convective and radiation heat transfer, gas species and energy dispersion by turbulence as well as mass transfer and mixing rate of volatiles and air in the bed. Subsequently, bed packing affects the amount of volatiles released, reaction zone thickness Yang et al. [28], operational limit of air flow rate [25], burning rate, Ryu et al. [29], and ignition front velocity, Porteiro et al. [30]. Despite the significance of fixed bed combustion technology in power generation, there are few studies of this technique in an oxy-fuel environment, Tanui et al. [31]. Most of the studies only cover combustion under air-fuel condition. Specifically, the effects of bed porosity on wood conversion in a fixed bed operated in O₂/CO₂ mixture have not been investigated.

The main aim of this study was to investigate the impact of particles packing density on fixed bed combustion of wood in an oxy-fuel burning environment. Fuels with different characteristic particle size were experimentally studied in a fixed bed operated in oxy-fuel environment. A detailed analysis of bed combustion in terms temperature profiles, species generations, reaction zone thickness and conversion rates were done using Euler-Lagrange model. The model was implemented in a commercial software CD-Adapco (STAR CCM + version 11.04) [32].

2. Material and method

2.1. Fuel sample properties

The fuel samples used in all experiments in this study were of eucalyptus wood. Eucalyptus is the main source of fuel for wood-fired boilers used for steam generation in process industries such as tea production in Kenya. Eucalyptus tree is an attractive source because it takes a short time to mature. The properties of fuel sample are presented in Table 1. Fuel sample sizes were determined using BS EN 15149–2:2010 standard [33]. Sieving of wood particles

was done using Fritsch vibratory shaker with sieves of size between 0.5 and 7.1 mm. In every sieving process conducted, an amplitude of 3 mm and time of 15 min was used.

The fuel particles were then grouped into three categories according to their sizes, namely, sawdust 1 (SD1), sawdust 2 (SD2) and wood chips (WC), as shown in Fig. 1. The characteristic size, $\bar{d}$, of each group was fitted using Rosin-Rammler distribution, Eq. (1) [34].

$$R(d) = 100 \left(1 - \exp \left(- \left(\frac{d}{\bar{d}} \right)^n \right) \right) \quad (1)$$

In Eq. (1), $R(d)$ is the percentage of accumulated undersize mass and the value of n was determined according to Brezání and Zelenák [35].

The particle diameter, D_{eq} , which is equivalent to that of a sphere with the same volume, was evaluated for each fuel sample using its characteristic size $\bar{d}$ and shape. Furthermore, the sphericity, ψ of the particle was determined [23].

$$\psi = \frac{\pi D_{eq}^2}{A_s} = \frac{\pi^{1/3} (6V_p)^{2/3}}{A_s} \quad (2)$$

Bed porosity, χ , was determined from the measured fuel bed density, ρ_b , and density of wood particle, ρ_p , which were related through Eq. (3) [25]:

$$\chi = 1 - \frac{\rho_b}{\rho_p} \quad (3)$$

The sphericity, equivalent diameters and bed porosity of different fuel samples used in this study are presented on Table 2.

2.2. Experimental set-up

All experiments in this work were done using a laboratory scale combustion test rig shown in Fig. 2. The combustion module was made from a 40 mm-diameter stainless steel tube which was 200 mm long. It was insulated with a refractory material, which was contained in a stainless steel tube. A full description of the combustion rig is provided in our previous paper, Tanui et al. [31].

Temperature distribution in the combustion region was obtained using Type K thermocouples that were located 10 mm from each other along the axial length of the rig. The temperature data were acquired and recorded in every second. Temperature measurement data at various heights in the bed were used to estimate ignition time and flame propagation speed. Combined measurement uncertainty for thermocouple data acquisition depends on the measured temperature and for the entire range was determined to be between $\pm 2.2^\circ\text{C}$ and $\pm 6.6^\circ\text{C}$. 21% O₂/79% CO₂ mixture was supplied, mixed in a chamber of glass particles and led into combustion chamber through a stainless steel grate. Gas volumetric flow rate was controlled by rotameters with a tolerance of $\pm 2\%$.

Experiments were done for five fuel particle types shown in Table 2, which form bed porosity in the range of 0.51–0.74. Three replicates were performed for each experiment. For all the cases studied, the fuel bed height was 60 mm. The bed was operated in a batch mode; the fuel particles were supplied once for each experiment. However, oxidizer was supplied continuously. Ignition was done at the top and the reaction front propagated downward into unreacted fuel particles.

2.3. Numerical model

Fixed bed combustion of wood was modeled using a commercial

Table 1
Proximate and ultimate analysis of the fuel sample.

Proximate Analysis	(wt %)	Standards
Moisture	10.3	CEN-TS 14774-2:2009
Volatile matter (wt% dry basis)	84.9	CEN-TS 15148:2009
Fixed carbon (wt% dry basis) - by difference	14.9	—
Ash (wt% dry basis)	0.2	CEN-TS 14775:2009
Ultimate Analysis	(wt % dry basis)	Standards
C	50.87	CEN-TS 15104:2011
H	5.73	CEN-TS 15104:2011
N	0.3	CEN-TS 15104:2011
O (by difference)	43.1	—
Gross calorific value (MJ/kg)	19.3	CEN-TS 14918:2009

(a) Wood chips (WC)

(b) Sawdust 2 (SD2)

(c) Sawdust 1 (SD1)

Fig. 1. Wood fuel samples.

Table 2
Properties of wood samples and fixed bed.

Fuel type	ρ_b (kg/m ³)	ρ_p (kg/m ³)	D_{eq} (mm)	ϕ (—)	χ (—)
Wood chips (WC)	597	1220	5.25	0.30	0.51
Sawdust 1 (SD1)	321	1220	1.28	0.25	0.74
Sawdust 2 (SD2)	477	1220	2.91	0.29	0.61
Mixture of WC and SD1 (25% WC) – WCD1	390	1220	2.27	0.28	0.68
Mixture of WC and SD2 (50% each) – WCD2	537	1220	4.08	0.30	0.56

software code CD-Adapco (STAR CCM + version 11.04) [32]. Euler-Lagrange simulation method was implemented in this work. In this technique, solid wood is simulated through a Lagrangian framework, Discrete Element Method (DEM), whereas fluid-phase is modeled using computational Fluid Dynamics (CFD). Governing equations for fluid-phase are presented in Table 3 while those for solid-phase are in Table 4. More details about these equations are described in our previous paper [31] and in Ref. [32]. The symbols are defined in the nomenclature section.

Exchange of mass and species between solid-phase and fluid-phase were enabled by coupling equations: $\sum_{i,g} w_{i,g}^{ps} = - \sum_{i,s} w_{i,s}^{fs}$ and

$w_{i,g}^{ps} = -w_{i,s}^{fs}$, respectively. Similarly, the energy source term in fluid-phase model is as a result of energy exchange between solid and fluid phases by convection and radiation. This term also accounts for the enthalpy of formation of heterogeneous species. The source terms appearing in fluid-phase energy Eq. (9) have the same magnitude as those in solid-phase energy Eq. (12) but have opposite sign. Turbulence in fluid-phase was enabled by using a standard $k - \epsilon$ model.

The chemical kinetic mechanism that is implemented in this

study is shown in Table 5. It consists of sub-models for drying, devolatilization, homogeneous reactions and char combustion, respectively. The chemical effect of CO₂ environment was accounted for by inclusion of reaction R (10), that was established as the most significant in such environment, Liu et al. [36,37]. Furthermore, R (10) is associated with reactions R (11) and R (12), which are also included. Kinetic data and rate expression for all reactions are specified in Table 5. Char combustion were modeled through oxidation reaction R (15). The char combustion rate were evaluated based on partial pressure of O₂, CO₂ and H₂O available at its surface, Evans and Emmons [38]. The stoichiometric ratio of CO₂ to CO was modeled in terms of particle temperature [39]:

$$Q = \frac{2(1 + 4.3 \exp[-3390/T_{particle}])}{2 + 4.3 \exp[-3390/T_{particle}]}$$

In this work, radiation energy exchange between continuous region and fuel particles was considered. The radiant energy equation was computed through Discrete Ordinate Method (DOM), Fiveland [45]. Both fuel particles and gases were considered to participate in radiation. The radiation property of the fuel particles

(a) Schematic diagram

(b) A photo of laboratory set-up

Fig. 2. Experimental set-up.

Table 3
Gas-phase conservation equations.

- Mass conservation equation:

$$\frac{\partial}{\partial t}(\chi \rho_g) + \nabla \cdot (\rho_g \mathbf{v}_g) - \sum_{i,g} w_{i,g}^p = 0 \quad (4)$$

- Momentum conservation equation:

$$\frac{\partial}{\partial t}(\chi \rho_g \mathbf{v}_g) + \nabla \cdot (\rho_g \mathbf{v}_g \mathbf{v}_g) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho_g \mathbf{g} + S_m \quad (5)$$

- Energy conservation equation:

$$\frac{\partial}{\partial t}(\chi \rho_g h_g) + \nabla \cdot (\rho_g \mathbf{v}_g h_g) - \frac{\partial}{\partial t}(\chi p) + \nabla \cdot (\lambda_{g,e} \nabla T_g) - \sum_{i=1}^{N_g} h_{i,g} \nabla \chi_i + \nabla \cdot (\mathbf{v}_g p) - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}_g) + S_E = 0 \quad (6)$$

- Species conservation equation:

$$\frac{\partial}{\partial t}(\chi \rho_g Y_{i,g}) + \nabla \cdot (\rho_g \mathbf{v}_g Y_{i,g}) - \nabla \cdot (\rho_g D \nabla Y_{i,g}) + w_{i,g}^p = 0 \quad (7)$$

- Momentum source term:

$$S_m = - \left(\frac{\mu}{C_1} \mathbf{v}_g + C_2 \rho_g |\mathbf{v}_g| \mathbf{v}_g \right) \quad (8)$$

- Energy source term:

$$S_E = A_g h_c (T_s - T_g) - \sum_{i,g} w_{i,g}^p H_{i,g} + q_R \quad (9)$$

was considered to be gray. On the other hand, gases radiation properties were modeled using unmodified Weighted-Sum-of-Gray-Gas-Model (WSGGM), Smith et al. [46].

Computation was done on an unstructured grid that consisted of cells which were made of polyhedral elements. The cells closest to the walls were made of prism layers. Solutions which are independent of grid size were carried out by performing a mesh independent test as shown in Fig. 3. The graphs represent temperature profiles for particle type WC and SD1 predicted by different grid sizes. Temperature predicted using a mesh size with 100,000 cells showed a significant difference from that predicted using a mesh

size of 200,000 cells. However, changing of mesh size to 300,000 cells and 400,000 cells, respectively, did not significantly change the prediction results when compared to that of 200,000 cells. Therefore, combustion of all fuel particle types were computed using a mesh with 200,000 cells.

The packing density, which determines the region porosity, is influenced by fuels' geometry. Size and shape were determined directly from fuel particles and used to evaluate the particle sphericity. All parameters of the wood particles which were input to the model are presented in Tables 1 and 2.

The inlet boundary was positioned on the lower side of the fixed

Table 4
Solid-phase conservation equations.

• Mass conservation equation:

$$\frac{\partial}{\partial t}((1-\chi)\rho_s) - \sum_{i,j} w_{i,j}^s = 0 \quad (10)$$

• Species conservation equation:

$$\frac{\partial}{\partial t}((1-\chi)\rho_s Y_{i,s}) - w_{i,j}^s = 0 \quad (12)$$

• Energy conservation equation:

$$\rho_s c_{ps}(1-\chi) \frac{\partial T_s}{\partial t} - \nabla \cdot (\lambda_{se} \nabla T_s) + A_p h_c (T_g - T_s) + \frac{A_p}{4} \Omega_{ap} (G - 4\sigma T_s^4) + \sum_{i,j} w_{i,j}^s H_{i,j} = 0 \quad (13)$$

Table 5
Biomass kinetic model.

Drying	Rate expression	Source
R (1) Wet wood $\rightarrow$ Dry wood + H ₂ O (g)	$R_{dry} = Y_{mf, wet} 1.6 \times 10^{27} \exp(-25000/T_s)$	[39]
Pyrolysis Reactions	Rate expression, $K_i = A_i T^n \exp(-E_i/RT)$	Kinetics: A (s ⁻¹), E (kJ/mol)
R (2) Dry wood $\rightarrow$ gas	$w_b' = K_2 \rho_{b, dry}$	$A_2 = 111 \times 10^9$, $E_2 = 177$
R (3) Dry wood $\rightarrow$ Tar	$w_b' = K_3 \rho_{b, dry}$	$A_3 = 9.28 \times 10^9$, $E_3 = 149$
R (4) Dry wood $\rightarrow$ char	$w_b' = K_4 \rho_{b, dry}$	$A_4 = 30.5 \times 10^9$, $E_4 = 125$
R (5) Tar $\rightarrow \gamma_t$ Tar _{inert} + γ_{CO} CO + γ_{CO2} CO ₂ + γ_{H2} H ₂ + γ_{CH4} CH ₄	$w_{tar}' = K_5 \rho_{tar}$	$A_5 = 9.55 \times 10^4$, $E_5 = 93.37$
Homogeneous Gas-Phase Reactions	Rate expression, $K_i = A_i T^n \exp(-E_i/RT)$	Kinetics: A (s ⁻¹), E (kJ/mol)
R (6) 2CO + O ₂ $\rightarrow$ 2CO ₂	$R_{CO} = K_6 [CO][O_2]^{0.25} [H_2O]^{0.5}$	$A_6 = 2.24 \times 10^{12}$, $n = 0$, $E_6 = 167.36$
R (7) CH ₄ + 2O ₂ $\rightarrow$ CO ₂ + 2H ₂ O	$R_{CH4} = K_7 [CH_4]^{0.7} [O_2]^{0.8}$	$A_7 = 11.58 \times 10^{13}$, $n = 0$, $E_7 = 202.5$
R (8) 2H ₂ + O ₂ $\rightarrow$ 2H ₂ O	$R_{H2} = K_8 [H_2][O_2]$	$A_8 = 2.19 \times 10^9$, $n = 0$, $E_8 = 109.2$
R (9) Tar + 2.9O ₂ $\rightarrow$ 6CO + 3.1H ₂	$R_{tar} = K_9 [Tar]^{0.5} [O_2]$	$A_9 = 9.2 \times 10^6$, $n = 0$, $E_9 = 80.2$
R (10) CO + OH $\rightarrow$ CO ₂ + H	$R_{CO} = K_{10} [CO][OH]$	$A_{10} = 4.76 \times 10^7$, $n = 1.3$, $E_{10} = 0.293$
R (11) H + O ₂ $\rightarrow$ O + OH	$R_H = K_{11} [O][OH]$	$A_{11} = 2.65 \times 10^{16}$, $n = -0.671$, $E_{11} = 71.347$
R (12) H ₂ + O ₂ $\rightarrow$ OH + OH	$R_{H2} = K_{12} [H_2][O_2]$	$A_{12} = 2.51 \times 10^{12}$, $n = 0$, $E_{12} = 163.075$
R (13) H ₂ O + CO $\rightarrow$ CO ₂ + H ₂	$R_{H2O} = K_{13} [H_2O][CO]$	$A_{13} = 2.78$, $n = 0$, $E_{13} = 12.55$
R (14) CO ₂ + H ₂ $\rightarrow$ H ₂ O + CO	$R_{CO2} = K_{14} [CO_2][H_2]$	$A_{14} = 93.69$, $n = 0$, $E_{14} = 46.594$
Heterogeneous Reactions	Rate expression, $K_i = A_i T^n \exp(-E_i/RT)$	Kinetics: A (s ⁻¹), E (kJ/mol)
R (15) Ω C + O ₂ $\rightarrow$ 2 ($\Omega - 1$) CO + ($2 - \Omega$) CO ₂	$w_{char, O2}' = K_{15} \rho_{O2} S_{a, char}$	$A_{15} = 2.54 \times 10^{-3}$, $E_{15} = 74.8$
R (16) C + CO ₂ $\rightarrow$ 2CO	$w_{char, CO2}' = K_{16} \rho_{CO2} S_{a, char}$	$A_{16} = 1.81 \times 10^{-2}$, $E_{16} = 130$
R (17) C + H ₂ O $\rightarrow$ CO + H ₂	$w_{char, H2O}' = K_{17} \rho_{H2O} S_{a, char}$	$A_{17} = 1.81 \times 10^{-2}$, $E_{17} = 130$

Fig. 3. Comparison of temperature profiles along the axial length of the bed for particle type (a) WC ($\chi = 0.51$) and (b) SD1 ($\chi = 0.74$) when reaction front is at 4 cm from the grate applying different computation mesh sizes.

bed. At the inlet, mass flow rate, species mole fraction and temperature were specified using Dirichlet boundary condition. The temperature for the oxidizer mixture, which consisted of 21% O₂ and 79% CO₂ at the inlet, was 295 K. Mass flow of the oxidizer mixture at the inlet was 0.1 kg/m²/s for all the fuel types. At outlet boundary, which was positioned at top of the fixed bed, species concentration and temperature gradients were fixed at zero. The thermal conditions at the fixed bed were considered to be both convective and radiative. The coefficient of convective heat transfer which was adopted at the fixed bed wall was 10 W/m².K. The fixed bed wall was made of stainless steel whose emissivity is 0.8 [47].

3. Results and discussions

The CFD-DEM model results were validated by data obtained from experiment. Fig. 4 presents a validation of temperatures at various heights in the bed for different fuel particle types. In general, deviations of 10% or less between the model and measured data indicate a good agreement. Particle type WC, WCSD2 have two distinct temperature peaks, Fig. 4(a)–(b), while particle type WCSD1 and SD1 have a single temperature peak, Fig. 4(d) and (e). Particle type SD2 is a transition case with a distinct first temperature peak and the temperature plateaus off in the second peak, Fig. 4(c). The first peak is attained during ignition front propagation phase while the second peak is attained during char oxidation phase, Khor et al. [48]. Fig. 4(a)–(b) indicate that beds with low porosity have substantial amount of char remaining in the bed after devolatilization. The char combustion phase peak temperatures for these fuel particle types are higher than ignition front propagation phase peak temperatures. In particle type SD2, some of the char produced are oxidized in the first peak region leading to a higher flame temperature being attained. Subsequently, its second peak region has a low temperature value. In case of high porosity beds, Fig. 4(d) and (e), they have a single peak temperature point with relatively higher values than those for the first peaks of the beds with low porosity. It is also observed that in all the fuel particles investigated the bed temperatures are relatively less than those for air-fuel environment in comparable burning conditions [31]. Temperature in a O₂/CO₂ mixture is reduced by its higher heat capacity.

Presented in Fig. 5 is the ignition time for the different fuel particles. Bed ignition time was considered to be the time in which the reaction front takes to start at the top surface of the bed. Reaction front starts when the bed temperature rises rapidly from ambient value to peak value. Ignition time was estimated from temperature profiles at various heights in the bed with an assumption that the flame propagation is steady, Yang et al. [49]. Ignition time decreases with increase in initial bed porosity. For the entire range, the ignition time values are higher than those reported for wood combustion under N₂ environment in the same conditions, Tanui et al. [50]. Higher ignition time in CO₂ environment could be due to its decreased flame temperature and heating rates. Furthermore, chemical reactions of CO₂ through reactions R(14) and gasification of char, R(16), contribute to retardation of ignition time. Reaction R(16) is endothermic and results in decreasing the amount of heat in the bed. Consequently, it increases the ignition time delay in the fuels.

The impact of porosity on air to fuel stoichiometry and flame front propagation speed is presented in Fig. 6. The values are compared to those obtained in N₂ environment under similar operating conditions. The equivalence ratio presented are the averaged values based on the total combustion time, fuel chemical composition and air flow rates. The actual equivalence ratio varies at different combustion stages as noted later in the analysis of gas species generation in the bed: It is higher during pyrolysis phase

and lower during char consumption phase. For both cases, flame front propagation speed increases with increases in bed porosity. It is correspondingly lower in CO₂ environment.

Fig. 6 also shows that as bed porosity is increased the burning condition is shifted from fuel-rich to fuel-lean side. Under the same air flow rate and O₂ volumetric concentration, this shift is more toward the porous region in a O₂/CO₂ mixture than in a O₂/N₂ mixture as a result of differences in molecular weight. Furthermore, as noted in the flame front propagation speed, the operational range with respect to porosity is narrowed in a CO₂ environment. This is due to its high heat capacity which causes earlier quenching effects than in N₂ environment.

Drying, pyrolysis, homogeneous reactions and char conversion in the bed occurs simultaneously. Overlapping of these processes depends on the burning conditions. Dry wood particles with the same amount of mass initially located at 4 cm from the grate for different particle types were tracked in order to monitor their conversion progression. Fig. 7(a) presents the conversion of these particles in the bed with respect to time. The mass of dry wood remains constant until the onset of pyrolysis. Amongst the cases investigated, the onset of pyrolysis in particle type WCSD1 occurred at 180 s, which is earlier than any other particle. Pyrolysis in particle type WC started to occur at 390 s and took longer a time to complete, 1110 s. This indicate that as porosity of the bed is increased, pyrolysis process takes a shorter time. Though it is observed that there is an optimum point at which pyrolysis times begins to increase even with increase in porosity. This optimum point occurs when porosity is about 0.71. This is as a result of combustion conditions becoming too lean and the flame starts to be quenched by excess CO₂ through convection cooling.

The amount of char produced in the bed decreases with increase in porosity, Fig. 7(b). Higher amount of char in low porosity bed indeed confirms the second peak temperatures attained in these particle types seen in Fig. 4(a)–(b), which arise from combustion of char that is left in the bed after devolatilization. Char, which is in essence carbon, is produced and consumed within a shorter period of time as bed porosity increases. The amount of char presented in Fig. 7(b) is the net amount at a given time for particle tracked. Char is produced from pyrolysis of dry wood through reaction R (4). Once it is produced, it is consumed through reactions R (15)–R (17) depending on bed temperature and availability of O₂, CO₂ and H₂O.

The actual rates for conversion of dry wood particles are presented in Fig. 8(a). Particle type WCSD1 and WC attained the fastest and slowest pyrolysis rate of 4.78 and 2.13 kg m^{−3} s^{−1}, respectively. The trend of influence of porosity is similar to what was observed before; pyrolysis rate increases with increase in porosity up to the optimum point, 0.71, where it starts to decrease. As porosity is increased, there is a quick release of volatiles. Oxidation of combustible volatiles through reaction R (6)–R (10) releases intense heat which increases the conversion rate. Since the conversion processes are fast, ignition is quick and flame propagation is also fast as noted in Figs. 5 and 6, respectively. In low porosity beds, volatiles are slowly released, heating rate is low and consequently, a slow conversion rate. Subsequently, low porosity beds have higher ignition time and low flame front propagation speed. Net char formation and consumption for the particles with respect to time are presented in Fig. 8(b). Just like wood pyrolysis rate, net char formation rates, positive values, increases as porosity is increased up to an optimum value, then it starts to decrease. However, the net consumption rates, negative values, have no optimum value. Particle type WC, WCSD2 and SD2 attained almost the same peak consumption rates. Char consumption rate is directly proportional to the char specific surface area, $S_{a, char}$ as indicated in reactions R (15)–R (17). Thus, the high specific surface area for char in porous

Fig. 4. Measured and predicted temperature profiles at various heights above the grate for particle types (a) WC ($\chi = 0.51$), (b) WCS2 ($\chi = 0.56$), (c) S2 ($\chi = 0.61$), (d) WCS1 ($\chi = 0.68$) and (e) S1 ($\chi = 0.74$).

bed increases their consumption.

Gas species concentration and temperature predicted during entire conversion of wood at a particular height is shown in Fig. 9. The values presented are taken at 4 cm from the grate for different particle types. The figures clearly depict the three distinct stages of wood combustion; drying, pyrolysis and char consumption. In all

the cases, drying starts when the temperature reaches about 50 °C, as evident in the drying front which is always slightly ahead of the ignition front. The decrease in CO₂ mole fraction at the onset of drying is due to introduction of water vapour in the bed and should not be viewed as a consumption. The absolute amount of CO₂ only changes in the reaction zone as it is a product of oxidation of char

Fig. 5. Measured and predicted ignition time for wood combustion under oxy-fuel condition for different initial bed porosity. Error bars are the standard deviations.

Fig. 6. Measured and predicted flame front propagation speed for wood conversion in 21% O₂/79% N₂ and 21% O₂/79% CO₂ mixtures for different initial bed porosity.

and volatiles which contain carbon in their molecular structure. Alternatively, its amount may change through its participation in gasification of char, through reaction R (16) and in the forward and backward reactions of H₂O and CO, in R (13) and R (14).

During pyrolysis, particles at a local point absorb heat energy from oxidation of volatiles released by adjacent particles located in the upper side through radiation and conduction. Once the particle attains devolatilization temperature, then the volatiles are rapidly released. Combustible volatiles, are oxidized through reactions R (5)–R (10) releasing intense heat which rapidly increases the temperature to the first peak point, as seen in Fig. 9 for all the cases. During this period, O₂ decreases gradually but does not go to zero immediately. Under the same oxidizer mixture mass flux as used in

this study, the extent to which O₂ concentration falls depends on the bed porosity. For particle type WC and WCSD2, Fig. 9(a) and (b), as pyrolysis progresses downward, the volatiles release at the lower part of the bed consume all the O₂. Consequently, O₂ is not able to reach the upper region. Since the wood fuels in this region are still undergoing pyrolysis, which is endothermic, the local temperature decreases. During this time, volatiles in upper region are not oxidized and their concentration remains almost constant. Similarly, char produced is not oxidized during this time. For this particle types, during devolatilization time, char is only consumed by gasification H₂O and CO₂. As a result, the amount of char is higher than for SD1, SD2 and WCSD1, as observed in Fig. 7(b).

Once the entire bed is completely pyrolyzed, volatiles in the

Fig. 7. Predicted (a) wood conversion and (b) char formation of the particles with the same amount of mass initially located at 4 cm from the grate for different fuel particle types.

Fig. 8. Predicted rate of (a) wood conversion and (b) char formation of the particles with the same amount of mass initially located at 4 cm from the grate for different fuel particle types.

lower region are the first to be completely oxidized since O_2 is supplied from the bottom. This is evident in the steep increase in temperature of thermocouple located close to grate, Fig. 4(a) and (b). After complete oxidation of volatiles in the lower region of the bed, excess O_2 is convected upward. The volatiles remaining in the bed are oxidized progressively from bottom to the top, as depicted in steep temperature rise at the end of devolatilization stage in Fig. 4(a) and (b). At a given height, CO_2 concentration sharply increases at the end of devolatilization stage. This is partly due to oxidation of CH_4 , CO and tar. Its increase is also caused by depletion of other species through complete oxidation. Complete oxidation of volatiles end at 1200 s and 860 s for particle type WC and WCS2, respectively, Fig. 9(a) and (b). After this point, there is excess O_2 in the bed and char oxidation through reaction R (15) starts. Concurrently, char is consumed by CO_2 through Boudouard reaction R (16). In overall, the amount of CO_2 decreases while that of CO increases. Finally, CO is completely oxidized to CO_2 toward the end of char combustion.

Pyrolysis and char consumption in particle types SD2, WCS1 and SD1 proceed in almost a similar way. They all operate under lean conditions throughout conversion process as depicted by excess O_2 in their reaction zones, Fig. 9(c)–(e). As a result, oxidation of volatiles continues in the upper part of the bed as pyrolysis progresses downwards. This is evident in the low concentration of

tar, CH_4 , H_2 and CO in these particles as compared to those of particle types WC and WCS2. In addition, char is oxidized concurrently with volatiles. This explains the high temperatures in the first peak of the porous fuels seen in Fig. 4(c)–(e). The low amount of char in the porous bed noted in Fig. 6(b) is also accounted for by this fact. For particle types SD1 and WCS1, the heat release from oxidation of the char remaining in the bed after complete devolatilization is not sufficient to raise the temperature to a second peak, Fig. 9(d) and (e). However, particle type SD2 still has a substantial amount of char whose oxidation is sufficient to increase the temperature to a second peak. Though it is not as high as for particle types WCS2 and WC1.

Flame structures along axial length of the bed for different particle types when the reaction front is at 4 cm from the grate are presented in Fig. 10. The graphs clearly illustrate the thickness of the reaction front for various fuel particles. Thickness of the reaction front was considered to be the axial length in the bed in which the temperature changes from ambient value to maximum as flame front passes, Yang et al. [49]. It is affected by several factors which include burning rates, flame front propagation speed and fuel particle size. In general, it was observed that reaction front thickness increases as porosity increases; the lowest and highest values being 21 mm and 35 mm for particle types WC and SD1, respectively. Thin reaction front indicates that the particles at a given

Fig. 9. Predicted species concentration and temperature profiles for particle types (a) WC ($\chi = 0.51$), (b) WCD2 ($\chi = 0.56$), (c) SD2 ($\chi = 0.61$), (d) WCD1 ($\chi = 0.68$) and (e) SD1 ($\chi = 0.74$).

height burn uniformly. For this case, higher amounts of volatiles are present at a given height, Fig. 10(a)–(c). On the other hand, a thicker reaction front as seen in Fig. 10(d) and (e) is associated with a high flame front propagation speed, high burning rates and fast pyrolysis. In this case, fuel particles at a lower region start releasing small amount of volatiles which are immediately oxidized. Consequently, the amounts of volatiles are not as high as for cases with thin reaction front thickness. Furthermore, radiation energy in low porosity beds have short penetration into fuel particles in

unreacted region. Therefore, their flame front propagation moves slowly as seen in Fig. 6, and the reaction zone is thin. This is opposite to high porosity bed which allows deep penetration of radiation energy to unreacted particles in the lower part of the bed making them to have high flame front propagation speed and a thicker reaction zone.

Volatiles released when the reaction front is at 4 cm from the grate, for all the cases, are not completely oxidized in the fuel bed, Fig. 10. Unreacted volatiles do not stay in the bed but instead, they

Fig. 10. Predicted major species concentration and temperature along axial length of the bed for particle types (a) WC ($\chi = 0.51$), (b) WCSD2 ($\chi = 0.56$), (c) SD2 ($\chi = 0.61$), (d) WCSD1 ($\chi = 0.68$) and (e) SD1 ($\chi = 0.74$).

are transported to freeboard region, height above 6 cm, where they are reacted as indicated by their decreasing levels. Unlike in the bed region, there are no endothermic processes, pyrolysis and gasification, in freeboard region. Therefore, oxidation of volatiles results in higher freeboard temperature in all the cases. It is noted that for fuels with thick reaction zone thickness, Fig. 10(c)–(e), H_2 is the dominant volatile in the low temperature region of about 300–800 K. A high amount of H_2 in these fuels is as a result of reaction R (13). This is supported by low amount of CO in this region. Furthermore, this reaction has been reported to have better prediction and works well in fuel lean conditions under which these fuels were operated, Andersen et al. [51] and Jones & Lindstedt [52].

4. Conclusions and recommendations

An investigation on the influence of particle packing density on wood conversion in the fixed bed under oxy-fuel environment in the entire possible operation range were done in this study. The following are the main findings of the study:

- The packing density affects the combustion process in an oxy-fuel environment by changing the burning conditions and flammability limits. The combustion condition is shifted from fuel-rich to fuel-lean side as bed porosity is increased. Consequently, the flame front propagation speed increases while the ignition time reduces. The reaction zones also thicken.

- As bed porosity is increased, volatiles and char are concurrently oxidized during pyrolysis stage leading to a single temperature peak. On contrary, bed with low porosity has two distinct temperature peaks since volatiles and char are oxidized sequentially due to O₂ deficit.
- There is an optimum packing density, $\chi = 0.71$, beyond which the efficiency falls off due to the onset of quenching in the spaces.
- Increasing the porosity of the bed positively affects the pyrolysis rate up to the optimum point. At the same time, the volatiles oxidation is increased due to fuel-lean combustion condition. This leads to low concentrations of tar, CH₄, H₂ and CO in high porosity beds.
- High porosity promotes char formation and consumption rates of the bed. The overall effect is a reduced amount of char in this bed.
- The operational range with respect to porosity was decreased in an oxy-fuel burning condition due to higher quenching effects of CO₂.

In this study, particle packing density was analyzed by considering initial arrangement of particles in the bed. In practice, the packing density and porosity changes as combustion proceeds due to bed shrinkage. Channeling in the bed could also arise as combustion takes place. These were not considered in this work. Hence, there is need to consider them in a future study.

CRediT authorship contribution statement

J.K. Tanui: Conceptualization, Methodology, Investigation, Writing - original draft. P.N. Kioni: Conceptualization, Methodology, Supervision. T. Mirre: Investigation, Software, Validation. M. Nowitzki: Software, Validation. N.W. Karuri: Supervision, Writing - review & editing.

Acknowledgement

This work was financially supported by both Dedan Kimathi University of Technology, Kenya and Technische Hochschule Wildau, Germany. The first author would like to thank the German Academic Exchange Service (DAAD), Germany, ID NO: 57314019 for the financial support for his stay in Technische Hochschule Wildau, Germany where the experiments were conducted.

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- D*: Diffusivity [$\text{m}^2 \text{s}^{-1}$]
D_{eq}: Diameter of the particle which is equal to that of volume-equivalent sphere [m]
E: Activation energy [J mol⁻¹]
g: Gravity [m s^{-2}]
G: Incident radiative heat flux [W m^{-2}]
h: Enthalpy [J kg⁻¹]
h_c: Convective heat transfer coefficient [$\text{W m}^{-2} \text{K}^{-1}$]
H_f: Enthalpy of formation of species *i* [J kg⁻¹]
J: Diffusion mass flux [$\text{kg m}^{-2} \text{s}^{-1}$]
K: Rate constant [s^{-1} (mol m⁻³)]
n: Rosin-Rammler distribution parameter [–]
N_g: Number of gas species [–]
p: Pressure [Pa]
q_R: Radiative heat flux [W m^{-2}]
Q_{ap}: Particle absorption coefficient [–]
R: Universal gas constant [J mol⁻¹ K⁻¹]
R(d): Percentage of accumulated undersize mass in Rosin-Rammler distribution [%]
S_g: Specific surface area [m^{-1}]
S_E: Energy source term [$\text{J m}^{-3} \text{s}^{-1}$]
S_M: Momentum source term [$\text{kg m}^{-2} \text{s}^{-2}$]
t: Time [s]
T: Temperature [K]
v: Velocity [m s^{-1}]
V_p: Particle volume [m^3]
w_i: Rate of production of species *i* [$\text{kg m}^{-3} \text{s}^{-1}$]
Y: Mass fraction [–]
- Greek symbols*
- ε*: Turbulent dissipation rate [J kg⁻¹ s⁻¹]
θ: Particle porosity [–]
κ: Turbulent kinetic energy [J kg⁻¹ s⁻¹]
λ: Thermal conductivity [$\text{W m}^{-1} \text{K}^{-1}$]
μ: Viscosity [$\text{kg m}^{-1} \text{s}^{-1}$]
ρ: Density [kg m^{-3}]
σ: Stefan-Boltzmann constant [$\text{W m}^{-2} \text{K}^{-4}$]
τ: Shear stress tensor [Pa]
χ: Bed porosity [–]
Ψ: Sphericity [–]
Q: Stoichiometric coefficient [–]
- Subscripts*
- b*: Biomass
e: Effective
g: Gas
i: *i*th reaction
ig: Gaseous species
is: Solid-phase species
p: Particle
s: Solid
- Superscript*
- g_x*: Heterogeneous reaction
n: Exponent
- Operators*
- ∇: Gradient operator
 ∇: Divergence operator

Nomenclature

A: Arrhenius pre-exponent factor [s^{-1} (mol m⁻³)]
A_p: Particle surface area [m^2]
c_p: Specific heat [J kg⁻¹ K⁻¹]
C_i: Permeability [m^2]
C₂: Inertia loss coefficient [m^{-1}]
d: Particle diameter [m]
δ: Characteristic size [m]