Computational Fluid Dynamics (CFD) Modelling of Oxy-Fuel Combustion Technique for Power Plants

A Thesis Submitted for the Degree of Doctor of Philosophy

By

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Declaration of Originality

This thesis contains no material, which has been previously accepted for the award of any other degree or diploma at any university and to the best of my knowledge and belief contains no material previously published or written by another person or persons except where due reference is made.

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Audai Hussein Al-Abbas

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List of Publications

The following papers have been published or submitted in high impact factor journals and conferences in support of the works in this thesis:

**Peer-reviewed journals:**


**Peer-reviewed conferences:**

List of Publications


7- Al-Abbas, AH, Naser, J, Dodds, D, and Blicblau, A 2012 “Numerical modelling of oxy-fuel combustion in a full-scale tangentially-fired pulverized coal boiler”, Proceeding of the 5th BSME International Conference on Thermal Engineering in Bangladesh.
Nomenclature
Nomenclature

\[ A_\phi \] Coefficient matrix of the unknown variable
\[ A_v \] Pre-exponential factor \((s^{-1})\)
\[ r \] Fuel consumption rate \((kg/m^3 .sec.)\)
\[ X_i, X_j \] Directions of Cartesian coordinate system
\[ C_\mu \] Turbulent model constant
\[ S_\varphi \] Variable source
\[ \tau_R \] Turbulent time scale \((s^{-1})\)
\[ i_{n+1} \] Total radiation intensity \((W/m^2 \text{sr})\)
\[ x_i \] Gases composition
\[ \Delta h_{fu} \] Enthalpy of combustion \((kJ/kmol)\)
\[ C_{e1}, C_{e2}, C_{e3}, C_{e4} \] Coefficients in \(k - \varepsilon\) turbulent model
\[ a_1, a_2, a_3 \] Stoichiometric relations
\[ C_{fu}, C_{pr} \] Combustion model constants
\[ C_nH_m \] Hydrocarbon fuel
\[ C_D \] Drag coefficient
\[ C_p \] Specific heat capacity at constant pressure \((kJ/kg \cdot K)\)
\[ D_P \] Diameter of the particle (\(\mu\)m)
\[ E \] Energy \((kJ)\)
\[ E_v \] Activation energy constant \((J \text{kmol}^{-1} \cdot K^{-1})\)
\[ f_j \] Linear interpolation factor
## Nomenclature

- \( f \)  
  Mixture fraction

- \( g \)  
  Residual gas mass fraction (kg/kg)

- \( h \)  
  Specific enthalpy (kJ/kg)

- \( K \)  
  Turbulent kinetic energy (m\(^2\)/s\(^2\))

- \( N_u \)  
  Nusselt number

- \( M \)  
  Molecular weight of species (kg/kmol)

- \( m_j \)  
  Mass flow rate through the face \( j \)

- \( m_{vp} \)  
  Mass of coal particles when devolatilization process occurs

- \( \min \)  
  Minimum value of operator

- \( P \)  
  Pressure (N/m\(^2\)), central node

- \( P_j \)  
  Neighbouring node

- \( Pr \)  
  Prandtl number

- \( R \)  
  Universal gas constant (8.314 J/mol. K)

- \( Re \)  
  Reynolds number

- \( S \)  
  Stoichiometric air/fuel ratio, swirl number, source or sink term

- \( t \)  
  Time (s)

- \( T \)  
  Temperature (Kelvin)

- \( T^* \)  
  Mean temperature (Kelvin)

- \( U^* \)  
  Mean velocity (m/sec)

- \( U_i \)  
  Velocity in the \( i \)th direction

- \( u,v,w \)  
  Velocity components (m/sec.)

- \( Y \)  
  Mass fraction (kg/kg)
Nomenclature

Greek Characters:

\( \lambda \)  
Equivalence ratio, thermal conductivity

\( \Delta \)  
Increment

\( \phi \)  
Variables

\( \Gamma \)  
Diffusion coefficient of the variable

\( \alpha_\phi \)  
Under-relaxation factor

\( \varepsilon \)  
Turbulent dissipation rate \((\text{m}^2/\text{sec}^3)\), emissivity

\( \mu \)  
Dynamic viscosity \((\text{Pa.s})\)

\( \rho \)  
Density \((\text{kg/m}^3)\)

\( \mu_t \)  
Turbulent viscosity \((\text{m}^2/\text{sec})\)

\( \tau_{\text{res}} \)  
Resident time of species \((\text{sec})\)

\( \sigma_{pr}, \sigma_{sc} \)  
Prandtl number, Schmidt number

\( \delta_{ij} \)  
Unit tensor

\( \tau_{ij} \)  
Stress tensor \((\text{N/m}^2)\)

\( \sigma \)  
Stephan-Boltzmann constant \((5.67 \times 10^{-8} \text{ W/m}^2 \text{K}^4)\)

\( \omega \)  
Angular velocity \((\text{rad/sec})\)

\( \xi \)  
Mixture fraction

\( \xi \)  
Normalized enthalpy loss

Subscripts:

\( t \)  
Turbulent

\( \text{th} \)  
Theoretical
Nomenclature

b                                    Blackbody, backward  
dr                                   Drag force  
react                                Reaction  
**eff**                                Effective  
f                                    Forward  
fu                                    Hydrocarbon fuel  
fu,b & fu,u                    Burnt and unburnt fuel  
k                                    Species  
Ox                                 Oxidizer $O_2$  
Pr                                   Product  
rg                                   Residual gas  
tot                                  Total  
st                                    Stoichiometric characteristics  
p                                    Particle  
g                                    Gas  
r                                    Radiation  
rel                                  Relative  

Superscripts:

k                                    Iteration number  
-                                     Ensemble-averaged  
,                                     Fluctuating component  
.                                     Signifies rate of change
Nomenclature

Units

µm  Micrometer ($10^{-6}$m)
mm  Millimeter ($10^{-3}$m)
cm  Centimeter ($10^{-2}$m)
m   Meter (distance)
m/s Meter per second (velocity)
°    Degree (angle)
kg  Kilogram (mass)
s   Second (time)

List of abbreviations:

AFT    Adiabatic flame temperature
ASU    Air separation unit
CIA    Carbon in ash
CFD    Computational fluid dynamics
CETC   CANMET energy technology centre
CMC    Conditional moment closure
CCS    Carbon capture and storage
CDS    Central differencing scheme
CTF    Combustion test facility
GHG    Greenhouse gas
DCKM   Detailed chemical kinetic mechanism
DDM    Discrete Droplet Method
DO     Discrete ordinary
DT     Discrete transfer
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>DTG</td>
<td>Differential thermal gravimetric</td>
</tr>
<tr>
<td>DTRM</td>
<td>Discrete transfer radiation method</td>
</tr>
<tr>
<td>DTF</td>
<td>Drop-tube furnace</td>
</tr>
<tr>
<td>EBU</td>
<td>Eddy breakup combustion model</td>
</tr>
<tr>
<td>ESP</td>
<td>Electrostatic precipitator</td>
</tr>
<tr>
<td>EWBW</td>
<td>Exponential wide band model</td>
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<tr>
<td>ETIS</td>
<td>Energy technology innovation strategy</td>
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<tr>
<td>ERC</td>
<td>Environment research corporation</td>
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<tr>
<td>EOR</td>
<td>Enhance oil recovery</td>
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<tr>
<td>FDM</td>
<td>Finite difference method</td>
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<tr>
<td>FEM</td>
<td>Finite element method</td>
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<tr>
<td>FVM</td>
<td>Finite volume method</td>
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<tr>
<td>FGD</td>
<td>Flue gas desulphurization</td>
</tr>
<tr>
<td>FGC</td>
<td>Flue gas condensation</td>
</tr>
<tr>
<td>HGOT</td>
<td>Hot gases off take</td>
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<tr>
<td>HHV</td>
<td>High heating value</td>
</tr>
<tr>
<td>IGCC</td>
<td>Integrated gasification combined cycle</td>
</tr>
<tr>
<td>IFRF</td>
<td>International flame research foundation</td>
</tr>
<tr>
<td>IEA</td>
<td>International energy agency</td>
</tr>
<tr>
<td>JAMIC</td>
<td>Japan microgravity centre</td>
</tr>
<tr>
<td>MEA</td>
<td>Monoethanolamine</td>
</tr>
<tr>
<td>MOHESR</td>
<td>Ministry of higher education and scientific research</td>
</tr>
<tr>
<td>NBM</td>
<td>Narrow band model</td>
</tr>
<tr>
<td>NGCC</td>
<td>Natural gas combined cycle</td>
</tr>
<tr>
<td>PDEs</td>
<td>Partial differential equations</td>
</tr>
</tbody>
</table>
Nomenclature

PC                                 Pulverized coal
PDF                               Probability density function
PF                                  Pulverized fuel
RFG                              Recycled flue gas
RTE                           Radiation transfer equation
SIMPLE                        Semi-implicit method for pressure linked equation
SKIPPY                        Surface kinetics in porous particles
TG                                 Thermal gravimetric
UDFs                            User defined functions
UDS                              Upwind differencing scheme
VM                                Volatile matter
VCRF                            Vertical combustor research facility
WBM                            Wide Band Model
WSGGM                       Weighted sum of gray gases model
Abstract
Abstract

At present, fossil-fuel power plants supply the majority of the world’s demand of electric energy. The environmental and health threats from anthropogenic emissions of greenhouse gases (GHG) of these power plants have been considered as one of the main reasons for global climate change. In order to make the existing fossil fuel energy sources more environmentally friendly, a new generation of advanced power plant with increased output and environmental performance is required to be built. Oxy-fuel combustion technique can potentially provide significant opportunities for near-zero emissions from the existing and new-build power plants by capturing and storing the carbon dioxide emissions from burning fossil fuels and biomass. To obtain a better understanding of the overall oxy-fuel combustion process, it is important to investigate the effects of oxy-fuel-fired conditions on the combustion characteristics and heat transfer performance as innovations in the energy used.

As a first step in developing and validating a computational tool to numerically model combustion of gaseous fuel, a computational fluid dynamics (CFD) modelling study has been carried out involving propane combustion with associated chemical reactions, radiative heat transfer, and turbulence. Three different combustion environments that were adopted experimentally in a 100 kW drop tube firing unit, were examined. One air-fired (reference case) and two oxy-fuel-fired cases (21 vol.% O₂ for one combustion case (OF21) and 27 vol.% O₂ for the other combustion case (OF27)) were investigated. The irreversible single-step and reversible multi-step reaction mechanisms were considered. The results obtained with the multi-step chemistry mechanism showed improved agreement, particularly in the flame zone. The unburnt fuel in air-fired and OF27 cases was less than that of the OF21 case due to the low oxygen concentration used in the latter combustion case.

As a second step of this research program, a comprehensive CFD modelling study was undertaken by integrating the combustion of pulverized dry lignite in several combustion environments. Four different cases were investigated: an air-fired and three different oxy-fuel combustion environments (25 % vol. O₂ concentration (OF25), 27 % vol. O₂ concentration (OF27), and 29 % vol. O₂ concentration (OF29) were considered. The available experimental results from a lab-scale 100 kW firing lignite unit (Chalmers’ furnace) were selected for the
Abstract

validation of these simulations. The findings showed reasonable agreement with the qualitative and quantitative measurements of temperature distribution profiles and species concentration profiles at the most intense combustion locations inside the furnace. Through the use of Computational Fluid Dynamics (CFD), it is concluded that the resident time, stoichiometry, and recycled flue gas rates are relevant parameters to optimize the design of oxy-fuel furnaces.

Under the same oxy-fuel combustion conditions as above, the appropriate mathematical models with the related kinetics parameters were implemented. The purpose was to accurately calculate the temperature distributions, species concentrations ($O_2$, $CO_2$, $CO$, $H_2O$, and $H_2$), $NO_x$ emission concentrations, and the radiation heat transfer. In this step of the modelling investigation, the multi-step chemical reaction mechanisms were conducted on the gas-phase and solid-phase of the coal reaction in one-, two-, and three-step reaction schemes. The predicted results showed a reasonably good agreement against the measured data for all the combustion cases, but in the three-step scheme the results were highly improved, particularly in the flame envelope zone.

In the final step of the investigation, a computational fluid dynamics (CFD) modelling study has been developed to investigate Victorian brown coal combustion in a 550 MW utility boiler under air-fired and three oxy-fuel-fired scenarios. User-defined functions (UDFs) were written and incorporated into the CFD code in order to calculate the following mathematical models: the PC devolatilization, char burnout, multi-step chemical reactions, mass and heat transfer, carbon in fly-ash, and $NO_x$ formation/destruction. A level of confidence of the CFD model was achieved by validating four different parameters of the conventional combustion case. The numerical results of OF29 combustion condition were considerably similar to the reference firing results in terms of gas temperature levels and radiative heat transfer relative to the OF25 and OF27 combustion cases. In addition, a significant increase in the $CO_2$ concentrations and a noticeable decrease in the $NO_x$ formation were observed under all oxy-fuel combustion scenarios. This study of oxy-fuel combustion in a large-scale tangentially-fired boiler is important prior to its implementation in real-life.
Chapter 1. Introduction
1. Introduction

1.1 Primary research theme

This thesis reports on an investigation of oxy-fuel combustion characteristics and heat transfer performance for a 100 kW firing facility unit and a 550 MW tangentially-fired utility boiler. A computational fluid dynamics (CFD) model has been developed to provide a good understanding of the mechanism of oxy-fuel combustion techniques in both the physical and chemical fields. The numerical simulations of the combustion of propane, pulverized dry lignite, and brown coal (a low rank coal contains around 62% water) have been conducted in several combustion environments. The subroutines required for the pulverized coal (PC) devolatilization, char burnout, multi-step chemical reactions, mass and heat transfer, carbon in fly-ash, and nitric oxidizes formation/destruction have been written and incorporated into the CFD code, as user-defined functions (UDFs). The validation of the predicted results was comprehensively carried out against the physical data of the lab-scale (100 kW) furnace for both the air-fired (reference combustion case) and oxy-fuel-fired scenarios at the most intensive combustion locations of the furnace. The validation of the CFD results with the power plant (550 MW) data has been conducted in the air-fired combustion. Four parameters: flue gas composition, gas temperatures, carbon in fly-ash, and hot gases off take (HGOT) mass flow were compared.

1.2 Background

This report is the documentation of a doctoral research program undertaken at Swinburne University of Technology in Melbourne, Australia under the sponsorship of the Iraqi Ministry of Higher Education and Scientific Research (www.mohesr.gov.iq) for developments and innovations in a clean energy sector. This research is specific to the improved model of oxy-fuel combustion technique in a large-scale tangentially-fired boiler in an attempt to improve modelling capabilities. This is of a great importance to achieve a high combustion efficiency, consistent thermal performance, and inherently low emissions in the existing or new-build power plants in the foreseeable future.
In the state of Victoria in Australia, there exists one of the largest basins of brown coal in the world. Loy Yang power plant located in the Latrobe Valley, Victoria has been designed to use the brown coal; it is suppling approximately one third of the electricity demands of Victoria (Li 2004). Generally, in Australia, around 85% of electricity production is obtained from solid fuel (coal). This vast reserve of brown coal will lead to a continuation of the low-cost of electricity in the near future. It is, however, a competitive resource of energy amongst the other sources of fossil fuel and renewable energies. On the other hand, it is a major contribution to the greenhouse gases (GHG) emissions and global warming. Based on this disadvantage from brown coal utilisation, innovations and research on the brown coal combustion in a tangentially-fired furnace can play an important role to develop this economical energy source. In addition, with increasing concerns from the Kyoto Protocol against the global climate change, this research on the brown coal combustion can also make it meet a suitable sustainable progress for power generations (Li 2004).

In order to adopt the continuous use of coal, as a cheap and reliable energy source in the future, several advanced combustion technologies have been recently developed. Pre-combustion capture, post-combustion capture, and oxy-fuel combustion are being considered the most efficient utilisation technologies to reduce CO\textsubscript{2}, NO\textsubscript{x}, and SO\textsubscript{x} emissions and fuel consumption (Doukelis et al. 2009; Kanniche et al. 2009; Wall et al. 2009). However, oxy-fuel (O\textsubscript{2}/CO\textsubscript{2}) combustion technology has been widely considered the most viable approach amongst the above-mentioned technologies in the PC power plants. The fundamental concept of the O\textsubscript{2}/CO\textsubscript{2} technology is to use pure oxygen (approximately 95vol.% O\textsubscript{2}), produced in air separation units, instead of air (O\textsubscript{2}/N\textsubscript{2}) in conventional combustion, to burn fuel. Due to this high purity of O\textsubscript{2}, a very high combustion temperature is achieved in the combustion zone; no nitrogen is introduced in this combustion process. This elevated temperature can be diluted by recycling part of the flue gas (about 60%) to the combustion chamber in order to reduce the radiation heat transfer to the furnace wall (see Fig. 1-1). At the end of this combustion process, the concentration (partial pressure) of carbon dioxide in the exhaust gas is highly increased, and thereby the capturing process of CO\textsubscript{2} will be easier, and economically efficient, compared to that in the air-fired furnace. Nevertheless, NO\textsubscript{x} and SO\textsubscript{x} are
Chapter 1- Introduction

decreased, and a high char burnout is achieved in the exit flue gas (Hjärtstam et al. 2009; Kakaras et al. 2007; Zhou and Moyeda 2010).

![Figure 1-1: Principal outline of the oxy-fuel combustion technique (adopted from Vattenfall AB).](image)

Before switching to apply oxy-fuel combustion approach on the conventional large-scale firing boiler, lab-scale and/or pilot-scale furnaces have to be initially examined under several oxy-fuel combustion conditions. This strategy of testing is strongly recommended to investigate the combustion characteristics and boiler performance with this challenging approach. However, when the oxy-fuel combustion campaign was commenced in the last decade (2000-2010), much research work has been implemented in terms of experimental (Andersson et al. 2008; Qiao et al. 2010; Sheng and Li 2008; Zhang et al. 2010) and theoretical studies (Chui et al. 2004; Khare et al. 2008; Normann et al. 2008), using different furnace size.

The main aspects of the research were focusing on the species concentrations, flame temperature levels, char burn-out, NO\textsubscript{x} and SO\textsubscript{x} formation, and heat transfer on the furnace wall. The values of these variables, under oxy-fuel combustion conditions, are very connected to the amounts and concentrations of oxygen and carbon dioxide used in the recycled flue gas (RFG). The differences in the thermodynamic properties between the CO\textsubscript{2}, in oxy-fuel, and N\textsubscript{2}, in the conventional firing atmosphere, can definitely lead
to some changes on the combustion characteristics inside the furnace. These modifications should be minimized as much as possible in order to be close to the characteristics of conventional combustion, i.e. avoiding major changes to the boiler design.

From recent literature, there are many innovations on oxy-fuel combustion techniques, which have been implemented under several operating conditions and combustion environments to reduce the retrofits for the conventional combustion system. However, in the present simulation study of the large-scale furnace, the oxy-fuel combustion approach conducted experimentally in the Chalmers’ lab-scale furnace (Andersson 2007) has been chosen. This selection was strongly dependent on the preliminary CFD study (Al-Abbas et al. 2011). Whilst the existing (reference) combustion case has been based on the drawings and operation conditions of Loy Yang A power plant that provided by the Energy Technology Innovation Strategy (ETIS) program (Staples and Marshall 2010).

1.3 Research objectives

The objectives of this research program are to perform:

- A CFD modelling investigation of gaseous fuel (propane) combustion with associated chemical reactions, radiative heat transfer, gas compositions, and turbulent models in a 3-D hybrid unstructured grid CFD code. Three different combustion environments that were adopted experimentally in a 100 kW drop tube firing unit were examined: one air-fired and two oxy-fuel-fired cases, (21 vol. % O\textsubscript{2} for one combustion case (OF21) and 27 vol. % O\textsubscript{2} for the other combustion case (OF27)) were investigated.

- A comprehensive CFD modelling investigation of the combustion of pulverized dry lignite in several combustion environments. Four different cases were investigated: an air-fired and three different oxy-fuel combustion environments (25 vol.% O\textsubscript{2} concentration (OF25), 27 vol.% O\textsubscript{2} concentration (OF27), and 29 vol.% O\textsubscript{2} concentration (OF29) were considered. The chemical reactions (devolatilization and
char burnout), convective and radiative heat transfer, fluid and particle flow fields (homogenous and heterogenous processes), and turbulent models were employed in 3-D hybrid unstructured grid CFD simulations. The available experimental results from a lab-scale 100 kW firing lignite unit (Chalmers’ furnace) were selected for the validation of these simulations.

- A CFD modelling investigation of gaseous and solid phase chemistry mechanisms for lignite. Multi-steps chemical reaction mechanisms and nitric oxides (NO\(_x\)) formation/destruction mechanisms were performed in the same combustion scenarios on a lab-scale 100 kW firing lignite unit.

- A comprehensive CFD modelling investigation of the Victorian brown coal combustion in a 550 MW utility boiler under the air-fired (reference case) and three oxy-fuel-fired scenarios. The reference firing case was modelled based on the operating conditions of Loy Yang A power plant located in the state of Victoria/Australia, while Chalmers’ oxy-fuel combustion approach was selected for the oxy-fuel combustion simulations in terms of thermodynamic and aerodynamic properties.

The work programme covered by this thesis achieves the development and comprehensive validation of the computational tool applied to the above-mentioned combustion systems which indicate the practical relevance and the long term viability for such a tool.

1.4 Overview of the research program

In this section, an overview of the research program will be briefly discussed. This will be classified into four main objectives of this research program described in the previous section.

I- A three-dimensional CFD model was developed to model the air-fired and two different oxy-fuel combustion cases (OF21 and OF27) in a 100 kW unit firing propane. The temperature distribution levels, species concentrations (CO\(_2\), CO, and O\(_2\)), velocity
distributions, and propane consumption were investigated at the most intense combustion locations in the furnace. An efficient turbulent combustion model, Eddy Breakup (EBU), with the most appropriate empirical coefficients was used in this numerical study. Primary and secondary swirl registers of the burner were employed to enhance an internal recirculation mechanism of flames and to ensure a well-mixing condition for turbulent non-premixed gaseous reactants.

II- The 3 D numerical simulations of pulverized dry lignite in a 100 kW test facility were conducted to simulate four different combustion environments (air-fired, OF25, OF27, and OF29) and to investigate the temperature distribution levels, species concentrations, velocity, and particles consumption in the furnace. The commercial CFD software was used to model and analyze all the combustion media. Several mathematical models with the appropriate related constants and parameters were employed for lignite coal combustion. The combustion conditions of oxy-fuel combustion cases were satisfied by modifying the following factors: oxygen concentrations in the feed gas and carrier gas, and recycled flue gas rates. The scope of this research is limited to the experimental data available.

III- The commercial CFD code was used again to precisely predict and analyze four different combustion scenarios (air-fired, OF25, OF27, and OF29), simulating the experiments on a 100 kW Chalmers’ lab-scale furnace. The temperature distributions, species concentrations (O₂, CO₂, CO, H₂O, and H₂), NOₓ emission concentrations were investigated at different locations inside the furnace, as well as, the radiation heat transfer on the furnace wall. The multi-step chemical reaction mechanisms were carried out on the homogenous and heterogeneous reactions of the pulverized lignite particles in terms of single-, two-, and three-step reaction models. The simplified approach of the chemical kinetics has been modelled to calculate the Fuel and Thermal NO formation, decoupled from the main fluid flow computations.

IV- The commercial CFD code was modified to investigate the Victorian brown coal combustion in a 550 MW tangentially-fired boiler under different combustion media.
Several mathematical models such as coal devolatilization, char burnout, combustion chemistry, convection and radiation heat transfer processes, carbon in fly-ash, and thermal and fuel nitric oxides models were developed through subroutines and added to the CFD calculations. The available experimental data from the power plant were used to validate the predicted results under air-fired condition; a good agreement was achieved. The oxy-fuel combustion approach adopted in a 100 kW facility unit (Chalmers’ furnace) was applied to the present large-scale furnace in three O$_2$/CO$_2$ mixture conditions, namely OF25, OF27, and OF29. These models were implemented to investigate the importance of including such models in conjunction with the newly developed oxy-fuel combustion model.

1.5 Thesis structure

Chapter two will discuss the current developments and innovations of modelling of carbon dioxide capture technologies through different geometric configurations. Both experimental investigations and numerical studies will be discussed covering a range of the fundamentals, pollutant formations and operating conditions of oxy-fuel-fired furnaces, which best suit this research direction.

Chapter three will cover the numerical solution methods used throughout this research. The mathematical models of both gas and coal combustions are discussed, from which the appropriate coefficients and detailed kinetic chemical parameters used in this study are tested and presented based on the combustion conditions. The mechanisms of multi-step reaction and nitric oxides (NO$_x$) formation/destruction are discussed and presented.

Chapter four consists of the comprehensive CFD investigation of the gaseous fuel reaction processes in the lab-scale furnace. The four-step chemistry mechanism is modelled and presented to improve the predicted results in terms of temperature distribution levels and species concentrations.

Chapter five covers the comprehensive CFD modelling study that was undertaken by integrating the combustion of pulverized dry lignite in several combustion
Chapter 1- Introduction

environments. Extensive validations of the CFD results are carried out against the available measured data of the lab-scale furnace.

Chapter six presents the findings of the numerical results conducted under multi-step reaction mechanisms for the same combustion environments used in the pulverized lignite particles firing. Discussions are covered with importance and influence of model improvements on the accuracy of the predictions of the temperature distributions and the species concentrations, particularly in the flame zone. The NO\textsubscript{x} concentrations are presented and compared in term of Thermal and Fuel NO mechanisms in the furnace for all combustion cases examined.

Chapter seven discusses the comprehensive CFD investigation of the combustion of the brown coal in a 550 MW tangentially-fired boiler under different combustion media. Combustion characteristics and heat transfer performance are discussed and presented at different locations of the boiler. This chapter represents the main objective of achieving the current research program for oxy-fuel power plants. Discussions will be made on the importance of the thermodynamic and aerodynamic conditions utilised in oxy-fuel combustion models and influence of model improvements on the thermal performance and emission levels.

The conclusions for this research program will be summarised in chapter eight with recommendations for future work also discussed in regards to better modelling of oxy-fuel combustion.

1.6 Perceived specific contributions of the research

This research project contributed to an understanding how oxy-fuel combustion conditions affect the combustion characteristics and boiler performance in comparison with those of the air-blown case. A comprehensive CFD study provided a basis to develop a turbulent combustion model for both the gas and pulverized coal in different scales of furnaces. The relevant parameters such as resident time, stoichiometry, and
recycled flue gas rates were utilised. This will provide useful information to optimize the design of oxy-fuel furnaces and ultimately reduce the greenhouse gas emissions.

Experimental results of the Chalmers’ furnace (100 kW) for firing propane and dry pulverized lignite were selected for validating combustion models. The multiple chemistry mechanisms of the homogenous and heterogenous reactions of fuel were performed to improve the CFD results, as well as nitric oxides formation. The Victorian brown coal combustion in a 550 MW utility boiler under the air-fired and three oxy-fuel-fired scenarios were investigated and compared with the available power plant data. This CFD modelling study can highlight the importance of the included improved models and also provide knowledge to be used to better simulate full-scale tangentially-fired furnace with more accuracy, which reduces the need for costly physical modelling.
Chapter 2. Literature Review
2. Literature Review

Recently, the environmental and health threat from anthropogenic emissions of greenhouse gases (GHG) of power plants has been considered as one of the main reasons for global climate change (Wall et al. 2009). The undesirable increase in global temperature is very likely because of increase the concentrations of these syngas in the atmosphere. The most important resource of these anthropogenic GHG emissions in the atmosphere is carbon dioxide emissions. At present, fossil fuels provide approximately 85% of the world’s demand of electric energy (Davison 2007). Many modern technologies in the electricity generation sector have been developed as sources of new and renewable energies. These new technologies include solar energy, wind energy, geothermal energy, and hydro energy. While these sources of renewable energy are often seen as having zero greenhouse gas emissions, the use of such technologies can be problematic. Firstly, sources of renewable energy are often still under development. Therefore, there can be a higher cost involved in their installation and in other related technical requirements. Secondly, the sudden switching of these energy sources (zero emission) has caused serious problems with the infrastructure of energy supply and global economy (Buhre et al. 2005).

In order to reduce the problem and obey the new environmental and political legislation against global warming, it is necessary to find an appropriate solution to cut pollution which is with cost-effective, from the energy sources. The most effective technique, which can achieve a high level of reduction in GHG emission to atmospheric zone, is to capture carbon dioxide from the conventional power generations. Figure 2-1 shows the emissions of carbon dioxide from fossil fuels used in different sectors of commercial operations. As can be seen, electricity power generation represents the largest source of CO$_2$ emissions compared with other commercial industries. Therefore, the existing power plants have to be studied and investigated in order to achieve less emissions and high combustion efficiency. At present, several organizations, energy research centres, companies, and universities, particularly in developed countries, are working to develop these conventional power plants in order to make them more environmentally friendly, with near-zero emissions sources. Improvements in the combustion characteristics and
boiler performance of power plants could, in the foreseeable future, help to protect our planet against dangerous increases in atmospheric temperature.

Figure 2-1: Emissions of carbon dioxide from fossil fuel consumption (Davison 2007).

This chapter continues with a literature survey on different CO$_2$ capture technologies such as pre-combustion capture, post-combustion capture, and oxy-fuel combustion capture. The developments on oxy-fuel combustion technology with different scales of furnaces in terms of experimental investigations and theoretical modelling are discussed. The fundamentals and operating conditions of oxy-fuel-fired power plants are reviewed due to the importance of these conditions on the flame stability and coal combustion behaviour relative to those of conventional combustion. The effects of particular factors and parameters on the oxy-fuel combustion characteristics and boiler performance are reported. Finally, the chapter closes with different kinds of emissions and pollutant formations from oxy-fuel combustion systems.
Chapter 2- Literature Review

2.1 Different CO₂ Capture Technologies

In order to understand the technologies that are used for CO₂ capture in the conventional power plants, it is important to understand the systems of leading technology for these power plants. The most popular leading technology systems are as follow: Integrated Gasification Combined Cycle (IGCC), Natural Gas Combined Cycle (NGCC) and Pulverised Fuel (PF) combustion steam cycles (some references called Pulverised Coal (PC)). As previously mentioned, large amounts of CO₂ emissions and other gases such as nitrogen oxides (NOₓ) and sulphur oxides (SOₓ) are produced by energy production from fossil fuel. Several techniques to capture carbon dioxide are being increasingly developed in order to comply with the new environmental and political legislation against global warming (Buhre et al. 2005; Vitalis 2008). The three main techniques, which have been developed for CO₂ capture from these different systems of leading technology, are pre-combustion capture, post-combustion capture, and capture of oxy-fuel combustion. The last technique is studied in this work.

The first approach (pre-combustion capture) converts the fossil fuel after gasification of coal or reforming of gas with oxygen into a split stream of carbon monoxide (CO) and hydrogen (H₂). A shift-conversion (water-gas shift) reaction process can be subsequently applied to convert CO and H₂O to CO₂ and H₂, and finally a physical sorbent is utilized to capture CO₂. The second approach (post-combustion capture) captures carbon dioxide from the flue gases, immediately as the fuel is completely burned with air (O₂/N₂), by using a chemical solvent such as amine or ammonia for scrubbing CO₂ out of the combustion flue gases (Plasynski et al. 2009). The third approach (oxy-fuel combustion) burns fossil fuels with a mixture of pure oxygen (around 99.5vol % O₂), which is produced in a cryogenic air separation unit (ASU), and with recycled flue gas (RFG) or CO₂ to produce a high concentration of CO₂ in the flue gas. The purpose of this process is to separate the CO₂ from the flue gas, and compression processes make it easier and more economical. The next subsections explain these three techniques in detail.
2.1.1 Pre-Combustion Capture

The pre-combustion capture technique excludes CO$_2$ from the fuel before the burning process in the combustion chamber. This technique can be achieved by installing special equipment which captures CO$_2$ between the gasifier and the combined cycle power plant. After gasification of coal or the reforming of natural gas with oxygen, the first step of this process leads to the production of a split stream of carbon monoxide (CO) and combustible gases (mainly hydrogen (H$_2$)). The second step is to convert CO to CO$_2$ with steam (synthetic gas with suitable amounts of water vapour) by a process called shift-conversion ($CO + H_2O \xrightarrow{yields} H_2 + CO_2$). After that, CO$_2$ can be separated by using a physical solvent, and finally the CO$_2$ becomes efficiently available for a sequestration process after it passes through a compression unit. The other remaining parts (mainly hydrogen (H$_2$)) will be sent to the combined cycle power plant to be used as input fuel for power production (Amelio et al. 2007). As shown in Figure 2-2, the clean syngas is supplied to a combined cycle power plant after several treatment processes such as gas cooling (for protecting equipment), particulate removal, and hydrogen sulphide (H$_2$S) removal. Although this method of CO$_2$ capture can be considered a good producer of hydrogen for the combined cycle power plant, it has a relatively high level of complexity compared with other CO$_2$ capture techniques (Ratafia-Brown J et al. 2002).

![Figure 2-2: Power plant with pre-combustion capture technology.](image-url)
2.1.2 Post-Combustion Capture

The post-combustion capture technique involves capturing CO₂, as well as reducing particulate matter, SOₓ, and NOₓ in the combustion flue gases (see Figure 2-3). As mentioned above, this technique requires adding a separation unit after firing systems of the PC or NGCC. Any of the following three separating technologies can achieve the sequestration of CO₂: chemical absorption, low temperature distillation, and gas separation membranes (Kanniche et al. 2009).

![Figure 2-3: Power plant with Post-combustion capture technology](image)

In the first separating technology, the chemical absorption of chemicals such as monoethanolamine (MEA) is used in an absorption tower to scrub CO₂ from the combustion flue gases. A high temperature level is used to separate CO₂ from the chemical solvent after delivering it to the regenerating tower. After that, a compression process is performed to capture CO₂ as seen in Figure 2-3. Because of the relatively high temperature and low partial pressure (concentration) of the carbon dioxide to be treated in the flue gases, this method offers a big design challenge for conventional power generation. This means that the chemical absorption process can only provide an economic benefit if it is applied to work at a small scale. On the other hand, this process needs a large amount of energy due to the large size of the main sequestration components, and thereby the energy penalty will introduce a higher operating cost if it is applied for large-scale power plant with CO₂ capture (Romeo et al. 2008; van Loo et al. 2007).
The second separating technology for post-combustion capture uses gas separation membranes such as solution-diffusion or molecular sieving, which can be used to capture CO₂ by separating it from the flue gases. These membranes can experience some technical problems if applied to the capture of CO₂ in flue gases from coal power plants due to the degradation of the absorbent by impurities existing in the flue gas. However, this technology has not yet shown its ability to be applied at a large-scale CO₂ capture power plant, and it is still under development. Finally, the third separation technology, low temperature distillation, can be used to capture CO₂ from the flue gas, but this process requires special conditions (above 75 psi pressure, and -75 °F temperature) to achieve a high purity of CO₂ (about 90% CO₂) in the flue gas. Due to these complicated conditions involved in the separating processes in a power plant, low temperature distillation is not considered an efficient technology for the CO₂ capture from power plants.

2.1.3 Oxy-fuel Combustion Capture

The oxy-fuel combustion technique captures carbon dioxide from the flue gases of combustion. It is approximately similar to the post-combustion capture technique in terms of separating the CO₂ from the exhaust gases as a final process of sequestration, but it is less chemically complicated. As described earlier, the partial pressure of CO₂ in the flue gas is low in conventional combustion (air-fired combustion), and it needs special treatments for the separation processes. The basic principle of oxy-fuel combustion is to increase the partial pressure of CO₂ in the flue gases in order to make its sequestration and compression process easier and more cost-effective. This technique can be performed by using a mixture of pure oxygen with part of a recycled flue gas (RFG) (mainly CO₂) instead of air in the combustion chamber. In this case of combustion, a high concentration of CO₂ (high partial pressure) can be achieved in the flue gas stream, and therefore the high cost of its capturing processes can be avoided unlike the post-combustion process. The oxy-fuel combustion technique is schematically shown in Figure 2-4. In Figure 2-4, the oxy-fuel technique shows that the first removal equipments extract particulates and sulphur dioxide, respectively. The
particulate removal can remove the fly ash from the flue gas, while the bottom ash is removed after accumulating at the bottom of the furnace, i.e. at the hopper zone.

After removing particulates and condensing water vapour from the flue gases, the concentration of CO$_2$ will be increased to around 75% vol. under wet basis or to around 95% vol. under dry basis so that it can be transported for permanent storage. The purity of CO$_2$ concentration is completely dependent on factors such as the purity of the oxygen feed (from ASU), air-leakage, and the excess of the oxygen/fuel (stoichiometry) ratio. As shown in Figure 2-4, a part of flue gas (around 60-70%) is recycled and mixed with pure oxygen. This process is used to prevent high temperature levels inside the furnace, i.e. to protect the furnace wall. Due to this recirculating of flue gases, the size of the furnace and the sizes of other gaseous removal equipment can be significantly reduced. The recycled gas process of oxy-fuel combustion technique can maintain the same flow field conditions of the burners in the conventional combustion case.

The air separation unit (oxygen production unit) produces two gas streams. The first is an oxygen stream, which supplies the furnace, and the second includes nitrogen and other minor constituent inert gases that are vented to the atmosphere. In the air separation unit (ASU), a large amount of energy is used to separate nitrogen and produce a pure stream of oxygen. Despite the high cost of this process, oxy-fuel combustion is definitely a competitive technique compared with the other CO$_2$ capture technologies due to the high reduction in NO$_x$ and SO$_x$ emissions besides its high CO$_2$
Chapter 2- Literature Review

capture. However, using pure oxygen and recycled flue gas (RFG) instead of air to burn pulverized coal (PC) in the combustion chamber leads to problems such as many changes in flame temperature levels, species concentrations, and radiation heat transfer problems inside the furnace. These modifications of the combustion characteristics are due to the following reasons: the high specific heat capacity of CO$_2$ with respect to nitrogen in conventional combustion, radiative properties of gas mixtures, low oxygen molecular diffusivity in CO$_2$ compared to N$_2$ and other transport properties of the gas mixture such as viscosity, thermal diffusivity, gas phase chemistry etc. (Al-Abbas et al. 2011; Buhre et al. 2005; Nikolopoulos et al. 2011; Wall et al. 2009). However, oxy-fuel combustion is a recent technique, and it needs further investigation and development in a number of combustion processes.

2.1.4 Comparison amongst Different Capture Technologies

In short, all these three CO$_2$ capture technologies have different outcomes, particularly with regards to reduction of power plant efficiency and in increasing the cost of electricity production. In general, to be successful post-combustion capture requires new developments in the process of chemical absorption of CO$_2$ in order to adequately reduce energy consumption in the absorption process, but this is very expensive. In contrast, pre-combustion capture is achieved by the conversion of fuel into carbon monoxide (CO) and hydrogen fuel (H$_2$) in which CO is converted to CO$_2$ by the shift-conversion process. This CO$_2$ capture approach can be developed by either physical or chemical absorption processes to avoid any extra complex in chemical design of power generation. However, both of these processes are very expensive and chemically complicated. Finally, capture of CO$_2$ by the oxy-fuel combustion technique is less expensive than the other two processes and less complex. It can be carried out by burning the fossil fuel with a mixture of pure oxygen (99.5 vol. %), produced in ASU, and recycled flue gas (RFG). The products of this combustion will be only CO$_2$ and H$_2$O in the flue gas. After the condensation process, CO$_2$ concentrations will be increased to a level more suitable for the separating and compression processes. Although energy consumption for O$_2$ production, in an air separation unit, is relatively high (about 10% of the net energy of power plant), new technologies for air separation
processes and O\textsubscript{2} production are under development in order to reduce the energy penalty for CO\textsubscript{2} capture power plants (Andersson and Johnsson 2006).

Recently, Kanniche et al. (2009) comprehensively made a comparison between the leading technology systems for the IGCC, NGCC, and PC power plants with the above-mentioned CO\textsubscript{2} capture technologies. The results showed that the efficiency of the PC power plant when it used post-combustion capture is lower than that of the IGCC power plant using pre-combustion capture. The NGCC and PC power plants obtained the highest efficiencies with post-combustion capture and with oxy-fuel combustion, respectively. Regarding the production costs, the lowest costs occurred when PC used oxy-fuel capture, but costs gradually increased for IGCC use of pre-combustion capture and NGCC use of post-combustion capture. The highest cost per tonne of CO\textsubscript{2} removal was for NGCC using pre-combustion capture, whereas the costs for PC using oxy-fuel combustion capture and PC using post-combustion capture were approximately at the same cost levels. Based on these results, Kanniche et al. recommended taking the following considerations into account during designing near-zero emissions power plants: pre-combustion capture in IGCC, post-combustion in NGCC, and oxy-fuel combustion in PC.

In addition, oxy-fuel combustion is a considerably competitive technique compared to other CO\textsubscript{2} capture technologies. Therefore, a large number of experimental and theoretical studies are being carried out in this area worldwide, particularly in developed countries using different scales of furnaces. Generally, these studies depend on solid fuel (coal) because it is a major source of energy in some of these countries. In order to identify any difficulties in using a large-scale boiler during switching from air-fired (conventional) combustion to oxy-fuel combustion, several studies using different scales of furnaces should be widely undertaken. These studies on oxy-fuel-fired scenarios will provide relevant information to maintain the similar combustion characteristics of PC without capture. Thereby, the most cost-effective basis can be achieved for retrofitting existing power plants or to build a new power plant unit under oxy-fuel combustion conditions. However, recent studies have concluded that the oxy-fuel combustion technology is technically feasible and can be applied in a large-scale pulverized coal-
fired power plant, and it certainly represents a competitive method relative to the other CO\textsubscript{2} capture technologies. As a result, investigations, developments, innovations and research in this technique are necessary to provide high level confidence and operational experience at a laboratory-scale and pilot-scale and then gradually at a large power plant scale. This technology could be used by long term electricity generation sectors in order to avoid higher levels of emissions. Finally, improvements to this challenging technique can highly reduce thermal efficiency loss, and make it more economically acceptable with appropriate safety and operating conditions.

2.2 Oxy-fuel Combustion Technology Developments

In order to reduce GHG emissions to the atmosphere, systematic research and development work on the existing electricity power plants for CO\textsubscript{2} capture are required. Research into CO\textsubscript{2} capture started two decades ago with both experimental investigations and numerical simulation methods. Lab-scale furnaces were initially used in order for researchers to identify and characterise the fundamentals and operations of oxy-fuel combustion issues under different operating conditions. The fundamental aspects of concern included, for example, flame stability (Andersson et al. 2008b; Moore and Kuo 2008), ignition behaviours (Hjärtstam et al. 2009; Zhang et al. 2010a), species concentrations (Croiset and Thambimuthu 2001), and fuel combustion rate (Liu et al. 2005). The heat transfer characteristics under different oxy-fuel-fired scenarios have been studied (Krishnamoorthy et al. 2009; Yin et al. 2011) in order to reduce the retrofits needed to convert conventional boiler designs to oxy-combustion processes. Globally, there have been some studies on pilot-scale oxy-fuel combustion facilities in Europe and some developed countries (Chui et al. 2003; Murphy and Shaddix 2006; Tan et al. 2002). These investigations revealed that power plants can simply switch from air-fired combustion to the oxy-firing at a large scale and produce higher concentrations of CO\textsubscript{2} in the flue gas. In addition, a significant reduction in NO\textsubscript{x} emissions can be achieved due to eliminating N\textsubscript{2} from the oxy-fuel combustion processes (Cao et al. 2010). These confirmations and support for oxy-fuel combustion technique for CO\textsubscript{2} capture show that there are no main crucial barriers in implementing this clean, efficient, and economic technology in industrial large-scale facilities.
However, switching to oxy-combustion is completely dependent on public support and government developing policies to address global climate change.

### 2.2.1 Experimental and theoretical laboratory-scale projects

With increasing concerns from the Kyoto Protocol about the CO$_2$ emissions and global warming, research into oxy-fuel combustion technology has widely increased. To overcome the difficulties in applying the oxy-fuel combustion and make it more appropriate and acceptable in the applicable fields, several experimental studies have been conducted with different combustor sizes such as lab-scale and pilot-scale furnaces as the basis for building a large-scale oxy-fuel furnace. Some of these investigations were not only conducted through experiments, but also through numerical modelling. The latter is comprehensively carried out in this project for different utility furnaces and for several fuel types. In the literature on oxy-fuel combustion, studies on lab-scale furnaces have mainly focused on some important points: ignition behaviour, chemical species characteristics, char combustion, flame propagation speed, NO$_x$ reduction and SO$_x$ formation, and heat transfer models were investigated.

Liu et al. (2005) used a 20 kW down-fired coal combustor (190 mm inner diameter and 3 m height) to test the UK bituminous coal combustion in air and in the mixture of O$_2$/CO$_2$. The authors showed that the char burnouts and gas temperatures obviously decreased in coal-O$_2$/CO$_2$ combustion due to the high specific heat capacity of carbon dioxide compared to nitrogen. They recommended that the concentration of oxygen in O$_2$/CO$_2$ mixture should be increased to 30% and 70% for CO$_2$ (or recycled flue gas) to achieve a corresponding temperature similar to the coal-air combustion.

The flame propagation behaviour of pulverized coal clouds in O$_2$/CO$_2$ combustion have been studied by Suda et al. (2007). The authors performed experimental investigations in a 200mm diameter spherical chamber under micro-gravity. Three different kinds of pulverized coal particles were used to investigate the effect of carbon dioxide on flame propagation behaviour. Their results showed that in an O$_2$/CO$_2$ mixture gas, the speed of
flame propagation reduced from about 1/3 to 1/5 compared to an \( \text{O}_2/\text{N}_2 \) (reference) mixture gas. Furthermore, they found flame stability can be improved in \( \text{O}_2/\text{CO}_2 \) combustion by decreasing the size of pulverized coal particles in order to allow a high amount of volatility to be released from the surfaces of these fine particles.

The influence of reactions, including the effects of char structure and heat transfer, on the ignition behaviour of low-rank Victorian brown coal and high-rank Chinese bituminous coal in air-fired and oxy-fuel combustion cases was experimentally investigated in a wire-mesh reactor by Qiao et al. (2010). As the gas mixture was set at 21% \( \text{O}_2 \) and 79% \( \text{CO}_2 \), a slight increase in the average ignition temperature was noted for both the coal types. In contrast, a noticeable decrease in the particle ignition temperature was observed with increasing \( \text{O}_2 \) concentrations for brown coal and bituminous coal during oxy-fuel-fired scenario. Qiao et al. concluded that the reason for that ignition behaviour was the thermal physical properties of the gases surrounding the particles (Qiao et al. 2010). As a continuation of the Victorian brown coal investigation into \( \text{O}_2/\text{N}_2 \) and \( \text{O}_2/\text{CO}_2 \) mixtures, Zhang and co-researchers (2010a) and (2010b) used a lab-scale drop-tube furnace (DTF). The measurements were conducted using a high-speed camera (MotionPro Y-3) and two-colour pyrometers, the first for photographic observation, and the second for particle temperature measurements. The authors concluded that the coal pyrolysis, coal combustion (volatiles ignition and char oxidation rate), and the surface temperature were highly influenced by the bulk gases in the \( \text{O}_2/\text{CO}_2 \) mixture. There was a clear delay in the coal ignition in the oxy-fuel combustion environment compared to that in the coal-air combustion. This was because a thick volatile cloud released remained attached to the char surface for a long time in the \( \text{O}_2/\text{CO}_2 \) mixture and led, as a result, to the high oxygen consumption on the char surface. Zhang et al. recommended increasing the \( \text{O}_2 \) concentration in the \( \text{O}_2/\text{CO}_2 \) mixture to 27% and 73% for \( \text{CO}_2 \). This increase leads to achieving good stability in the volatile flame, and obtaining a corresponding char particle temperature to that of the air-fired case.
Regarding the gaseous fuel combustion, Kim and co-workers (2006) and (2007) experimentally examined the flame structure, combustion characteristics, and NO\textsubscript{x} formation in a 0.03 MW oxy-fuel combustor for a wide range of oxidant streams and fuel (methane) flow rates. The aims of their investigations were to obtain a good understanding of the effects of the inlet flow velocities of fuel and oxidizers, with and without quarls, on the above-mentioned combustion and emission characteristics under oxy-methane combustion. Their results found that the length of the flame, in the oxy-fuel combustion, decreases when the input flow fields of fuel and oxygen are increased because of the higher turbulent mixing and entrainment. In the laminar flow region, the flame size depended strongly on the mass flow rate of feed oxidizer gases, and was independent of the diameter of the nozzle. On the other hand, in the turbulent flow region, the flame size was highly dependent on the nozzle diameter, and it was nearly independent on the fuel flow rates. As the quarl was not fitted, the level of NO\textsubscript{x} emissions also decreased with increasing inlet flow fields of oxidizers due to the decrease of the combustion residence time, resulting in a reduction in the temperature level at the flame zone, and vice versa when the quarl was fitted. Therefore, they suggested installing a quarl in the oxy-fuel burner in order to improve the combustion conditions and to eliminate emissions.

An experimental study on the combustion instabilities of oxy-methane flame was presented by Ditaranto and Hals (2006). They noted that the heat release and pressure fluctuations have a significant effect on the flame instability patterns by changing the values of Reynolds number (R\textsubscript{e}). Furthermore, they found O\textsubscript{2} enrichment levels should be minimized to 30% in the feed oxidizer gases in order to stabilize the flame, resulting in a decrease in the pressure oscillations. In the same context, Moore et al. (2005) performed an experimental investigation to examine the effect of the initial temperature of gaseous reactants on the stability of a non-premixed CH\textsubscript{4}/O\textsubscript{2} flame at a constant oxygen-to-fuel (stoichiometry) ratio of 1.3. Their measurements revealed that the ignition time and R\textsubscript{e} decreased with an increase in the initial gas temperature, and therefore led to accelerating the transient time from a stable flame regime to an unstable flame regime.
Computational fluid dynamics (CFD) modelling studies can comprehensively provide a wide range of information for the design of furnace and burner that can reduce the cost of time-consuming experimental investigations. The CFD has the ability to predict well the flame structure, gas temperatures distributions, chemical species concentrations, radiative heat transfer etc., under different combustion conditions. One of the CFD benefits is that the multiple chemistry mechanisms discovered can be used in simulations of the fuel reaction, which are often conducted on the assumption of a chemical balance, finite-rate chemistry scheme, or an approach of mixed-is-burned model (Breussin et al. 2000; Brink et al. 1999).

Recently, Venuturumilli and Chen (2009) performed a CFD analysis between the four-step reduced mechanism and its starting mechanism on axisymmetric laminar diffusion (non-premixed) methane flames. The reduced mechanism included 8 major species ($\text{CH}_4$, $\text{H}$, $\text{H}_2$, $\text{H}_2\text{O}$, $\text{CO}$, $\text{CO}_2$, $\text{O}_2$, and $\text{N}_2$), while the starting mechanism had 18 species and 65 elementary reactions. The comparison between these two different chemical mechanisms showed that the temperature distributions and axial velocity profiles were similar at the flame base location, whereas the four-step reaction mechanism was not able to provide precise information about the ignition characteristics of the methane flame. Furthermore, the authors estimated the computational time required for the starting mechanism was around 3-4 times as long as for the four-step reaction mechanism.

Andersen et al. (2009) modified two global multi-step reaction schemes that were based on the detailed chemical kinetic mechanism (DCKM): the two-step mechanism by Westbrook and Dryer (WD) (Westbrook and Dryer 1981) and the four-step mechanism by Jones and Lindstedt (JL) (Jones and Lindstedt 1988). Their CFD investigations were to test and refine the chemical species concentrations and temperature distributions of hydrocarbon fuel under air-fired and oxy-fuel combustion conditions. The modified WD scheme showed better improvements on the predicted CO concentrations, while a slight
improvement was achieved on the CO profiles with the modified JL scheme compared to the original mechanism.

Due to the importance of the role of combustion chemistry and radiation heat transfer models in the oxy-fuel-fired calculations, Yin and co-researchers (2011) performed a CFD modelling study in a lab-scale 0.8 MW oxy-natural gas (NG) flame furnace. For the air-NG and oxy-NG combustion environments, the two detailed chemistry models, the two-step reaction for WD, and the four-step reaction for JL, were also modified. This development of the DCKM was carried out in order to better predict the intermediate species that are formed in the flame zone due to the thermal dissociation mechanism, especially in oxy-fuel combustion. The improvements observed in the simulation results were similar to those found by Andersen et al. in terms of intermediate chemical species such as CO and H₂. In the original two-step WD reaction, the flame temperature was over-predicted compared to the oxy-fuel experiments, and under prediction of the CO level was largely observed. A good agreement in the CFD results was achieved between the modified WD two-step and JL four-step reaction mechanisms under oxy-fuel combustion. Regarding the gaseous radiative properties, the authors also modified the weighted sum of gray gases model (WSGGM) proposed firstly by Smith et al. (1982). Insignificant differences in the predicted results were found between the original and modified WSGGMs in the lab-scale oxy-fuel furnace.

In addition to the above experimental investigations and numerical modelling, the literature includes a number of relevant findings (Bejarano and Levendis 2008; Li et al. 2009; Sturgeon et al. 2009; Toporov et al. 2008) from small lab-scale oxy-fuel furnace experiments. These lab-scale studies under oxy-fuel combustion conditions are useful, and can provide some technical insights and fundamental engineering techniques for this challenging technology. The uncertainties about the heat transfer characteristics, flame behaviour, corrosion problems and pollutant control units in lab-scale furnaces lead to the need for research on the application of this technology with pilot-scale furnaces prior to industrial full-scale boiler development.
2.2.2 Experimental and theoretical pilot-scale projects

A better understanding of the effects of oxy-fuel combustion with recycled flue gas (RFG) on the combustion characteristics and boiler thermal performance can definitely increase the potential for CO₂ capture. This also can provide key parameters for the necessary modifications to the conventional boiler, such as the flue gas recycle system and an air separation unit. Therefore, pilot-scale studies are highly required for this purpose. Below is a brief description of the different experimental investigations and numerical simulation methods of oxy-fuel combustion under pilot-scale plants reported in the literature.

One of the first studies into the combustion of pulverized coal (PC) with waste carbon dioxide and oxygen in the pilot-scale facility was conducted by the Environment Research Corporation (ERC) in a 3 MW unit (Wang et al. 1988). The objective of the study was to characterize and compare a one-dimensional computer code with actual measurements tested in the laboratories of Battelle Columbus, USA. The predicted results showed reasonably good agreements with the experimental data in terms of temperature distributions and species concentrations. The researchers noted that the complete combustion of PC under oxy-fuel conditions can be achieved over a range of CO₂/O₂, from 2.23 to 3.65 in the oxidant stream.

A detailed study carried out by the International Flame Research Foundation (IFRF) was performed to characterize the PC combustion in a mixture of oxygen and recycled flue gas (Woycenko DM 1995). In general, this project was part of three project areas funded by the European Commission to evaluate the technical and economic feasibility of CO₂ capture from the flue gas of PC power plants, and then to enhance oil recovery (EOR) in the storage site. The results showed that the combustion characteristics such as flame behaviour, heat transfer performance, and pollutant emissions of oxy-fuel combustion can be similar to those of the air-fired operation. A high CO₂ concentration (91.4 %) was achieved by use of the optimum ratio of RFG, which equals to 0.61. Furthermore, a low NOₓ burner configuration was tested to demonstrate its effect on the nitrogen oxide reduction under use of oxy-fuel combustion technology.
Numerical simulation and combustion tests were performed in a pilot-scale furnace at a 1.2 MW facility unit to investigate four different combustion cases of pulverized coal combustion with oxygen and recycled flue gas (Nozaki et al. 1997). The combustion facility unit had a tunnel (horizontal) furnace (1.3 m inner diameter and 7.5 m long), which was equipped with a swirl-stabilized burner used for injecting oxygen in the central position of the pulverized coal burner. The results showed that the direct injection of O\textsubscript{2} into the burner leads to improved flame stability compared to other O\textsubscript{2}/CO\textsubscript{2} combustion cases (without injecting extra oxygen). The dry recycled flue gas has a more significant effect on the increase of gas temperature than does wet recycled flue gas. The results of comparisons between the measurements and numerical simulation showed that there was under-prediction of the numerical results, especially for gas temperature along a furnace axis. The authors indicated this discrepancy was due to inaccurate evaluation of the radiation mathematical models of the gas components H\textsubscript{2}O and CO\textsubscript{2}.

CANMET Energy Technology Centre (CETC) (Chui et al. 2003; Chui et al. 2004) has used a 0.3 MW cylindrical, down-fired vertical combustor (0.61 m inner diameter and 8.3 m height) with two different burner configurations to evaluate burner and combustor design concepts in both experimental investigations and numerical modelling of oxy-coal combustion. The authors tested two modes of oxy-fuel combustion: O\textsubscript{2} enriched air (OEA) and recycled flue gas (RFG). The study was conducted both experimentally and numerically. Computational fluid dynamics (CFD) was used in the numerical study to model the coal combustion, heat transfer and pollutant characteristics. They examined the changes of the species concentrations and the temperature distributions inside the combustor by using Western Canadian sub-bituminous coal. Results showed that both OEA and RFG have the ability to increase the CO\textsubscript{2} concentration in flue gas, but the OEA mode leads to enhanced nitric oxide production. This was due to an increase in oxygen concentration levels along the furnace centreline that was coupled with the high flame temperatures. In addition, there were highly unsymmetric coal particle trajectories inside the furnace because of the impact of the burner configuration which led to the tendency of the flame to move towards one side of the combustor.
In the same organization of CANMET Vertical Combustor Research Facility (VCRF) in Canada, Tan et al. (2006) also investigated the combustion characteristics by using three different Canadian coals. Eastern bituminous (EB), Sub-bituminous (SB), and Lignite (LN) coals were tested. The authors noticed that in O$_2$/CO$_2$ combustion, there was a slight increase in the heat flux values inside the furnace with a 35 vol. % O$_2$ and 65 vol. % CO$_2$ in the gas mixture compared to the air-firing (reference) case. However, with 28 vol. % O$_2$ and 72 vol. % CO$_2$ the heat flux values were slightly lower than the reference combustion. In terms of emissions, for the oxy-SB coal combustion, the concentration of NO emissions increased twice times (1183 ppm) compared to the air-firing (707 ppm) because of the reduction in the volumetric flue gas. But, for the oxy-LN coal combustion, the NO concentration was lower than that of SB coal (i.e. 555 ppm for oxy-LN coal combustion, and 771 ppm for air-LN coal combustion). This improvement in the NO concentration in the latter combustion was due to the use of a different design of burners. Lower CO$_2$ concentration in the flue gas was noticed in the oxy-LN coal combustion (92 vol. % CO$_2$) compared to the oxy-EB coal (97 vol. % CO$_2$) and oxy-SB coal (98 vol. % CO$_2$) combustion cases due to poorly-sealed boiler system.

Vattenfall 30 MW Schwarze Pumpe Power Station (Anheden 2008) commenced a research project on the oxy-fuel combustion technology in 2001. This pilot-scale plant is part of a broader research and development (R&D) project for clean carbon energy conducted by the power station. The furnace used either PC black coal or pre-dried lignite as a feed fuel. A series of removal equipments was built to treat the combustion flue gas such as fly ash, NO$_x$, SO$_x$, and H$_2$O prior to the CO$_2$ sequestration and compression processes. The purpose of the research was to optimize and validate the fundamental operations of the pilot-scale oxy-fuel plant and would provide a basis for retrofitting the commercial large-scale 600 MW facility unit.

Kaß et al. (2009) investigated the combustion of dry lignite under oxy-fuel process conditions in a 0.5 MW test facility. The research program focused on the flue gas compositions (CO$_2$, O$_2$, H$_2$O, NO, SO$_2$, CO) in two different combustion atmospheres (air and oxy-fuel combustion cases). Under the oxy-fuel combustion conditions, reduction in SO$_2$ concentration in the flue gas, due to the use of desulphurization
additives (CaCO$_3$) in the combustion chamber, was found to reduce the corrosion problems in the boiler. In addition, the implementation of staged combustion (variation of the oxygen concentration) was found to be an effective method in reducing NO concentration in the furnace. For optimum operation conditions in the test facility, the experimental results showed that the optimal CO$_2$ concentration (about 92% vol. in the dry flue gas) with lower concentrations of NO and SO$_2$ can be achieved when an oxygen content in the primary air level is smaller than in the secondary air level of the combustion chamber.

Until recently, the technology of oxy-fuel combustion in pilot-scale units has been tested without including electricity generation. The major technical attentions of investigations were concentrated on evaluating the large-scale burner and estimating the carbon capture and storage (CCS) processes. A 30 MW test facility, the Babcock and Wilcox (B&W) USA project, was recently modified to work under oxy-fuel combustion operations. The project included all removal, cleaning and condensing equipments (McDonald and Zadiraka 2007). The large-scale oxy-fuel burner demonstration was conducted in both the OxyCoal-UK project, at 40 MW, and the Pear Power station-USA (Jupiter Oxygen) with a 22 MW four-burner oxy-fuel firing system (Zheng 2011).

Finally, in light of the above-mentioned investigation in regard to the pilot-scale oxy-fuel studies, it can be concluded that the oxy-fuel combustion technology can be implemented at commercial PC power plants with higher CO$_2$ concentrations and less NO$_x$ and SO$_x$ formation. In addition, no major technical barriers could affect the combustion performance and heat transfer characteristics of the boiler during the switching process.

### 2.2.3 Industrial large-scale demonstration developments

Developments in the lab-scale and pilot-scale oxy-fuel facilities as a result of experimental investigations and numerical simulation methods have led to new approaches being used in large-scale facility units. These developments have allowed, effectively, a good compromise between the expensive experimental tests and complete
simulation of commercial large-scale with CCS plants. Therefore, the knowledge and technical experience gained from these studies and investigations can be utilized directly to design industrial demonstration large-scale boilers (>250 MW) for the next few years. However, the pollutant control units are not completely understood in oxy-fuel combustion systems, and as a result more research work is required, particularly in the mercury removal units. A lot of information in regard to the international demonstration of oxy-fuel combustion can be found in the International Energy Agency (IEA) Greenhouse Gas Programme, which has been supported by the Asia partnership project. Recently, there have been a number of projects investigating PC oxy-fuel combustion demonstrations, some focussing on electricity production and other on CCS processes in industrial large-scale boilers such as Vattenfall, Endesa, FutureGen 2.0, and KOSEP/KEPRI, as summarized in Table 2-1 (IEA 2009). The implementation of these industrial-scale oxy-fuel combustion projects will greatly reduce the technology costs, especially in the ASU and CO\textsubscript{2} compression equipment, and make it more appropriate for commercial applications in 2022, as reported in the sequence project developments by Wall et al. (2009).

Up to date, in the field of numerical simulation on the commercial-scale facility unit, there has been unfortunately little research work conducted on oxy-fuel combustion conditions. Zhou and Moyeda (2010) conducted a process analysis and main calculations on an 820 MW facility to compare the furnace temperature profiles for the air-fired and the oxy-fuel combustion with both wet and dry recycled flue gas modes. The authors proposed several design criteria for both oxy-fuel combustion cases as follows: they would use the same total heat fuel, the same boiler exit O\textsubscript{2} and the same gas flow rate in order to reduce the retrofit impact on the conventional boiler performance. They showed that the flue gas recycle ratio depends on the stoichiometric (air-to-fuel) ratio and ash content in coal. Their results also indicated that the moisture content in O\textsubscript{2}/CO\textsubscript{2} combustion was 3.5 times higher than that of the conventional combustion. As a result, a clear reduction in the adiabatic flame temperature was noticed due to the increased moisture content, and therefore 75% of the recycled dry flue gas should be used to increase the flame temperature. The significant resulting
increase in the $H_2O$ and $CO_2$ concentrations in the flue gas of $O_2/CO_2$ combustion cases was accompanied by a clear decrease in $NO_x$ formation due to the reduction in the flame temperature and thermal NO production.

Table 2-1: Developments of oxy-fuel combustion demonstration projects in the worldwide (adopted from IEA 2009).

<table>
<thead>
<tr>
<th>Project</th>
<th>Location</th>
<th>MW$_{th}$</th>
<th>Start Up Year</th>
<th>Boiler Type</th>
<th>Main Fuel</th>
</tr>
</thead>
<tbody>
<tr>
<td>B &amp; W</td>
<td>USA</td>
<td>30</td>
<td>2007</td>
<td>Pilot PC</td>
<td>Bit, Sub B, Lig.</td>
</tr>
<tr>
<td>Jupiter</td>
<td>USA</td>
<td>20</td>
<td>2007</td>
<td>Industrial</td>
<td>NG, Coal</td>
</tr>
<tr>
<td>Oxy-coal UK</td>
<td>UK</td>
<td>40</td>
<td>2009</td>
<td>Pilot PC</td>
<td>Bituminous</td>
</tr>
<tr>
<td>Alstom</td>
<td>USA</td>
<td>15</td>
<td>2009</td>
<td>Pilot PC</td>
<td>Bit, Sub B, Lig.</td>
</tr>
<tr>
<td>Vattenfall</td>
<td>Germany</td>
<td>30</td>
<td>2008</td>
<td>Pilot PC</td>
<td>Lignite (Bit)</td>
</tr>
<tr>
<td>Total, lacq</td>
<td>France</td>
<td>30</td>
<td>2009</td>
<td>Industrial boiler</td>
<td>NG, Coal</td>
</tr>
<tr>
<td>Callide</td>
<td>Australia</td>
<td>90</td>
<td>2011</td>
<td>PC-with Electricity</td>
<td>Bituminous (Sub B)</td>
</tr>
<tr>
<td>CIUDEN-PC</td>
<td>Spain</td>
<td>20</td>
<td>2010</td>
<td>Pilot PC</td>
<td>Anthra, Bit, Lig.</td>
</tr>
<tr>
<td>CIUDEN-CFB</td>
<td>Spain</td>
<td>30</td>
<td>2011</td>
<td>Pilot CFB</td>
<td>Anthra, Bit, Lig.</td>
</tr>
<tr>
<td>ENEL HP Oxy</td>
<td>Italy</td>
<td>48</td>
<td>2012</td>
<td>Pilot-High pressure</td>
<td>Coal</td>
</tr>
<tr>
<td>Vattenfall</td>
<td>Germany</td>
<td>1000</td>
<td>2014</td>
<td>PC-with Electricity</td>
<td>Lignite (Bit)</td>
</tr>
<tr>
<td>Endesa</td>
<td>Spain</td>
<td>1000</td>
<td>2015</td>
<td>CFB-with Electricity</td>
<td>Anthra, Bit, Lig.</td>
</tr>
<tr>
<td>FutureGen 2.0</td>
<td>USA</td>
<td>600</td>
<td>2017</td>
<td>PC-with Electricity</td>
<td>Coal</td>
</tr>
<tr>
<td>KOSEP/KEPRI</td>
<td>Korea</td>
<td>400</td>
<td>2018</td>
<td>PC-with Electricity</td>
<td>Coal</td>
</tr>
</tbody>
</table>

More recently, Nikolopoulos et al. (2011) performed CFD simulations for a 330 MW facility consisting of a tangentially fired pulverized-lignite boiler located in Greece under three different combustion conditions: air-firing (reference), partial oxy-fuel, and full oxy-fuel scenarios. The partial oxy-fuel concept was adopted based on the work published by Doukelis et al. (2009), while the full oxy-fuel-fired concept for the lignite power plant was selected because it had been studied earlier at the same mentioned power plant (Kakaras et al. 2007). The Discrete Ordinates (DO) model, with the Exponential Wide Band Model (EWWB) which provides more accurate figures for the absorption coefficient of the gas mixture was used in a radiation model to obtain
accurate calculations in both air-firing and oxy-fuel combustion cases. Regarding the
coal combustion, the reaction of volatile matter was modelled by means of one-step and
two-step reaction mechanisms, while char combustion was modelled using a three-step
semi global intrinsic kinetic law mechanism. NO\textsubscript{x} formation mechanisms were
modelled in terms of thermal and fuel NO\textsubscript{x} mechanisms which were based on the source
terms of NO, NH\textsubscript{3}, and HCN in transport equations. The main comparison results for
the combustion scenarios showed that the high emissivity of the flue gas (H\textsubscript{2}O and
CO\textsubscript{2}), in the partial and full oxy-fuel combustion environments, resulted in an increase
in the radiation heat fluxes of the furnace wall, but it was still within the allowable
operating limits of the boiler materials. The wall heat fluxes were 326.9 MW, 374.4
MW, and 418.5 MW for air-fired, partial oxy-fuel, and full oxy-fuel combustion
scenarios respectively. The reduction of NO\textsubscript{x} emissions is evident in oxy-fuel
combustion cases in the decrease in fuel NO\textsubscript{x} production which is caused by the
destruction mechanisms. Evidence, NO\textsubscript{x} reduction is also found in the decrease of
thermal NO\textsubscript{x} formation.

2.3 Fundamentals and operations of oxy-fuel combustion power plants

In this section, some of the fundamental issues affecting the operations of oxy-fuel
power plant, e.g. coal ignition, flame stability, and char combustion are briefly
surveyed. For better understanding of these aspects of the combustion processes, the
survey includes both the experimental results and theoretical methods. Other important
issues that will be reviewed include the effects some parameters, such as oxygen
content, particle size, RFG ratios, and air leakages have on the combustion
characteristics. These parameters are considered to have a significant influence on the
performance and reliability of oxy-fuel power plants.

2.3.1 Coal ignition

Kiga et al. (1997) used a microgravity drop shaft facility of the Japan Microgravity
Centre (JAMIC) to investigate the ignition characteristics of the PC in a CO\textsubscript{2}-rich
environment. The investigations measured the flame propagation speed inside the
facility with conditions of a homogenous distribution of the PC which allowed an increase in the accuracy of measurements by avoiding the mixing that occurs in natural convection. It was found that there is poor ignition in an O$_2$/CO$_2$ environment, compared to in an O$_2$/N$_2$ environment, resulting in a decrease in the flame propagation speed in the oxy-fuel case. They pointed out that delay was due to the higher heat capacity created by increased amount of a CO$_2$ in the gas mixture. Yamamoto et al. (2004) reported the same reason for a decrease in a flame propagation velocity when investigating the effect of carbon dioxide on coal ignition. This important observation was also confirmed by the experimental studies of Molina and Shaddix (Molina and Shaddix 2007; Shaddix and Molina 2009). They determined the ignition point of particles by using charge-coupled device (CCD) camera images of the CH chemiluminescence. The authors concluded that the high heat capacity of CO$_2$ was not only the main reason for the ignition delay, but it was also due to the effect of O$_2$ concentrations on the reactivity of the local gas mixture. For that reason, they suggested increasing the O$_2$ concentration to 30% in an O$_2$/CO$_2$ mixture to obtain similar particle ignition as that in air-coal combustion. In another study, Arias et al. (2008) used an entrained flow reactor to study the ignition and burnout of coal in O$_2$/CO$_2$ mixtures and in air (as reference). An ignition delay was detected in the oxy-fuel combustion case at 21% O$_2$. At an O$_2$ concentration of 30% or higher, a clear improvement in the ignition was observed in O$_2$/CO$_2$ mixture, in comparison with air-firing.

Khare et al. (2008) used experimental studies and numerical modelling (by using CFD code, Fluent 6.2) of the IHI pilot-scale vertical furnace (1.2 MW) to investigate the mechanism of flame ignition in air-fired and oxy-fuel combustion cases. A low-swirl, Type-0, burner (without internal recirculation) was used for this investigation. For both the experiments and CFD studies conducted under oxy-fuel combustion conditions, the results showed a delay in the ignition timing and decrease in the flame propagation speed in comparison with coal-firing in an air environment. The differences in gas density, heat capacity, and thermal conductivity were the reasons for that delay in coal ignition between the two mentioned combustion cases, as well as the differences in the flow momentum ratio between the primary and secondary registers (Khare et al. 2008).
The authors suggested installing a high-swirl, Type-2, typical burner (with internal recirculation) for the oxy-fuel retrofits instead of Type-0.

To understand the impact of the specific heat capacity of the gas mixture on the coal ignition process, the following mathematical equations can be inferred from the above observations. Once the volatile matter has been released during the volatilization process, the auto ignition time of coal particles can be determined based on the assumptions of ignition and explosion theory (Law 2006). For a one-step overall reaction and no heat loss, the ignition delay of volatile gases is given as follows:

\[ \tau = \frac{c_v}{Q_c Y_{F,O} A \exp(-T_o/T_a)} \frac{T_o^2}{T_a} \]  

(2.1)

Where, \( c_v \) is a specific heat capacity at constant volume, \( Q_c \) is the combustion heat release per mass of fuel, \( Y_{F,O} \) is the mass fraction of fuel at initial time value \( t=0 \), \( T_o \) is the initial temperature of reactants, \( T_a \) is the ambient temperature and \( A \) is a kinetic factor in the Arrhenius expression.

According to Eq. 2.1, it is clear that the ignition delay time increases with an increase in the specific heat capacity \( (c_v) \) of gases and decreases in proportion to the combustion heat release \( (Q_c) \). Therefore, the high specific heat capacity can play an important role in increasing the ignition delay. As mentioned earlier, the specific heat capacities of the gaseous combustion products such as CO\(_2\) and H\(_2\)O are higher than that of N\(_2\). As reported in many oxy-fuel experimental investigations (Arias et al. 2008; Hjärtstam et al. 2009; Molina and Shaddix 2007), the ignition delay can be reduced by increasing the oxygen concentration in the gas mixture in order to enhance the chemical reaction rate, as explained in Eq. 2.1. As a result, a higher O\(_2\) concentration can be used to dilute the carbon dioxide effect on the ignition mechanism and to yield the same ignition time for oxy-fuel combustion as that of coal-firing in the air.

In addition, the chemical effects on the coal particles, due to the elevated concentrations of CO\(_2\) and H\(_2\)O in the flue gas of oxy-fuel combustion, have been considered an
another reason for the coal ignition delay. This chemical phenomenon was observed in two experimental studies, which were conducted in lab-scale drop-tube furnaces (DTF) in Australia (Rathnam et al. 2009; Zhang et al. 2010a). The authors used different types of Australian coals and a wide range of O$_2$ levels to investigate the coal pyrolysis behaviour, ignition extent, and char burnout in air-fired and oxy-fuel-fired environments. Zhang et al. (2010a) noted that when the nitrogen is replaced by carbon dioxide in the gas mixture, this enhances coal pyrolysis prior to ignition and as a result produces a large cloud of thick volatile matter on the char surface. Thereby, ignition of the volatile cloud occurred instead of single particle ignition. Approximately 30% of O$_2$ concentration in the O$_2$/CO$_2$ mixture was recommended to be used in order to achieve similar coal ignition like that in the O$_2$/N$_2$ mixture. Rathnam et al. showed that the apparent volatile yield measured in the DTF for O$_2$/CO$_2$ mixture at 1673 k was around 10%, as high as that in air-firing for all coal types.

### 2.3.2 Flame Behaviour

In general, the physical parameters of the flame, for instance shape, brightness, extinction, oscillation frequency, and temperature level, can be used to characterise the flame behaviour and control the stability of flame in the furnace to improve combustion efficiency. As a consequence, flame stability is an important issue and needs to be studied and taken into consideration when designing burners in order to improve flame characteristics and reduce emission levels. The replacement of air by CO$_2$ in the feed oxidizer gases has been found to have a significant effect on flame stability. However, to maintain a better flame stability in an oxy-fuel furnace, Chui et al. (2003) tested two different burners’ configurations (A and B) to compare which has optimal efficiency. Both experimental investigation and numerical modelling studies on a pilot-scale furnace were conducted. The main difference between the designs of the two burners was the location of the pure oxygen injection into the primary gas stream. For burner A, the annulus high-O$_2$ jet was located inside the primary stream, while in burner B, the annulus high-O$_2$ jet was located between the primary and secondary streams and without a cyclone chamber for coal delivery. The experimental and numerical results showed that burner A improved the flame stability and achieved a significant decrease
in the NO\textsubscript{x} level in the combustion flue gas in comparison with burner B, particularly when the swirl number was increased in the secondary stream. The improvement was due to the enhancement of the internal recirculation zone of reactants in the near-burner region.

The edge flame structure of the oxy-CH\textsubscript{4} combustion has been numerically studied by Choi et al. (2009) to identify the influence of pure oxygen and air on the premixed (non-diffusion) flame structure over a mixing layer. The species concentrations, momentum, and energy equations were solved using CHEMKIN-III and TRANSPORT packages. The multi-step reaction mechanism was applied in the calculations. The effect of pure O\textsubscript{2} and air on the structures of methane flames was taken into account by dividing the flame into three different regions: lean premixed-flame, rich premixed-flame, and non-premixed flame. In the fuel-rich region of the oxy-CH\textsubscript{4} flame, the partial oxidation was dominant and produced CO and H\textsubscript{2} rather than CO\textsubscript{2} and H\textsubscript{2}O as final reaction products relative to the same region in the air-CH\textsubscript{4} flame. In the fuel-lean region of air-CH\textsubscript{4} flame edge, the concentrations of CO and H\textsubscript{2} were also less than those of the oxy-CH\textsubscript{4} flame edge. In the non-premixed air-CH\textsubscript{4} flame region, CO was additionally oxidized to CO\textsubscript{2} in a broad reaction zone due to the OH radical that produced from the fuel-lean flame front. Generally, in the whole region of the oxy-CH\textsubscript{4} flame, the CO and H\textsubscript{2} productions were much stronger than in those of the air-CH\textsubscript{4} flame, and that adverse increases of intermediate species led, as a result, to decreasing the brightness of oxy-fuel flame (Choi et al. 2009).

Using state-of-the-art turbulence-chemistry interaction, several advanced turbulent combustion models have been developed such as Eddy-Breakup (EBU) model, Probability Density Function (PDF) transport model, and Conditional Moment Closure (CMC). Most of these mathematical combustion models have only been utilized for the calculations of air-fired flame. For that reason, Kim et al. (2009) adopted the CMC model to analyse the characteristics of turbulent combustion of natural gas (NG) flame in air-fired and oxy-fuel combustion environments. The authors coupled the CMC model with a flow solver. The detailed chemical kinetics mechanism model was implemented to calculate the intermediate species (CO and H\textsubscript{2}) formed in the flame.
envelope because of the enhanced thermal dissociation. The normalized enthalpy loss variable \( \xi \) used to calculate the effect of convective and radiative cooling terms on the turbulent flame, and it is defined as follows:

\[
\xi = h - h_{\text{min}}/h_{\text{ad}} - h_{\text{min}}
\]  

(2.2)

Where, \( h_{\text{ad}} \) is the conditional adiabatic enthalpy, and \( h_{\text{min}} \) is the conditional minimum that is calculated when the conditional temperatures are reduced to the surrounding temperature.

The numerical results showed that the oxy-fuel flame produced a much broader region in the hot-flame zone, particularly in the lean-fuel side of the mixture fraction, in comparison with the air-NG flame. They also noted that the temperature value of oxy-fuel flame is higher than that of air-firing. The predicted temperature levels for both combustion cases were overestimated compared to the experiments. That discrepancy arose because of the inadequacy of the modified \( k - \epsilon \) turbulence model used in the calculations and to the measurements uncertainties.

Suda et al. (2007) conducted experimental investigations (as mentioned in the previous section) and numerical studies to investigate the effect of \( \text{CO}_2 \) on the flame propagation speed of PC firing in different oxy-fuel combustion conditions. The simple one-dimensional numerical simulation was carried out separating the PC cloud into many \( N \) elements with constant length. The numerical Monte Carlo method was performed to provide accurate radiant calculations between the elements. Mie scattering and Gray-gas theories were used to calculate the scattering and absorption of radiation, respectively, which happened in the combustion zone due to the interaction between PC and carbon dioxide (Bohren and Huffman 1983). The temperatures of particle and gas in each element were calculated by energy equations, and their mathematical expressions are given as follow:

\[
C_{pc} \cdot \frac{n \cdot D_p^3 \cdot p_p}{6} \cdot N_p \cdot \frac{dt_p}{dt} = Q_{rp} - Q_f + \alpha \cdot Q_{reac}
\]  

(2.3)

\[
C_{pg} \cdot V_g \cdot \rho_g \cdot \frac{dt_g}{dt} = Q_{rg} + Q_f + (1 - \alpha) \cdot Q_{reac}
\]  

(2.4)
Where, $C_{pc}$ and $C_{pg}$ represent the specific heat capacities of particles and gas, respectively, $\rho_p$ and $\rho_g$ are densities of particle and gas, respectively, $D_p$ is the diameter of the particles, $V_g$ is the volume of gas in the element, $Q_{rp}$ and $Q_{rg}$ are the heat flux from the absorption of radiation by the particles and gas, respectively, and $Q_f$ and $Q_{reac}$ represent the heat flux by conduction between the particles and gas, and by the combustion of volatile matter released, respectively (Suda et al. 2007).

The combustion reaction rate ($Q_{reac}$) of the volatile matter was calculated by using a single reaction model of devolatilization, while the conductive heat transfer model ($Q_f$) was calculated assuming a constant value of the Nusselt number ($N_u=2.0$), and no heat flux by convection around the particles was considered.

The numerical results showed that the effect of absorption of radiation by CO$_2$ on ignition behaviour in oxy-fuel combustion case was relatively significant, but a small effect on flame propagation speed was noted. That was due to a slight chemical effect of CO$_2$ on the radiant heat transfer between coal particles. Compared to air-fired condition, the larger specific heat capacity of CO$_2$ led to a noticeable decrease in the flame propagation speed of O$_2$/CO$_2$ mixture, but the latter maintained the same distribution trends of the flame propagation velocity over a range of coal concentrations. Furthermore, the authors stated that the effect of the PC diameter on the propagation of the flame was important, since flame stability in the oxy-fuel combustion can be improved by decreasing the diameter of the coal particles.

The oscillation frequency of the oxy-fuel flame was measured by Smart et al. (2010) in a 0.5 MW combustion test facility (CTF) by using digital imaging systems. The CTF was a horizontal refractory lined unit with a 0.8 m square cross-section and 4.3 m in length. The effects of RFG ratios, total flows, and the oxygen levels of O$_2$/CO$_2$ mixtures on the flame stability were investigated for two different coal types. The experimental results illustrated that the higher RFG ratios used in oxy-fuel combustion led to a decrease the flame oscillation frequency, and therefore unstable flames were provided. From the investigating point of view, the authors noted that the oscillation
frequency of the oxy-fuel flame in the flame root region was less than in the flame middle region. In general, the oxy-fuel flame was lower in a flame propagation speed than in the air-fired case, indicating that a high RFG ratio has a negative impact on the flame behaviour. In order to increase the flame temperature and maintain the same stability in the oxy-fuel flame as that in air-firing, the oxygen and carbon dioxide concentrations have to be from 30 to 35 Vol. % and from 65 to 68 Vol. %, respectively in the gas mixture (Smart et al. 2010).

In order to mathematically demonstrate the chemical effect of CO\textsubscript{2} on the reduction of propagation flame speed, the extinction theory of diffusion and non-diffusion flames will be considered. The Damkohler number (D) is a dimensionless number, and can be used to interpret the extinction characteristics of flames, as follows (Williams 2000, 1981):

\[ D = \frac{\tau_r}{\tau_{ch}} \]  

(2.5)

Where \( \tau_r \) represents the residence timescale of reactants in the combustion zone, also known as the mixing timescale, and \( \tau_{ch} \) is the chemical reaction timescale and it is equal to a ratio of the characteristic thermal diffusivity of the gas divided by the square laminar burning speed (i.e. \( \tau_{ch} = \frac{\alpha}{S_{ch}^2} \)). The numerator of the D number is completely dependent on the fluid dynamics of the flame, but the denominator of D is a function of the flame reaction rate. Therefore, the mathematical expression of the Damkohler number can be rewritten using the Arrhenius kinetic rate formula, as follows:

\[ D \propto \frac{\tau_r}{\alpha} \exp\left(-\frac{E_A}{R T_f}\right) \]  

(2.6)

According to Eqs. 2.5 and 2.6, flame velocities in oxy-fuel combustion environments will observably be lower than those in air-fired environment at the same level of oxygen concentration. This is due to the lower values of thermal diffusivity and adiabatic flame temperature in O\textsubscript{2}/CO\textsubscript{2} mixtures compared to those in O\textsubscript{2}/N\textsubscript{2} mixture. As a result, the flame stability of the oxy-fuel combustion will definitely be affected by that reduction attained in propagation flame speed.
2.3.3 Char combustion

After the devolatilization process of the coal particles finishes, the char combustion subsequently starts in the firing system. This combustion process has been considered the dominant factor constraining several reaction parameters such as the total burnout time, unburned carbon level, and radiation from burning char particles. A better understanding of the effects of these parameters on the combustion characteristics and boiler heat transfer under oxy-fuel conditions enables engineers optimize the applications of both the existing and new coal power plants.

A comparison of the burning rate of coal char particles between the air-fired and oxy-fuel combustion environments was experimentally performed by Kaß et al. (2009). The authors used a thermo gravimetric analysis reactor to investigate the combustion behaviour of pre-dried lignite, and the gas composition effects on the burnout time and combustion rate were measured. The experimental results indicated that if an O\textsubscript{2}/CO\textsubscript{2} mixture is used rather than air in the feed oxidizer gases the burnout time of char is obviously less than that in an air filled chamber with the same oxygen content, especially for higher gas temperatures. The reason for that decrease of combustion time in an oxy-fuel atmosphere is due to the additional reaction of CO\textsubscript{2} with the carbon, as well as to coal combustion which is regarded as the main reactant in the gas mixture. Therefore, the heterogeneous reaction of carbon dioxide to the carbon has a significant influence on both the char content and the combustion rate of coal, particularly in O\textsubscript{2}/CO\textsubscript{2} atmospheres. This results in an increase in the CO production in the flue gas, as given in the Boudouard reaction, $CO\textsubscript{2}/C\textsubscript{char} \xrightarrow{\text{yields}} 2CO$, (Nagase et al. 1999).

In order to reduce the char burnout time and increase the combustion rate of char particles in O\textsubscript{2}/CO\textsubscript{2} mixtures, oxygen-enriched atmosphere must be used in the gas mixture (Murphy and Shaddix 2006). However, the literature shows that the combustion rate affects the reaction order of the bulk oxygen partial pressure. This means that the combustion rate when measured in terms of the chemical kinetic control reaches a high reaction order (0.6-1) for O\textsubscript{2} below 900K, but a low reaction order in the oxygen partial
pressure is exhibited when the global reaction rate is above 1200K (Hurt and Calo 2001). Based on these findings, the reaction rate of coal char particles has been interpreted to be subject to an n-th order law governing oxygen partial pressure and the Arrhenius kinetic rate model of char reaction. The overall rate of gasification is given as follows:

$$r_{gas} = k_s(T_p) P_{O_{2,s}}^n,$$ \hspace{1cm} (2.7)

Where $n$ represents the reaction order, $T_p$ is the temperature of the coal particle, and $k_s$ is a coefficient of temperature dependent rate and can be written according to the Arrhenius expression: $k_s(T_p) = A \exp\left(-E/R T_p\right)$.

The elevated CO$_2$ and H$_2$O concentrations in the flue gas of oxy-fuel combustion will influence the reaction rate of char particles. As previously mentioned, this can be attributed to the relatively high specific heat capacities of the main gaseous products (CO$_2$ and H$_2$O) compared to the nitrogen in the air-firing. These dominant species will act with the remaining char particles following the endothermic process and thereby reduce the char particle temperature, resulting in a decrease in the rate of char oxidation. Furthermore, the diffusivity of oxygen on the char surface in an O$_2$/CO$_2$ mixture is lower than that in an O$_2$/N$_2$ atmosphere, and this could be why a lower char oxidation rate is observed in an O$_2$/CO$_2$ mixture. Due to the importance of the elevated gases on the gas temperature and char burning rate, Hecht et al. (2010) used a computer model to study the effect of the endothermic CO$_2$ gasification reaction on the char consumption under different oxygen-enriched environments. Numerical modelling was implemented employing the Surface Kinetics in Porous Particles (SKIPPY) code over a range of potential CO$_2$ oxidation rates for bituminous coal particles. The SKIPPY depends on the FORTRAN program to solve the conservation mass, momentum, energy, and species concentration equations by assuming a multicomponent gaseous phase. The results showed that where there was 12% oxygen in an O$_2$/CO$_2$ mixture, the endothermicity of the CO$_2$ gasification led to a significant decrease in the char particle temperature, and thus reduced the reaction rate of char oxidation. For up to 24% O$_2$, the global consumption rate of char particles enhanced with increasing the reaction rate of CO$_2$ gasification. With more than 24% O$_2$, the overall rate of char reaction decreased with an
increase in the gasification rate of carbon dioxide. Using the gasification mechanisms, Nikolopoulos et al. (2011) recently performed a numerical study to scrutinize the influence of CO$_2$ and H$_2$O gasification on the oxidation rate of Greek lignite particles. The authors employed a CFD code (FLUENT, 2008 v.12.0.16) with user defined functions for the above-mentioned models under air-fired and two challenging oxy-fuel-fired cases.

2.3.4 Effect of some parameters on oxy-fuel characteristics

When a mixture of pure oxygen and recycled flue gas is used instead of air as the combustion gases in oxy-fuel-fired power plants, many modifications to the combustion characteristics of the power plant boiler will occur under normal operating conditions. Therefore, in order to address these challenges and ensure the oxy-fuel power plants are working at high combustion efficiency, consistent thermal performance, and with low emissions, several major parameters can be utilized to achieve that remarkable goal. Based on the design and operating conditions of the existing power plants, the effects of different parameters under oxy-fuel combustion conditions such as oxygen concentration, particle size, recirculation of flue gas, and leakages have been investigated. In this subsection, a brief summary of research under the effects of these different parameters is presented.

2.3.4.1 O$_2$ concentration

The oxygen concentrations in the mixed oxidizer stream have a significant impact on the flame stability and heat transfer characteristics in the oxy-fuel firing facilities. In order to maintain the same aforementioned characteristics as in the conventional firing systems, the desirable value of the O$_2$ concentration has to be precisely determined. Due to the physical and chemical differences between the properties of carbon dioxide and nitrogen, it seems that 21% O$_2$ concentration (by volume), in a mixed stream of oxy-fuel conditions, does not provide the same combustion characteristics as conventional operations. This can be explained, as mentioned earlier, as a result of the delay in the ignition time of volatile matter released and to the difficulties in oxidation of the coal char particles. Therefore, higher oxygen concentrations are required to work safety and
provide more efficient operations. However, the RFG enriched with 28 vol. % O\(_2\) is safer than of 21% O\(_2\) in the secondary stream of a pilot-scale burner in oxy-fuel combustion tests for high-volatile subbituminous coal (Chui et al. 2003).

The literature shows that the oxy-fuel combustion scenarios offer the opportunity to supply different amounts and concentrations of RFG enriched with O\(_2\) to both the fuel carrier gas and feed oxidizer gas streams. Many studies have shown that a range between 25% and 36% oxygen (by volume), at the burner inlet, is preferable in oxy-fuel-fired conditions to maintain the same flame behaviour and heat transfer characteristics as those in the air-fired (Andersson et al. 2008a; Andersson et al. 2008b; Huang et al. 2008; Suda et al. 2007; Zhang et al. 2010a). In addition to the safety reasons, this range of oxygen content in the gas mixture was basically found to result in a lower level of pollutants in the flue gas such as NO\(_x\), SO\(_x\), CO, and trace elements during the burning of several coals types. By increasing the O\(_2\) concentrations to more than 21 vol. % in both the primary transport gas and RFG streams at the commercial low NO\(_x\) swirl burner, Sturgeon et al. (2009) noted some improvements were achieved in different areas of investigation compared to the standard conventional firing. For example, the level of CO concentration was decreased, a stable flame was attained, and a low content of carbon in the ash was noticed.

2.3.4.2 Particle size

The findings on the effect of coal particle diameters on the oxy-coal firing have shown that there are recognizable influences on the flame propagation speed, devolatilization process, and ignition temperature. Suda et al. (2007) used two different particle diameters (50 µm and 100 µm) to investigate the effect of coal particle size on the propagation behaviour of flames. The results showed that the flame propagation velocity slightly decreased with coal particle size. However, the reason for that decrease is the lower heat transfer conduction process between the coal particles and gas. Moreover, the authors concluded that the flame stability in the O\(_2\)/CO\(_2\) mixture could be increased using smaller PC particles.
Huang and co-researchers (2008) investigated the effect of the coal particle size on the combustion characteristics of TieFa (Tf) bituminous coal in different mixtures of O\textsubscript{2}/CO\textsubscript{2} atmospheres during the experimental tests. The experiments were conducted using a differential thermal analyser (DTA). Three different particle sizes (11.34, 18.95, and 33.68 µm) and four different O\textsubscript{2} concentrations (10, 20, 50, and 80%) in the gas mixture were used in order to carry out comprehensive investigations into the effect of these two important parameters. The authors used a ratio of thermal gravimetric (TG) to the differential thermal gravimetric (DTG) to clarify the combined effect of the above-mentioned factors on both the devolatilization and char combustion processes. The results of the TG/DTG curves showed that the weight loss of coal samples was augmented as the coal particle size decreased. That contributed to an increase in the surface area of coal particles that led, as a result, to enhance the overall reactivity of coal char, particularly when the O\textsubscript{2} concentration was increased from 10% to 80% at a constant heating rate. In addition, there was a clear decrease in both the ignition and burnout temperatures at the small coal particle size. The effect of the particle size on the reaction rate was relatively negligible at oxygen-rich conditions (50% and 80%). The combustion property index (\(S\)) was also used to give an inclusive estimation of the combustion characteristics under these specified conditions and practical operations. The index (\(S\)) was defined as the coal reaction rates divided by the square of ignition temperature and burnout temperature, as follows (Xiumin et al. 2001):

\[
S = \frac{\left(\frac{dW}{dt}\right)^c_{\text{max}} \left(\frac{dW}{dt}\right)^c_{\text{mean}}}{T_i^2 T_b}
\]  

(2.8)

Where \(\left(\frac{dW}{dt}\right)^c_{\text{max}}\) and \(\left(\frac{dW}{dt}\right)^c_{\text{mean}}\) represent the coal burning rates at the maximum and mean values, respectively. The \(S\) values were determined with a constant heating rate of 30 °C/min.

The plotting of the combustion property index against the coal particle sizes show that the index \(S\) not only increased with a decrease in the particle size, but also with an increase in the oxygen concentration. Consequently, they concluded that the \(S\) values become superior with these two intensified combustion parameters (Huang et al. 2008).
2.3.4.3 Flue gas recirculation

The recirculation of flue gas or recycled flue gas (RFG) is an important process in oxy-fuel combustion. In this process, a large amount of combustion flue gases is recycled to the furnace in order to maintain the same combustion temperature and heat transfer characteristics in the boiler as in the conventional coal-fired power plant. The recycle ratio of flue gas can be defined according to the following simple mathematical expression (Smart et al. 2010):

\[
\text{Recycle ratio} = \left( \frac{\text{Recycled gas mass flow rate}}{\text{Recycled gas mass flow rate} + \text{Product gas mass flow rate}} \right) \times 100\% \quad (2.9)
\]

Typically, 60% to 80% of produced flue gas, mainly CO₂ and H₂O, is recycled in the oxy-fuel plants, and this ratio is basically dependent on the coal type and the options of RFG (Zhou and Moyeda 2010). As previously illustrated in Fig. 2-4, the oxy-fuel technique offers two options to draw the flue gas, either wet RFG or dry RFG can be practically used for the same purpose, depending on from which locations the flue gas is taken from the system. Generally, when using the wet RFG option, the produced combustion gas is extracted before the condensing process, whereas the dry RFG is extracted downstream from the condenser, and both of these options are carried out after the removal of particulates. Under the same volumetric flue gas flow rate, the dry RFG has higher adiabatic flame temperature (AFT) than that in the wet RFG. However, the combination of wet and dry RFG options may provide an attractive option, especially for the PC oxy-fuel power plants. The dry RFG can be utilized to transport coal particles from the mill to the furnace and other miscellaneous uses, while the wet RFG is used to control the combustion temperature due to its high content of water vapour which is much more than in dry RFG. This combined attractive option has recently been used by the Vattenfall project in Germany on the 30 MW oxy-lignite pilot-scale utility boiler (Rehfeldt et al. 2011).

In addition to the aforementioned effects of using RFG on the combustion characteristics and the reduction it causes in NOₓ formation, use of RFG will lead to both the concentrations of carbon dioxide and water vapour largely increasing in the exhausted gases. In order to ensure a higher CO₂ concentration produced in the flue gas,
all combustion gases and auxiliary gases of the air-coal firing have to be replaced by RFG (or principally CO₂) during the switching process in the oxy-coal combustion. Thus, as stated earlier, these desirable results can be achieved by mixing the RFG with about 30 vol. % pure oxygen prior to entering it into the combustion system. On the other hand, the increased CO₂ and H₂O concentrations yielded in the flue gas of oxy-fuel-fired environments lead, as a result, to an increase in the gas emissivity compared to the yield in air-firing environments. Much research conducted into oxy-fuel conditions (Andersson et al. 2008a; Guo et al. 2003; Yin et al. 2011) have shown that the majority of radiation heat transfer in the PC furnace is caused by the presence of particulate matter in the firing region. Therefore, no considerable measures can be taken to reduce the effect of higher concentrations of CO₂ and H₂O on the furnace wall.

Sturgeon et al. (2009) demonstrated the effect of the RFG ratio on the amount of furnace exit carbon in ash (CIA), on the adiabatic flame temperature, and on the coal residence time in the combustion zone. By increasing the RFG ratio, the flame temperatures and residence times of PC were gradually decreased, resulting in an increase in the exit of CIA from the furnace. In order to avoid making major modifications to the heat exchange equipment of the conventional large-scale boiler, the recycle ratio of flue gas, in the oxy-fuel scenario, has to be precisely determined. The best value of RFG can bring another benefit to the oxy-fuel power plant through eliminating the slagging and fouling formation problems on the water wall and on the convective tubes bank of the boiler such as superheaters and reheaters. This problem can be avoided by keeping the furnace exit gas temperature below the ash melting temperature of coal combustion (Al-Abbas et al. 2011; Hjärtstam et al. 2009; Nikolopoulos et al. 2011). This specific temperature is substantially dependent on the ash depositing behaviour of the coal used, as will be seen in the discussion sections of chapters five and seven.

2.3.4.4 Leakages

The major objective of the oxy-fuel combustion technique is to augment the flue gas stream with a higher CO₂ concentration in order to facilitate the sequent processes of
compression and sequestration of CO\textsubscript{2} in the power plant. Leakages in the boiler are considered the main reason for the potential decrease of CO\textsubscript{2} concentration in the flue gas. The leakages in the large-scale power plants can be classified into two types: air ingress and flue gas egress. Both of these types are undesirable and have to be minimized as much as possible in any oxy-fuel power plant. The first type leads to a significant decrease in the CO\textsubscript{2} concentration, whilst the second can increase the concentrations of pollutants such as NO\textsubscript{x} and SO\textsubscript{x} that escape along with the flue gas to the atmosphere. The gas egress can potentially lead to serious safety risks (Tan et al. 2006; Zheng 2011). In the boiler, the following three areas are considered the main sources of leakage: the mill-duct system, the firing group system, and the hopper region. Therefore, proper sealing of all piping systems and ports of the boiler is of great importance to minimize these technical problems during building or modifying the boiler system under oxy-fuel combustion operations. However, this leakage problem could offer the opportunity for using the wet RFG option rather than the dry RFG option because it includes a less complex piping system compared with the dry RFG, which has to pass through several removal and scrubber equipments. Alternatively, for safety and health reasons, the boiler must be operated under slightly negative pressure in order to minimize the flue gas egress through the ports, which is usually practised in many commercial power plants (Dodds et al. 2011).

Regarding the effect of air leakage on the NO\textsubscript{x} formation, Andersson et al. (2008c) conducted experimental tests in a lab-scale oxy-fuel facility unit (detailed information in relation to the simulation of furnace and operating boundary conditions can also be found in chapter six). The authors made use of the air leakage in the firing system by maintaining the air (O\textsubscript{2}/N\textsubscript{2}) as a carrier gas instead of using the O\textsubscript{2}/CO\textsubscript{2} mixture. Using the air leakage, the measured results showed that there was a slight increase in the nitric oxide compared to that which occurred without using the air leakage. That was due to the activation of thermal NO under this condition as well as the effect of the fuel NO. But, there was an obvious decrease in the CO\textsubscript{2} concentration using the air leakage, which was around 4% of the total feed oxidizer gases.
2.4 Heat transfer properties in oxy-fuel furnaces

In oxy-fuel combustion scenarios, several changes in heat transfer can be occurred in the radiative and convective passes of the boiler. These changes in the heat transfer properties are caused due to the recycling process of CO\(_2\) and H\(_2\)O instead of air to the furnace inlet, and thereby affecting the radiative heat transfer and thermal heat capacity of the combustion products (gases and particles). For retrofitting an existing furnace into oxy-fuel conditions or building a new oxy-fuel furnace, it is necessary to understand the influence of change of these intrinsic variables on temperature distributions and heat transfer characteristics. Under oxy-fuel combustion conditions, fuel combusts with a mixture of pure oxygen and part of RFG (wet or dry) producing gases and particulate matter. The gaseous product includes higher CO\(_2\) and H\(_2\)O concentrations with other minor intermediate species, while the particulate matter comprised of char, ash particles, and soot in a case of coal firing. The heat transfer processes between these combustion products and the water wall (radiative pass) and convective tubes bank (convective pass) determine thermal boiler efficiency. Then, the emissivity, thermal diffusivity, density, and heat capacity of the combustion products have a significant effect on the heat transfer properties of oxy-fuel boiler. For that reason, the accurate adjustment between the recycle ratio and O\(_2\) concentration provided to the oxy-fuel furnace is considered a key parameter and can probably achieve the same heat transfer characteristics of the existing power plant.

Over the past few years, there have been many investigations on the flame and radiation characteristics in terms of theoretical modelling (Khare et al. 2008; Krishnamoorthy et al. 2009; Yin et al. 2011) and experimental studies (Andersson et al. 2008a; Andersson et al. 2008b; Hjärtstam et al. 2009). Andersson and co-researchers (2008a) and (2008b) used the narrow angle probe to measure the radiation intensity of the flame and the combustion products in the furnace. The effect of the high temperature of the furnace wall on the measurement devices was avoided making the radiometer in a parallel appearance with a water-cooled suction body. While the collimating tube, that carries purge argon, utilized to prevent the absorption of radiation by the gases and the fouling of the tube. The measured results illustrated that the influence of RFG on the radiation
intensity was resulted in a change in the temperature and emissivity of oxy-fuel flames. They also observed that the soot formation is distinctly enhanced the flame radiation with the oxygen concentration (Andersson et al. 2008b).

2.4.1 Comparison between air-fired and oxy-fuel radiation flames

Compared with air-fired flames, the emissivity of the combustion products for oxy-fuel-firing atmospheres in both the wet and dry RFG is comparatively higher due to the increased concentrations of CO$_2$ and H$_2$O and some intermediate solid particles. The thermal diffusivity in the O$_2$/CO$_2$ mixture is lower by around 60% than that of the air-coal firing. In the elevated temperatures, the specific heat capacity (at constant volume) of CO$_2$ is as high as that of N$_2$ by 1.7 times, while the specific heat capacity of H$_2$O is 1.3 times that of N$_2$. The densities of the dominant combustion gases are completely different because of the differences in their molecular weights (the molecular weights of CO$_2$, H$_2$O, and N$_2$ are 44, 18, and 28 g/mol. respectively) (Buhre et al. 2005; Wall et al. 2009). Based on the above information, it can be said that these intrinsic and essential variables have a clear impact on the combustion behaviour and heat transfer properties in oxy-fuel environments. However, these differences in the radiative heat transfer can be seen clearly in the luminous appearance of flames, which divided into luminous and non-luminous flames. On the same O$_2$ concentration, the luminosity of air-fired flame is much higher than that of O$_2$/CO$_2$ flame. This phenomenon is not only attributed to the contributions of higher CO$_2$ and H$_2$O concentrations, but also to the reduced soot formation in the O$_2$/CO$_2$ mixture, resulting in a decrease in the combustion temperature. The soot formation is strongly connected with the flame temperature through the soot radiation (Wang et al. 2005). With increasing O$_2$ concentrations in the O$_2$/CO$_2$ mixture, the soot volume fraction is highly increased, particularly in the combustion zone, leading to increase in the luminous appearance as that of the air-fired flame. In the hydrocarbon combustion with the 21 vol. % O$_2$ and 79 vol. % N$_2$, and 27 vol. % O$_2$ and 73 vol. %CO$_2$, the luminosity of flames was identical compared with the flame of 21vol. % O$_2$ and 79 vol. % CO$_2$ mixture (Andersson et al. 2008b). Due to the importance of these systematical variables and essential variables on the radiation predictions of oxy-fuel boiler, the next subsections will briefly discuss the radiative models.


2.4.2 Radiation heat transfer models

The radiation transfer equation (RTE) has been shown to be a very appropriate method in three-dimensional and non-homogeneous participating media (Hottel and Sarofim 1967). The RTE can solve by several integral methods such as discrete transfer (DT), discrete ordinary (DO), P-1, and Monte Carlo. The total emissivity of the dominant combustion gaseous products is valued based on many parameters such as gas temperature, absorption coefficient, total pressure, and geometric path length (Hottel and Sarofim 1967). This estimation has been initially established for the combustion products of the conventional air-coal firing. Therefore, there is no strong certainty in regards to its validation for oxy-coal combustion conditions. Currently, there are several radiative heat transfer models, which are coupled with the flow solver of the CFD code (FLUENT, ANSYS, and AVL Fire of which the latter is used in this work). These radiative models have been employed in many numerical studies (Chen et al. 2008; Nikolopoulos et al. 2011; Yin et al. 2011) to solve the radiative heat transfer problems in oxy-fuel furnaces. In open literature there are many radiative models used to predict total gray (radiative) properties of combustion gases, including Hottel’s charts, Total Emissivity Model, Narrow Band Model (NBM), Wide Band Model (WBM), Weighted Sum of Gray Gas Model (WSGGM), and Exponential Wide Band Model (EWBM). The improvement of the radiative models was based on the experimental spectroscopic analysis of gas absorption. The most popular models used in calculations of the oxy-fuel furnaces were WSGGM (Yin et al. 2011; Zhou and Moyeda 2010) and EWBM (Chen et al. 2008; Nikolopoulos et al. 2011). The WSGGM approach was first developed by Hottel and Sarofim (1967) to solve the general RTE in non-scattering and non-gray radiation medium. This approach was modified later by Modest (1991) to be able to solve any radiative solution method by substituting the media by a small number of gray media, using the accepted P-1 for the equivalent gray radiation solutions. The total emissivity for the WSGGM approach is given according to Smith et al. (1982) as follows:

\[ \varepsilon = \sum_{i=0}^{I} a_{\varepsilon,i}(T)[1 - e^{-k_iPS}] \]  

(2.10)

Where \(a_{\varepsilon,i}\) denotes the emissivity weighted factor for \(i\)th gray gas and is dependent only on gas temperature, \(1 - e^{-k_iPS}\) is \(i\)th gray gas emissivity, \(k_i\) is the absorption
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coefficient of \( i \)th gray gas\((atm-\text{m})^{-1}\), \( P \) represents the sum of the partial pressure of the absorbing gases \((atm)\), \( S \) denotes the path length \((\text{m})\), and \( I \) is the number of gray gases. Then, in the WSGGM, the emissivity is represented a combination between the weighted factor and the gray emissivity for a gas mixture (CO\(_2\) and H\(_2\)O). The characteristics of emissivity for specific gas compositions are valid only in a small range of path length (Yin et al. 2011).

The EWBM first proposed by Edwards (1976) was based on the concentration method of absorption and emission of gases within several bands. In this model, the integrated band intensity \((\alpha)\), the line-width-to spacing parameter \((\beta)\), and the bandwidth parameter \((\omega)\) are used to describe a total gas band over a wide range of gas temperature, path length conditions, and pressure. These parameters \(\alpha\), \(\beta\), and \(\omega\) are a function of gas temperature and wave number \((\nu)\) (Edwards and Balakrishnan 1973). The ratio of the mean line intensity to the spectral line spacing \((S/d)\) is described in three limited functions based on the position of the band head (Strohle and Coelho 2002):

\[
\frac{S}{d} = \begin{cases} 
(\alpha/\omega)e^{-(\nu_u-\nu)/\omega} : \text{upper limit} \\
(\alpha/\omega)e^{-(\nu-\nu_l)/\omega} : \text{lower limit} \\
(\alpha/\omega)e^{-2|\nu_c-\nu|/\omega} : \text{band centre}
\end{cases} 
\tag{2.11}
\]

Where \(\nu_u\), \(\nu_l\), and \(\nu_c\) represent the upper, lower, and centre wave number, respectively. A detailed description regarding this radiative model can be found in Edwards (1976).

Krishnamoorthy et al. (2009) examined numerically three total gray models for their capability to predict well radiative properties of combustion gases in a large-scale boiler under oxy-fuel combustion conditions. The EWBM, WSGGM, and Perry models were fully coupled with the flow solver of the commercial CFD code (FLUENT). These total property models were based on a combined of the narrow and wide band model parameters in order to deal with different H\(_2\)O/CO\(_2\) composition ratios of the combustion products. The DO model was employed for the radiation calculations, considering the absorption coefficients obtain from the computed gas emissivity at each control volume of the computational domain. The assessment of the performance of
these property models revealed that when the \( \text{H}_2\text{O}/\text{CO}_2 \) composition ratios were in a range between 0.5 and 2.5 the predictions of the radiative properties were approximately similar. On the outside of these \( \text{H}_2\text{O}/\text{CO}_2 \) ratios, the Perry and WSGGM models could cause an error in the gas emissivity calculations. Therefore, the EWBM was the best choice for a wide range of gas composition, but it needs much computer time in comparison with other radiative models.

### 2.5 Emissions and pollutions from oxy-fuel combustion systems

In this section it can be seen how oxy-fuel combustion can impact on the major pollutants concentrations of air-coal firing, such as \( \text{NO}_x \), \( \text{SO}_x \), slagging and ash formation, and small particulate matters. As previously stated, the purpose of the oxy-fuel-fired technique is to capture the \( \text{CO}_2 \) enriched in the flue gas after the final removal processes. During the recirculating process of dirty flue gas to the oxy-fuel furnace a large amount of certain pollutants may be accumulated, specially compounds of sulphur. This undesirable accumulation could have negative impacts on the equipments of particulate removal and boiler performance. Therefore, these pollutants need to be reduced in the recycled flue gas to as a lowest level as possible.

Despite the higher \( \text{O}_2 \) concentration used with the recycled flue gas in the oxy-fuel combustion, there is a little change in the mechanisms of formation and destruction of the combustion products as the air-fired combustion, except for \( \text{NO}_x \) formation. The major change between the air-fired and oxy-fuel combustion cases in terms of pollutions is the higher \( \text{CO}_2 \) concentration formed in the flue gas in the latter case. It noted that this \( \text{CO}_2 \)-rich has a slight effect on the formation and destruction mechanisms of the major pollutants (Normann et al. 2009). For that reason, the oxy-fuel power plant needs little modifications in regards to the boiler design with respect to the conventional power plant. This means that the oxy-fuel boiler can utilize the same equipments of pollutants removal as that in the existing power plant such as the electrostatic precipitator (ESP), \( \text{NO}_x \) removal, flue gas desulphurisation (FGD), and flue gas condensation (FGC). One of these modifications required in the oxy-fuel firing system is to use the advanced low-\( \text{NO}_x \) burner, which has been established due to the sensitivity of \( \text{NO}_x \) formation to the
way of injecting oxygen (Kurose et al. 2004). However, this modification is not longer required for the retrofitted tangentially-fired PC boiler because it originally designed for low NO\textsubscript{x} formation in the furnace, considering a reliable recirculation flow for the reactants in the combustion zone.

2.5.1 Carbon dioxide (CO\textsubscript{2}) emission

The major objective of establishing oxy-fuel combustion technique is to increase CO\textsubscript{2} concentrations in the flue gas. This is also considered the main difference between the air-fired and oxy-fuel-fired environments in terms of emission, and in addition to the higher reduction in NO\textsubscript{x} formation. In general, the flue gas from the oxy-fuel firing systems includes from about 75% to 85% carbon dioxide on a dry basis. While the remaining part, as mentioned earlier, may likely consist of carbon dioxide (CO), NO\textsubscript{x}, SO\textsubscript{x}, particulate matter, and a small amount of trace elements and mercury. Under normal combustion conditions, it chemically found that CO\textsubscript{2} does not change the entire mechanisms for those pollutants, excepting higher CO concentrations in the combustion zone due to enhancing the dissociation mechanism (Hu et al. 2003; Tan et al. 2006). The CO\textsubscript{2} has to be purified from these impurities in the flue gas to reach to about 95% to be suitable for capturing and sequestrating processes and then transporting it to its eventual underground storage.

The experimental studies on lab-scale oxy-fuel furnaces pointed out that the CO\textsubscript{2} concentration in the combustion flue gas of firing pulverized coal particles might increase to around 95% (by volume) on a dry basis (Buhre et al. 2005; Hu et al. 2000). This desirable value could be decreased in pilot-scale oxy-fuel furnaces due to unwell-sealed firing systems. Chui et al. (2004) and Tan et al. (2006) indicated that the purity of CO\textsubscript{2} in the flue gas is reduced to 92% during firing lignite coal particles in the 0.3 MW vertical combustor research facility (VCRF). From 80% to 85% of CO\textsubscript{2} concentration may be achieved in the well-sealed large-scale oxy-fuel boiler. Otherwise, this value could be dropped down if the air leakage was unavoidable in the retrofits and piping systems. This fact has been approved through the numerical simulations conducted on the large-scale boiler under O\textsubscript{2}/CO\textsubscript{2} mixtures. For instance, Chen et al. (2008) conducted
a CFD modelling study on a 520 MW opposed-wall fired unit under both the air-fired and oxy-fuel combustion atmospheres. COMO\textsuperscript{SM} code was employed to predict the coal particles flow, combustion characteristics, and heat transfer processes. The predicted results showed that the CO\textsubscript{2} concentration is increased from 14.42 vol. \% (under air-firing process) to 66.84 vol. \% (under oxy-fuel-fired process). However, with a higher CO\textsubscript{2} concentration in the oxy-fuel flue gas, the capturing and sequestrating processes for CO\textsubscript{2} will be chemically easier, and no further purifying or separating processes are required.

2.5.2 Nitrogen oxide (NO\textsubscript{x}) emissions

Due to concerns regarding the nitric oxides (NO\textsubscript{x}) emissions from the PC air-fired boiler systems, the literature includes a large number of experimental investigations and numerical modelling (Díez et al. 2008; Habib et al. 2009; Kurose et al. 2004; Sheng and Li 2008; Xu et al. 2000). The findings on these emissions could be applied for the oxy-fuel power plants, although the higher O\textsubscript{2} concentration with RFG is introduced into the furnace inlet instead of air.

In general, the NO\textsubscript{x} formation from the coal combustion stems from three main sources: Thermal NO, Prompt NO, and Fuel NO. The Thermal NO forms due to the dissociation of the molecular air-nitrogen at the higher combustion temperatures. The Prompt NO creates due to the attack of hydrocarbon radicals such as CH, C\textsubscript{2}H, and CH\textsubscript{2} on the air-nitrogen. However, the NO formed from this source is always negligible in the prediction of the overall NO\textsubscript{x} formation because it is relatively small in comparison with that of Thermal NO process (Kurose et al. 2004). The Fuel NO produces from the reaction of oxygen with the nitrogen bound in the fuel, both of the volatile-N, such as HCN and NH\textsubscript{3}, and char-N (Díez et al. 2008). The mathematical expressions and chemical equations of NO\textsubscript{x} formation for the low-rank coal combustion will be addressed in the next chapter in terms of the Thermal NO and Fuel NO production mechanisms in detail.
Below 1673 k, the NO production from the fuel NO source is dominant compared with other NO formation sources, while above 1773 K the thermal NO will exceed the fuel NO. This is attributed due to the enhancement of the dissociation mechanism of air-N and then react it with oxygen to produce NO at the oxygen-rich region. However, the literature pointed out the NO\textsubscript{x} formation in O\textsubscript{2}/CO\textsubscript{2} mixtures is mainly dependent on the coal types and atmospheric environments as well as combustion temperatures (Chui et al. 2004; Hu et al. 2003; Liu and Okazaki 2003). Under oxy-fuel combustion conditions, the amount of NO formation in the flue gas is drastically decreased by more than 30% relative to the air-blown conditions. That obvious reduction in the NO formation was referred to the following potential reasons: decreasing in the thermal NO, recirculating process of the combustion flue gas, and adopting an air-staging and fuel-staging in the oxy-fuel firing systems (Croiset and Thambimuthu 2001; Hu et al. 2001; Okazaki and Ando 1997).

Cao et al. (2010) conducted a CFD modelling study to investigate the NO\textsubscript{x} formation and destruction mechanisms from firing an Australian sub-bituminous coal under air-firing and oxy-fuel firing conditions in a 1.2 MW pilot-scale facility unit. The numerical calculations were performed incorporating the source terms of the modified pathways of NO formation/destruction, HCN, and NH\textsubscript{3}, as a user defined functions, in the CFD code. Due to the slower processes of NO\textsubscript{x} formation relative to the coal combustion process, the sources of NO, HCN, and NH\textsubscript{3} were added to the CFD calculations as a second step, i.e. after finishing the main chemical reactions of volatile matter and coal char. The HCN was assumed to be released from the volatile-N, and subsequent reaction of HCN produces NH\textsubscript{3}, as explained in the following chemical reactions (Stanmore and Visona 2000):

\begin{align}
2 \text{HCN} + 2.5 \text{O}_2 & \xrightarrow{\text{yields}} 2 \text{NO} + 2 \text{CO} + \text{H}_2\text{O} \\
\text{HCN} + \text{H}_2\text{O} & \xrightarrow{\text{yields}} \text{NH}_3 + \text{CO}
\end{align}

The predicted results of Cao and co-researchers (2010) showed a good agreement with the measured data in both the air and oxy-fuel combustion cases. On a heat input basis of milligrams per mega joule of the NO emission, the NO formation for the oxy-fuel
case, without NO recycle, was more than 35% as lower as that in the air-fired case. While with adopting the 1000 ppm of NO recycle, this ratio was slightly decreased.

At CANMET organisation, comprehensive investigations on the effect of coal types, O$_2$-enriched atmospheres, and burner configurations on the NO$_x$ formation in an O$_2$/N$_2$ and several O$_2$/CO$_2$ mixtures were performed experimentally and numerically. The findings on the effect of the coal types was reported in subsection 2.2.2 (Tan et al. 2006). Regarding the effect of O$_2$ concentrations in the gas mixtures, Croiset and Thambimuthu experimentally used a US eastern bituminous coal at three different combustion categories: in the air, in O$_2$/CO$_2$ mixtures, and in a real recycled flue gas. They noted that the NO$_x$ formation rates increase with the higher O$_2$ concentrations, resulting in an increase in the combustion temperatures. In the air combustion media, the NO$_x$ emissions were noticeably higher in comparison with other oxy-fuel tested cases due to presenting nitrogen in the firing system, enhancing as a result the thermal NO mechanism. While the results from using a recycled flue gas indicated that the NO$_x$ emission rate was lower than that of the O$_2$/CO$_2$ mixtures. The authors explained the reason for that reduction was due to the extra reactions between the recycled NO and hydrocarbon radicals, producing an intermediate nitrogen species (HCN) in the flame zone (Croiset and Thambimuthu 2001).

For regarding the effect of burner’s design on the pollutant formation characteristics, Chui and co-workers (2004) numerically used two different burners (A and B); detailed descriptions in regards to the burners’ configuration can also be found in subsection 2.3.2. The burners were designed to work over a wide range of operating conditions and fuel types (natural gas and coals). The authors noted a significant decrease in the NO formation along the furnace when burner A is adopted compared with that of burner B. At the furnace exit, the predicted results of NO emissions reduced from 1160 ppm to 295 ppm for burners B and A, respectively. That was indicating that burner A promoted better mixing conditions between the fuel and oxidants at a near-burner region and led as a result to lowering NO$_x$ formation.
2.5.3 Sulphur oxide (SO₃) emissions

The reaction process of pulverized coal particles with oxidants in the firing systems is considered the main source of sulphur oxide (SO₃) emissions in the atmosphere. The sulphur bound in the coal reacts with oxygen (oxidant agent) to form sulphur dioxide (SO₂), and then further reactions with oxygen radicals could happen at higher flame temperature conditions to form SO₃, as explained in the following equations:

\[ S + O_2 \xrightarrow{yields} SO_2 \]  \hspace{1cm} (2.14)

\[ SO_2 + O + \ldots \leftrightarrow SO_3 + \ldots \]  \hspace{1cm} (2.15)

The content of S-bound in the coal varies from coal to other, for an instant lower-rank coals (lignite and sub-bituminous) include less sulphur content than high-rank coals (bituminous). Similar to NOₓ emissions in the oxy-fuel combustion, the recycled flue gas could drawback to the furnace either upstream or downstream of the FGD equipments. The latter gas stream, i.e. after the desulphurization process, can achieve a higher reduction level of SOₓ emission in the flue gas compared to that if the gas stream is recycled before eliminating emissions. However, these flue gas recirculation options are completely dependent on the sulphur content in the coal, in which the low-sulphur coals can improve the oxy-fuel power plant efficiency during reducing the operating costs of FGD (Wall et al. 2009; Zheng 2011).

Although few investigating studies have been done on the sulphur compounds in the O₂/CO₂ mixtures, it was found that there is a clear decrease in the SOₓ mass emissions compared to that in air-blown conditions. The experimental results conducted in the 160 kW test facility unit (Sturgeon et al. 2009) were showed that for oxy-fuel firing, on the heat input basis, SO₂ concentration was as less as 25% relative to that in the air-firing. That was attributed due to increasing the mass fraction of SO₂ in the fly ash during oxy-fuel firing, resulting in a decrease in the proportion of SO₂ in the flue gas.

The experimental investigations of Croiset and Thambimuthu done on the three firing categories, as mentioned earlier above, have shown that these atmospheric firing types
have a significant effect on the conversion ratio of S-bound in the coal to SO$_2$. In the air, the conversion to SO$_2$ was 91%, but for the O$_2$/CO$_2$ mixtures and recycled flue gas were 75% and 64%, respectively. In addition to the above-mentioned reason by Sturgeon et al., Croiset and Thambimuthu (2001) explained that the reduction was due to the further oxidation of SO$_2$ with available O radical to produce SO$_3$.

The effect of oxy-fuel combustion on the sulphur compounds was also studied in the VCRF test unit (Tan et al. 2006). The measured results showed that the concentrations of SO$_2$ in the oxy-fuel furnace were as high as 3-4 times in comparison with that of the corresponding air-firing case. This increase was caused due to recirculating the flue gas without SO$_2$ removal, i.e. it is recircled upstream the FGD, leading as a result to accumulating SO$_2$ in the flue gas. However, for a better oxy-fuel power plant design, it is necessary to maintain the boiler material above the acid dew point to prevent corrosion problems if the latter flue gas recirculation option is adopted.

2.5.4 Ash and slag formations

Ash deposition and slag formation from burning pulverized coal particles are significant parameters in the thermal boiler design, particularly on the heat transfer surfaces such as radiation zone (water-wall furnace) and convection zone (superheater, reheater, and economizer). Therefore, it is necessary to understand how these parameters change when the feed gas mixture replaces from O$_2$/N$_2$ to O$_2$/CO$_2$ mixtures in the furnace inlets. However, the full knowledge of the effects of these intrinsic parameters on the combustion characteristics and power plant efficiency is still not completely available, and more extensive research is needed under oxy-fuel combustion conditions.

The higher oxygen concentrations, in oxy-fuel combustion, lead to increasing the combustion temperature and then enhancing the potential for increased slag formation in the furnace. Thus, the suitable distributing conditions of fuel and oxidants have to be precisely taken into consideration prior to injecting O$_2$ to the oxy-fuel furnace. Regarding the bottom ash formed in the hopper zone, the reduction in the volumetric flow rate of feed oxidizer gases adopted in most oxy-fuel-fired scenarios showed a clear
effect on the ash content at the bottom of the furnace. This was due to that the lower gas velocity does not have the ability to burn larger ash particles, resulting in an increase in the quantity of bottom ash in comparison to that amount produced in the air-blown condition (Pedersen et al. 2009; Sheng and Li 2008; Wall et al. 2009).

In order to compare the impact of O$_2$/CO$_2$ and O$_2$/N$_2$ combustion atmospheres on the ash particle formation behaviour, Sheng et al. (2007) experimentally burned three typical Chinese coals in a drop tube furnace (DTF). The ratios of gas compositions of both the O$_2$/CO$_2$ and O$_2$/N$_2$ mixtures used in the tests were 1:4 and 2:3, supplying a wide range of O$_2$ concentrations as in practical operating conditions. For all three coals used, the measured results showed that there is no significant effect on the size distribution of ash particles under various O$_2$/CO$_2$ combustion conditions. But, there were noticeable effects on the mass and distributions of composition size for both the fine and coarse particles examined. The authors also noted that the increased O$_2$ concentrations in O$_2$/CO$_2$ mixture had considerable impact on the ash particle formation compared to that in the O$_2$/N$_2$ mixture (Sheng et al. 2007).
Chapter 3. Mathematical Models, Modelling Techniques, and Methodology
3. Mathematical models, modelling techniques, and methodology

3.1 Introduction

In the past few decades, the numerical solution of the engineering problems was considered as a complete research, from which the software packages were prepared. That was carried out by using one of the numerical methods such as Finite Volume method (FVM), Finite Element method (FEM), or Finite Difference method (FDM). With the time the uses of these packages became very useful and simple, especially with increasing the development of computerized technology that enhances the potential of computer simulation techniques. Some CFD packages such as ANSYS, FLUENT, etc. are available to solve and analyse any real engineering problem. For instance, more realistic and significant problems in mechanic, chemistry, environmental engineering can be solved and optimized by using these CFD codes. Optimization in these problems can definitely produce a cost-effective basis in equipment with associated large energy savings.

The selection of a CFD code for an appropriate application should obey several assumptions and accurate criteria. For instance, the appropriate CFD code should be able to define a wide range of geometry (two- or three-dimensional) in order to cover any complicated engineering problem. As well, it should have the capability to define the physical aspects in a wide range of applications to give an accurate numerical solution. Moreover, and it should make an easy and effective analysis of the numerical results in the entire simulation domain. Consequently, the appropriate selection of CFD code might bring many advantages in analysing the specific engineering problems.

As previously mentioned, it was necessary to start this project with a small scale furnace in order to ensure the ability of the CFD code to simulate the combustion process in the large-scale furnace under oxy-fuel combustion conditions. Therefore, the purpose of this work was not only to model the combustion processes in the laboratory-scale furnace for gaseous and solid fuels under air-fired and oxy-fuel combustion environments, but
also to develop appropriate computational models to simulate the large-scale
tangentially-fired furnace. The suitability of the CFD code can be certainly utilized for
optimizing the burners and furnace (combustor) of CO$_2$ capture from power plants
under safety conditions and accepted operations.

In this study, the commercial CFD code, AVL Fire ver.2008, was selected to solve
mathematical equations using the finite-volume technique in different 3-D hybrid
unstructured grid systems. The solution algorithm employed in the AVL Fire CFD code
is forceful and enables flexibility in the usage of any structured and unstructured grids.
The finite-volume approach is different from other numerical methods (e.g. FEM and
FDM) in terms of discretisation method and numerical solution. The main difference is
that the conservation equations are integrated prior to the discretisation scheme over the
finite control volumes (cells are generated by the adopted numerical mesh).

In addition, this CFD code includes a range of more recent turbulent models and
differencing schemes, which can provide accurate calculations of turbulent flow
problems. Different types of combustion models are available, from which their kinetic
chemical parameters can be changed and modified. But, the main reason of selection
this CFD code was due to its capability to implement user subroutines (user defined
functions) in the FORTRAN and user formula in C++. This gives the opportunity to
develop and modify many complicated mathematical models such as turbulent
combustion, evaporation, devolatilization, char oxidation, particle tracking, convection
and radiation heat transfer, multi-step reactions, NO$_x$ modelling. This also allows the
programmer or researcher to have access to a wide range of computational domains at
different sections of the code.

Based on all these interesting features and necessary observations, the AVL Fire code
was chosen for modelling the gas (propane) combustion and pulverized coal particles
(lignite and brown coals) combustion for different scales of furnaces. The reliability of
this CFD code was based on the extensive validation of the present predicted results
with the experimental data in different combustion scenarios. It is noteworthy to
mention here that this developed CFD code can also be used for further research in regards to the scrubbing process of $\text{CO}_2$ from the power plants and new design optimisation of the boiler.

The numerical solution techniques in this chapter start with the finite volume discretisation and solution method to solve the governing equations. An overview of the mathematical models of both gas and coal combustions is discussed. A detailed description of the turbulence model and heat transfer models in the computational domain and between the gas and coal particles is also presented. Appropriate coefficients and detailed kinetic chemical parameters used in this study are tested and presented based on the combustion conditions. The multi-step reaction mechanisms in terms of single-, two-, and three-step reaction models are discussed and presented for coal reaction processes, while one- and four-step chemistry mechanisms are used for gas reaction. The chapter closes with the nitric oxides ($\text{NO}_x$) modelling in terms of thermal and fuel NO formation/destruction mechanisms.


3.2 Numerical solution procedure

3.2.1 Mathematical models

The mathematical model is considered the basis for any numerical calculations. In this project the set of Eulerian partial differential conservation equations (PDEs) is solved for mass, momentum, turbulent kinetic energy, turbulent dissipation rate, enthalpy and a number of species mass fractions. Several sub-models are coupled via the source terms of PDEs for calculating the heat transfer (convection and radiation), turbulence, coal particle temperatures and trajectories, coal devolatilization, and char combustion models. The general form of non-steady state Eulerian transport equation used is (Patankar and Spalding 1972):

\[
\frac{\partial}{\partial t} (\rho \phi) + \frac{\partial}{\partial x_i} (\rho U_i \phi) = \frac{\partial}{\partial x_i} \left( \Gamma \frac{\partial \phi}{\partial x_i} \right) + S_\phi
\]

(3.1)

Where \( \rho \) is the fluid density, \( x_i \) is the distance in the ith direction, \( U_i \) represents the velocity in the ith direction, \( \Gamma \) is the diffusion coefficient of the variable \( \phi \), and \( S_\phi \) represents a source or sink term for the variable \( \phi \).

The first and second terms on the left hand side of Eq. (3.1) represent the unsteady term and convection term, respectively. On the right hand side, the first term is the diffusion term. In this study, several mathematical models were used to simulate the combustion processes and heat transfer characteristics of both the gaseous and solid fuels. Therefore, these mathematical models classified into two kinds, in this chapter, based on the combustion environments. The chemistry reaction mechanisms of main and intermediate species and the NO\(_x\) formation/destruction mechanisms were also presented and discussed in detail.

3.2.2 Finite volume discretisation

A suitable discretisation method has to be chosen after selecting the mathematical models. The discretisation method yields a large number of non-linear differential equations. Thus, the methods of solution of these equations are dependent upon the nature of physical problem and boundary conditions. However, there are three main
methods: finite difference (FD), finite volume (FV), and finite element (FE). These discretisation methods are used for approximating the differential equations by a system of algebraic equations at the discrete locations. In this work, the FV method was used with unstructured grids due to the complicated shape of the geometry.

3.2.2.1 Basic approach and numerical grid

The FV approach in this CFD code rests on the integral conservation principles describing the behaviour of a substance when it interacts with its surroundings, which is considered numerically a more suitable method for fluid flow and heat transfer problems. The first step of the finite volume method is to divide the computational domain into a finite number of non-overlapping control volumes (CVs) which constitute a numerical grid. The FV method uses the integration of the conservation equations over a control volume to yield a discretised equation at each nodal point of CV. The variable values of these equations are calculated at the central node (computational node) of each CV as shown in Figure 3-1. The faces of control volumes are located at a midway between the adjacent (neighbouring) nodes. Vertices \( \mathbf{v}_n \) are basic objects since they define physically the numerical grid through their position vectors. The vertices are connected by straight lines (segments), which lead to make cell faces. The cell-faces are divided into internal faces and boundary faces that share by only two control volumes.
In Figure 3-1, the neighbours of an internal face-based $j$ are defined by an array $lf$ as $ip1 = lf(1,j)$ and $ip2 = lf(2,j)$ and the face area vector $A_j$ points out from a cell with the index $ip1$ to a cell with the index $ip2$. Similar to the internal faces, for a boundary face $ib$ the neighbouring cell $ip1$ is identified by an array $lb$ as $ip1 = lb(ib)$. The boundary face always points out from the neighbouring cell. The surface vector ($A_j$) is computed using formula for a triangular face ($M_p$) and can be given in the following expression (AVL Fire CFD Solver v 8.5 manual 2008):

$$A_j = \frac{1}{2} \sum_{i=3}^{M_p} [((\vec{r}_{i-1} - \vec{r}_i) \times (\vec{r}_i - \vec{r}_3))]$$

(3.2)

Where $\vec{r}_j = x_j\hat{i} + y_j\hat{j} + z_j\hat{k}$ is the position vector at the cell centre. The geometric centre of a control volume around the central node $P$ is given as follows:

$$\vec{r}_p = \frac{1}{v_p} \int \vec{r} \, dv$$

(3.3)

Based on this brief description, the finite volume method is suitable for complex geometries and can be applied to any type of grid systems, where the grid identifies just the CV boundaries and need not be related to a coordinate system. Therefore, as a
comparison, the finite volume (FV) method is approximately the easiest discretisation method to understand and to apply in the CFD code.

3.2.2.2 Differencing schemes

The method used to calculate the variable values at cell faces has an important effect on the numerical stability of the numerical calculation, particularly when considering the evaluation of face values for the convective transport equation. The reason of this importance is a fundamental problem with the discretisation of second-order accurate linear interpolation. However, if this interpolation is used on inadequate refined numerical grids it could lead to producing unphysical oscillations and the unbounded variable values. In this study, two standard differencing schemes were used. The first was a central differencing scheme (CDS) that was adopted for calculating the continuity equation. Whilst the second was an upwind differencing scheme (UDS) which used for momentum, turbulence, scalar, and energy equations.

Central differencing and upwind differencing schemes

In common approximation procedures, the central differencing applies to represent the diffusion term of the Eq. (3.1). Simple linear interpolation between grids, which amounts to the CDS, gives the face values of a scalar variable ($\phi$) as follows:

$$\phi_j = f_j \phi_P + (1 - f_j) \phi_{P_j}$$  \hspace{1cm} (3.4)

Where $\phi_j$, $\phi_P$, and $\phi_{P_j}$ represent the scalar variables at the cell-face centre, nodal point, and neighbouring node, respectively and $f_j$ is the linear interpolation factor of the cell face value and can be defined in terms of distances between the node $P$, cell-face centre $j$ and the neighbouring node $P_j$ as shown in the following equation:

$$f_j = \frac{|r_{P_j} - \bar{r}_j|}{|\bar{r}_j - \bar{r}_P| + |r_{P_j} - \bar{r}_j|}$$  \hspace{1cm} (3.5)

Although this above treatment can be used for most terms in the discretised equations, it showed its inability to identify the strong flow direction at the convective flux term of
the transport equation. For that reason, the first-order- and second-order-accurate upwind differencing schemes were adopted in this study, in which the value at face \( j \) is taken to be that which succeeds at the upwind nodes. In the UDS, the scalar variable at the face value \( j \) is determined based on the values of mass flow rate through the face \( j \) and can be described by the following equation:

\[
\phi_{j}^{UDS} = \begin{cases} 
\phi_p & \text{if } \dot{m}_j \geq 0 \\
\phi_{p_j} & \text{if } \dot{m}_j < 0 
\end{cases}
\] (3.6)

Where \( \dot{m}_j \) is the mass flow rate through the face \( j \).

The first-order upwind differencing scheme is unconditionally bounded but creates an unwarranted numerical diffusion and may lead to wrong impact on the numerical results, particularly when the flow direction is not aligned with the grid lines. Therefore, the second-order-accurate UDS was adopted, in this study, for the species concentrations, momentum and energy equations. Detailed information regarding this numerical issue will also be given in the computational method description of the coal combustion processes in chapter five.

### 3.2.3 Solution procedure

The outcome of the discretisation procedure is a set of non-linear equations. The method of solution these algebraic equations depends on the nature of the problem. The general form of the discretised equations can be written as follows:

\[
a_p \phi_p = \sum_{j=1}^{n_i} a_j \phi_{p_j} + S_{\phi}
\] (3.7)

Where \( n_i \) is the number of internal faces, \( a_j \) represents the coefficients associated with the values of the dependent variable \( \phi \) at neighbouring nodes \( P_j \), \( S_{\phi} \) is the source term, and \( a_p \) is the central coefficient and can be calculated as:

\[
a_p = \sum_{j=1}^{n_i} a_j + \sum_{b=1}^{n_b} a_b + a_t + S_{\phi} ; a_t = \begin{cases} 
\frac{(\rho \nu)^{n-1}}{\Delta t} & \rightarrow 1^{st} order \\
\frac{4 (\rho \nu)^{n-1} - (\rho \nu)^{n-2}}{2\Delta t} & \rightarrow 2^{nd} order
\end{cases}
\] (3.8)
For unsteady flow problems, the transient run mode used for initial value problems in the ordinary differential equations, for which an elliptic problem has been solved at each time step. The determination of pressure considers the principal difficulty in solving the momentum equation. One of the iterative solution procedure used for calculating the Navier-Stokes equation is the semi-implicit method for pressure linked equations (SIMPLE) algorithm (Patankar and Spalding 1972). In this iterative SIMPLE algorithm, the discrete form of the continuity equation is converted into an equation for the pressure correction. The pressure-corrections are then used to update the pressure and velocity fields so that the velocity components obtained from the solution of momentum equations satisfy the continuity equation.

For a finite number of control volumes, a system of non-linear algebraic equations (Eq. 3.7) needs to be solved for dependent variables ($\phi$). The equations are coupled with more than one considerable variable in each equation. Due to the non-linearity, a segregated approach was implemented in this study to solve these equations. In this iterative solution approach, each equation for the substantial variable is decoupled by assuming other variables as known values. This method leads as a result to produce a sub-set of linearized algebraic equations for each dependent variable, reducing the storage requirements of the solution procedure. The coefficients $a_j$ and the source term $S_\phi$ in Eq. (3.7) are computed by using variable values from the previous result of the time step. A matrix form of the sub-set of linear equations can be written as:

$$A_\phi \phi = S_\phi$$

(3.9)

Where $A_\phi$ is the coefficient matrix and $\phi$ is a vector of the unknown variable.

After solving the linearized system of Eq. (3.9), the oscillation of the variable values over successive iterations could happen. Therefore, such divergence in the iteration process can be avoided by using an under-relaxation technique, which is described in the next subsection.
3.2.3.1 Under-relaxation

Under-relaxation promotes stability by slowing down the changes of variable values from the previous iteration \( \phi^{k-1} \) to the next iteration \( \phi^k \). This limitation ensures the convergence of the numerical solution, and this relaxation formula can be given as proposed by Patankar (1980):

\[
\phi^k = \phi^{k-1} + \alpha_\phi (\phi^{new} - \phi^{k-1})
\]  

(3.10)

Where \( \phi^{new} \) is the solution of Eq. (3.9) and \( \alpha_\phi \) is the under-relaxation factor (its values from 0 to 1). The implementation of this formula leads to modifying the central coefficient \( (a_p) \) and the source term of the discretised algebraic equation (Eq.3.7) as follows:

\[
a_p^* = \frac{a_p}{\alpha_\phi} , S_\phi^* = S_\phi + \frac{1-\alpha_\phi}{\alpha_\phi} a_p \phi_p^{k-1}
\]

(3.11)

Substituting Eq. 3.11 into Eq. 3.7, the modified equation will take the following linear form:

\[
a_p^* \phi_p = \sum_{j=1}^{n_l} a_j \phi_{p_j} + S_\phi^*
\]

(3.12)

As far as the under-relaxation factor is concerned, there are no general rules for choosing the best value of \( \alpha_\phi \). The optimum values depend upon a number of factors, such as the nature of the problems, the number of grid points, grid spacing, and iterative procedure used. Typically, a suitable value of this factor can be determined from the experience and from examining calculations for the given problem.
3.2.3.2 Convergence criterion

The monitor on the convergence of the numerical solution called a convergence criterion which was used in this study as the normalized sum of absolute residual values for all variables. The residual sum of any variable ($\phi$) at node ($P$) is defined as follows:

$$R_\phi = \sum_{i=1}^{M} \left| a^i P \phi_P - \sum_{j=1}^{M} a_j \phi_P - S^i \phi \right| / \sum_{i=1}^{M} |a^i P \phi_P|$$  \hspace{1cm} (3.13)

Improvements in the convergence properties require a good initialization in the early iterations, particularly for the transient mode applications. However, for any exact solution, the residual sum must be zero to satisfy the partial differential equations. But, for the nearly exact solution, this solution procedure provides sufficiently small residuals for all variables solved in the field. In the present study, the value of the residual sum is typically less than $10^{-4}$ for all variables in each control volume.
3.3 Mathematical models of gas combustion

The Computational Fluid Dynamics (CFD) code was used to model and analyse a 3-D computational domain system involving chemical reaction mechanism, radiative heat transfer, fluid flow, and turbulence parameters. The numerical simulations of non-premixed propane flame under an air-fired and two different oxy-fuel combustion conditions were carried out using a commercial CFD, AVL Fire ver.2008.2 code. Subroutines for the multi-step propane reaction were written in this study and incorporated into the CFD code. To illustrate the applications of CFD on the turbulent non-premixed gaseous combustion, it is important to define all the mathematical models used in this combustion study.

3.3.1 Flow field model

To model the turbulent non-premixed flame characteristics in the combustion of C\textsubscript{3}H\textsubscript{8}-O\textsubscript{2}/N\textsubscript{2} and C\textsubscript{3}H\textsubscript{8}-O\textsubscript{2}/CO\textsubscript{2} mixtures, the three-dimensional governing equations of mass conservation, momentum, and energy transport equations in the transient conditions have been solved in the Cartesian tensor form:

- Mass conservation equation

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \]  

(3.14)

- Momentum conservation equation

\[ \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} (\tau_{ij})_{\text{eff}} + \frac{\partial}{\partial x_j} (-\rho u_i u_j) \]  

(3.15)

- Energy transport equation

\[ \frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_i} [u_i (\rho E + P)] = \frac{\partial}{\partial x_j} \left( k_{ij} \frac{\partial T}{\partial x_j} + u_i (\tau_{ij}) \right) + S_\phi \]  

(3.16)

Where \( P \) is the pressure of fluid, \( u_i \) and \( u_j \) are the fluctuating velocity components in the \( i \)th and \( j \)th directions, respectively. \( \phi \) denotes enthalpy and concentration of species, while term \( S_\phi \) represents the appropriate source of the variables \( \phi \). The local density of
the mixture is dependent on pressure, reactants, products concentrations, and temperature and determined through the equation of state:

$$\rho = \frac{P}{RT \sum_{k} \frac{Y_k}{(MW)_k}}$$  \hspace{1cm} (3.17)

While the temperature values can be calculated from the enthalpy:

$$T = \frac{h - \sum_{k} Y_k \Delta h_{fu}}{c_p}$$  \hspace{1cm} (3.18)

The effective stress tensor and thermal conductivity are given by the following equations:

$$\left(\tau_{ij}\right)_{eff} = \mu_{eff} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right) - \frac{2}{3} \mu_{eff} \frac{\partial u_i}{\partial x_i} \delta_{ij}$$  \hspace{1cm} (3.19)

$$K_{eff} = K + \frac{c_p \mu_i}{\sigma_i}$$  \hspace{1cm} (3.20)

Fuel and feed oxidizer gases (air or O$_2$/CO$_2$ mixture) were non-premixed before entering into the furnace. Detailed information regarding the burner configuration and fluid flow conditions can be found in chapter four. In this numerical study, it was assumed that the swirls created by the primary and secondary registers for ensuring a perfectly mixed reactants. This is also used to avoid any external recirculation in the flame structure and to keep it in stable form during burning reactants.

### 3.3.2 Species transport model

In order to reduce the number of equations to be solved and to save the computational time, dimensional quantities are introduced in this study to express the reactive system. The mass fraction, residual gas mass fraction, and mixture fraction are given by (AVL Fire CFD Solver v 8.5 manual 2008) as follows:
Chapter 3- Mathematical Models and Modelling Techniques

\[ y_{fu} = \frac{m_{fu,u}}{m_{tot}} \]  
(3.21)

\[ g = \frac{m_{rg}}{m_{oxid}} \]  
(3.22)

\[ f = \frac{m_{fu,u} + m_{fu,b}}{m_{tot}} \]  
(3.23)

The solution of transport equations for the density weighted mean quantities \( y_{fu}, f, \) and \( g \) is illustrated in the following equations:

\[ \frac{\partial}{\partial t} (\rho y_{fu}) + \frac{\partial}{\partial x_i} (\rho U_i y_{fu}) = \frac{\partial}{\partial x_i} \left( \Gamma_{fu} \frac{\partial y_{fu}}{\partial x_i} \right) + S_{fu} \]  
(3.24)

\[ \frac{\partial}{\partial t} (\rho f) + \frac{\partial}{\partial x_i} (\rho U_i f) = \frac{\partial}{\partial x_i} \left( \Gamma_{f} \frac{\partial f}{\partial x_i} \right) \]  
(3.25)

\[ \frac{\partial}{\partial t} (\rho g) + \frac{\partial}{\partial x_i} (\rho U_i g) = \frac{\partial}{\partial x_i} \left( \Gamma_{g} \frac{\partial g}{\partial x_i} \right) \]  
(3.26)

In the simulation of the one-step reaction mechanism, the chemical reacting system consists of five species which are fuel (C₃H₈), O₂, CO₂, H₂O, and N₂. The mass fraction of these species can be computed in terms of the total mixture mass with the following algebraic expressions:

\[ y_{o_2} = a_1 \left[ (1 - f) - S(f - y_{fu}) \right] \]

\[ y_{N_2} = (1 - a_1)(1 - f) \]

\[ y_{pr} = 1 - y_{fu} - y_{o_2} - y_{N_2} \]

\[ y_{co_2} = a_2 y_{pr} \]

\[ y_{H_2O} = a_3 y_{pr} \]  
(3.27)
The parameters $a_i$ and $S$ are summarised in Table 3.1, while $n$ and $m$ represent the number of carbon and hydrogen atoms in the hydrocarbon fuel ($C_nH_m = C_3H_8$) and the molecular weights of the individual chemical species are expressed by $M_{fu}, M_{O_2}, M_{CO_2}$, and $M_{H_2O}$.

Table 3-1: Chemical and mathematical meanings of symbols in Eq. (3.27)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Chemical meaning</th>
<th>Mathematical meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_1$</td>
<td>Mass fraction of oxygen in air</td>
<td>0.232</td>
</tr>
<tr>
<td>$a_2$</td>
<td>Mass fraction of $CO_2$ in products</td>
<td>( \frac{n M_{CO_2}}{M_{fu} + M_{O_2} \frac{n+m}{4} a_1} )</td>
</tr>
<tr>
<td>$a_3$</td>
<td>Mass fraction of $H_2O$ in products</td>
<td>( \frac{m}{2} M_{H_2O} \frac{n+m}{4} a_1 )</td>
</tr>
<tr>
<td>$S$</td>
<td>Stoichiometric air/fuel ratio</td>
<td>( \frac{(n+m) M_{O_2}}{a_1 \cdot M_{fu}} )</td>
</tr>
</tbody>
</table>

Regarding the four-step chemistry reaction mechanism, seven species (fuel, $O_2$, $N_2$, $CO_2$, $CO$, $H_2$, and $H_2O$) were sufficiently considered to predict well the thermodynamic equilibrium temperatures and $CO/CO_2$ production rates, as well as the equilibrium between the $H_2$ and $H_2O$ in the flame zone. A simplified approach of the chemical equilibrium for propane oxidation processes has been modelled for both one-step and four-step reaction mechanisms.
3.3.3 Combustion model

The numerical simulation of the mean chemical reaction rates has been considered to be a main problem in the determination of chemical kinetic processes. This is due to reaction rate being non-linear functions of the local temperature values and species concentrations. Though it is better to use a detailed chemical kinetic mechanism, kinetic parameters are not computationally available to deal with thousands of elementary reactions and hundreds of intermediate radical species. For that reason, the fuel reaction process was initially modelled, in this study, by a one-step (single-step) reaction. Subsequently, the modelling of the four-step (multi-step) reaction mechanism was carried out to improve the predicted results with the measured data. However, the single-step irreversible reaction of a hydrocarbon fuel (C\textsubscript{3}H\textsubscript{8}) with air or O\textsubscript{2}/CO\textsubscript{2} mixtures was considered for these turbulent combustion processes, as explained in the following balance chemical equations with 15% excess air:

\[
C_{3}H_{8} + 5.75O_{2} \rightarrow 3CO_{2} + 4H_{2}O + 0.75O_{2}
\]  
(3.28)

While the multi-step reaction mechanism consists of two irreversible reactions for hydrocarbon oxidation processes and two reversible reactions to control the reaction rates for H\textsubscript{2} and CO, as follows:

\[
C_{3}H_{8} + 0.575O_{2} \rightarrow 3CO + 4H + 0.075O_{2}
\]  
(3.29)

\[
C_{3}H_{8} + 3H_{2}O \rightarrow 3CO + 7H_{2}
\]  
(3.30)

\[
2H_{2} + O_{2} \leftrightarrow 2H_{2}O
\]  
(3.31)

\[
CO + H_{2}O \leftrightarrow CO_{2} + H_{2}
\]  
(3.32)

In this numerical simulation, the modified turbulence controlled combustion model (Magnussen and Hjertager 1977), the Eddy Breakup (EBU) model, was used to calculate the mean reaction rates for these combustion simulations. The mean reaction rate can be written according to Magnussen and Hjertager as follows:

\[
\rho r_{f_{u}} = \frac{C_{fu}}{\tau_{r}} \rho \min \left( y_{fu}, \frac{\bar{y}_{O_{2}}}{S}, \frac{C_{pr} \bar{y}_{pr}}{1 + S} \right)
\]  
(3.33)
The turbulent mixing time scale ($\tau_m$) in the above reaction equation is proportional to the eddy breakup time and can be defined based on the turbulent kinetic energy to its dissipation rate. In the operator “\text{min}”, the three terms are simply used to control the mixing rate of chemical species. $C_{mu}$ and $C_{pr}$ are empirical coefficients, and the value of the $C_{mu}$ is dependent on turbulence and fuel parameters (Cant and Bray 1989; Nicolleau and Mathieu 1994). For that reason, several allowable values were tested in this study to adjust the appropriate values with the measured combustion data (Andersson 2007). The adjustments have been conducted on the air-fired combustion case at 384 mm from the burner exit plane, as illustrated in Figure 3-2.

![Figure 3-2: Effect of empirical coefficient ($C_{fu}$) of EBU combustion model on the turbulent reaction rate at 384 mm from burner exit plane in the air-fired combustion case.](image)

It can be seen that when the values of the coefficient ($C_{mu}$) increase from 3.0 to 9.0, the turbulent reaction rates are increased, particularly in the flame envelope zone. This
means that the gas temperature levels are gradually increased with the coefficient \( (C_{fu}) \) values with respect to the experimental data due to an intensification of the turbulent reaction rates. As can be seen that the value of coefficient \( (C_{fu}) \) of 6.0 was more appropriate for this turbulent reaction rate. The same procedure of calibration of the empirical coefficient \( (C_{fu}) \) was conducted (not repeated for brevity) for the oxy-fuel combustion cases. Therefore, under these special conditions of the combustion cases, \( C_{fu} \) and \( C_{pr} \) were kept 6.0 and 0.5, respectively for air-fired case. In contrast, for the oxy-fuel combustion cases, \( C_{fu} \) and \( C_{pr} \) were kept 3.0 and 0.5, respectively for the same above-mentioned reason. These values are within the range recommended in literature (Cant and Bray 1989; Nicolleau and Mathieu 1994). Detailed information related to the aforementioned mathematical model can also be found in the preliminary CFD papers (Al-Abbas et al. 2011; Al-Abbas and Naser 2012).

3.3.4 Turbulence model

The \( k-\varepsilon \) is a commonly accepted model for turbulence modelling, especially for industrial applications and is available in most CFD codes. In spite of numerous shortcomings that have been discovered over the past decade, it is generally accepted that the \( k-\varepsilon \) model usually yields reasonable and realistic predictions of major mean-flow features in most complicated situations. Fan et al. (2001) used RNG \( k-\varepsilon \) model as an alternative for standard \( k-\varepsilon \) model to predict flows with swirling flow and sharp change in the tangentially fired furnace. However, in this simulation, near-wall treatment is introduced (details in boundary condition section of chapter four) in order to predict the wall-bounded turbulent flows that can manipulate the swirling effect of primary and secondary registers in the near burner region with sufficient accuracy. The standard \( k-\varepsilon \) model can be described by Launder et al. (1974):

- Turbulent kinetic transport equations:

\[
\frac{\rho}{\partial t} + \rho U_j \frac{\partial k}{\partial X_j} = P + G - \varepsilon + \frac{\partial}{\partial X_j} \left( \mu + \frac{\mu_s}{\sigma} \frac{\partial k}{\partial X_j} \right) \tag{3.34}
\]

- Rate of dissipation of energy from the turbulent flow:
\[
\rho \frac{D \varepsilon}{Dt} = \left( C_{\varepsilon_1} P + C_{\varepsilon_3} G + C_{\varepsilon_4} k \frac{\partial U_k}{\partial X_k} - C_{\varepsilon_2} \varepsilon \right) \frac{\varepsilon}{k} + \frac{\partial}{\partial X_j} \left( \frac{\mu_t \partial \varepsilon}{\sigma_\varepsilon \partial X_j} \right)
\]  
(3.35)

Where:

\[
P = -2 \mu_t S : S - \frac{2}{3} \mu_t (tr S) + k \] (tr S)  
(3.36)

\[
G = - \frac{\mu_t}{\rho \sigma_\rho} \nabla \rho \]  
(3.37)

\[
\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \]  
(3.38)

Where \( P \) is the shear production, \( G \) is production due to the buoyancy force and \( \mu_t \) is the turbulent viscosity that is calculated from the solution of the transport equations for the turbulent kinetic energy and its dissipation rate. The standard values of the coefficients of Eqs. (3.34 – 3.38), which are used in this simulation, are tabulated in Table 3-2.

<table>
<thead>
<tr>
<th></th>
<th>( C_\mu )</th>
<th>( C_{\varepsilon_1} )</th>
<th>( C_{\varepsilon_2} )</th>
<th>( C_{\varepsilon_3} )</th>
<th>( C_{\varepsilon_4} )</th>
<th>( \sigma_k )</th>
<th>( \sigma_\varepsilon )</th>
<th>( \sigma_\rho )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.09</td>
<td>1.44</td>
<td>1.92</td>
<td>0.8</td>
<td>0.33</td>
<td>1</td>
<td>1.3</td>
<td>0.9</td>
</tr>
</tbody>
</table>
Chapter 3- Mathematical Models and Modelling Techniques

3.4 Mathematical models of coal combustion

Numerical simulation of pulverized dry lignite and brown coal under air-fired and O₂/CO₂ combustion environments was carried out by a commercial computational fluid dynamics (CFD), AVL Fire ver.2008.2 code. The CFD code was used to model and analyze the (3-D) computational domain system. Appropriate subroutines were written and coupled with the CFD code FIRE to account for chemical reactions (devolatilization and char burnout) and convective and radiative heat transfer models. CFD code FIRE can solve for fluid and particle flow fields (homogenous and heterogeneous) and turbulence. In this numerical simulation, a Lagrangian/Eulerian approach was employed for gas-solid two-phase fluid flow.

3.4.1 Gas phase model

The continuous turbulent flow of multicomponent gaseous phase is described by three-dimensional non-steady state Eulerian partial differential conservation equations (PDEs) for mass, momentum, turbulence kinetic energy, turbulent dissipation rate, enthalpy and a number of species mass fractions. The heat transfer (convection and radiation), turbulence, coal particle temperatures and trajectories, coal devolatilization and char combustion models are coupled through the sub-models of source terms of PDEs. The general form of Eulerian transport equation used is (Patankar and Spalding 1972):

$$
\frac{\partial}{\partial t} (\rho \Phi) + \frac{\partial}{\partial x_i} (\rho U_i \Phi) = \frac{\partial}{\partial x_i} \left( \Gamma \frac{\partial \Phi}{\partial x_i} \right) + S_\phi + S_{\rho \phi}
$$

(3.39)

where, $\rho$ is the gas density, $x_i$ is the spatial distance in the $i^{th}$ direction, $\Gamma$ is the diffusion coefficient of the variable $\Phi$, $S_\phi$ is a source term for the variable $\Phi$, and $S_{\rho \phi}$ is the additional source term due to the exchange between the gas and the coal particles. While additional sources for $k$ and $\varepsilon$ are used to calculate the effect of particle-to-gas turbulence flow.
3.4.2 Particulate phase model

The particulate (Lagrangian) phase is modeled by using the Discrete Droplet Method (DDM) (Dukowicz 1980). This DDM has been widely used in modeling the low rank coals combustion. The particle is generally assumed to be spherical in shape in which each group of identical non-interacting particles termed parcels. This method operates by introducing the particle parcels in the flow domain, and then they are tracked through the computational grid used. Equations are solved for the exchange of momentum, heat and mass transfer between particles and gas phase.

The differential equations for a solid particle can be written as:

\[
m_p \frac{d u_{id}}{dt} = \vec{F}_{idr} + \vec{F}_{ig} + \vec{F}_{react}
\]  \hspace{1cm} (3.40)

The left side of the equation describes the particle mass multiplied by the inertia of the particle phase, while the right side illustrates the magnitudes of all external forces that are acting on the particle phase.

Where

\[
\vec{F}_{idr} = \frac{1}{2} \cdot \rho_p \cdot A_p \cdot C_D \cdot |u_{rel}| \cdot u_{rel}
\]

is the drag force, \(C_D\) is the drag coefficient which is based on the formulation of Schiller and Naumann (1933). The accurate value of drag coefficient is considered as a function of the Reynolds number and the cross-sectional area of the particle \(A_p\). The relative velocity is calculated by considering the gas velocities and particle velocities. \(\vec{F}_{ig} = V_p \cdot (\rho_p - \rho_g) g_i\) is the gravitational force calculated based on the density difference between the particle and the gas phase.

\[
\vec{F}_{react} = V_p \cdot \left( -\frac{m_{vp}}{dt} \right)
\]

is the reaction force exerted on the coal particle and \(m_{vp}\) is the mass of coal particles when devolatilization process occurs. The reaction force is small compared to the drag and gravitational forces, but it has some influence on the particle trajectory. The direction of reaction force is determined by stochastic means.
3.4.3 Coal combustion models

The numerical simulation of raw coal combustion is considered as a complex process compared with the combustion of others fossil fuel sources because it includes several complicated physical and chemical processes, which have not been completely understood. The basic steps of coal combustion are thermal decomposition and the consequent burnout of the volatile matter and the oxidation of char to leave the incombustible ash as a final undesirable part. The physical properties (proximate and ultimate analysis) of German Lignite and Victorian brown coal, used in the present study are summarized in Tables 3-3 and 3-4, respectively.

Table 3-3: The physical properties (proximate and ultimate analysis) of lignite coal particle.

<table>
<thead>
<tr>
<th>Proximate analysis (wt %, as received)</th>
<th>VM (%d.a.f)</th>
<th>Ultimate analysis (wt %, d.a.f.)</th>
<th>HHV (MJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ash, Combustibles, Moisture Fraction</td>
<td>59.4</td>
<td>C 69.9, H 5.4, O 23.1, N 0.6, S 1.0</td>
<td>20.9</td>
</tr>
<tr>
<td>5.0, 84.8, 10.2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3-4: The physical properties (proximate and ultimate analysis), specific energy, and moisture content of Latrobe brown coal particle.

<table>
<thead>
<tr>
<th>Proximate analysis (%wt, db)</th>
<th>Ultimate analysis (%wt, db)</th>
<th>Specific energy (MJ/kg)</th>
<th>Moisture content (M.C.) (%wt, ar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed carbon, Ash content, Volatile content</td>
<td>C 67.7, H 4.63, N 0.52, S 0.3, Minerals &amp; Inorgs 1.89, O 24.96</td>
<td>Gross dry 27.6, Net wet 8.8</td>
<td>62.0</td>
</tr>
</tbody>
</table>
3.4.3.1 Coal combustion gas phase

The numerical modeling of coal combustion was carried out using a particle transport calculation for the coal particles coupled with the Eulerian transport equations for the combustion of the volatile gases and char. The effect of turbulence in the chemical processes of finite rate chemistry of combustion is widely described by Molemaker and VilÀ-Guerau de Arellano (1998). In the gas phase, the instantaneous mass fraction of product \( y_{pr} \) can be calculated according to the volatile \( y_v \), oxidant \( y_{ox} \) and char \( y_c \) mass fractions as follows:

\[
y_{pr} = 1 - y_v - y_{ox} - y_c
\]  

(T3.41)

Turbulence controlled combustion model, Eddy Breakup (EBU) model, is used for these combustion simulations. The Eddy Breakup model is a popular and an efficient model in combustion calculation, which was firstly proposed by Spalding (1971) and modified later by Magnussen and Hjertager (1977). The mean reaction rate used in this study was early described and can be found in section 3.2.3 with full details.

3.4.3.2 Coal combustion particle phase

The combustion of dry coal particles mainly includes two complex reaction processes. The first reaction process is the devolatilization of the dry coal particle, which includes the reaction of the released hydrocarbon fuel (volatile) with the oxygen to produce essentially the water vapor \( (H_2O) \) and carbon dioxide \( (CO_2) \) as final products. This reaction process can be conducted by either single-step or multi-step chemical reaction mechanisms. The complete description of these chemistry mechanisms will be given in the next section. The second reaction process is the oxidation of the residual char which is slower than the devolatilization process.

1-Devolatilization

In the present simulation, the single reaction model of Badzioch and Hawksley (1970) (Badzioch and Hawksley 1970) is applied to simulate the coal pyrolysis. The coal is considered, in this model, to have fixed fraction of volatile matters, char and ash, and its
reaction depends on the local temperature experience, as well as its temperature history. The rate of production of the volatile is given by the first order reaction as follows:

\[
\frac{dV}{dt} = K_v \left( V_f - V \right)
\]  

(3.42)

Where \( V \) is the product of volatiles that have already released from unit mass of pulverized coal at time \( t \), \( V_f \) is the ultimate product of volatiles and \( K_v \) is the rate constant given by the Arrhenius form as: \( A_v \exp\left( -\frac{E_v}{T_p} \right) \), where \( T_p \) is the temperature of coal particle, \( A_v \) and \( E_v \) are the pre-exponential factor (s\(^{-1}\)) and the activation energy (J kmol\(^{-1}\).K\(^{-1}\)) constants, respectively, that are determined experimentally for the particular coal. These factors are usually obtained from the proximate analysis of the coal.

The appropriate selection of the kinetic factors of Arrhenius expression can be considered as a key issue towards the appropriate prediction of devolatilization rate, particularly in the near burner region (Badzioch and Hawksley 1970; Lockwood et al. 1998). Therefore, the devolatilization kinetic factors of the specific lignite were chosen to be \( 0.2 \times 10^5 \) (s\(^{-1}\)) and 5941 (J.kmol\(^{-1}\).K\(^{-1}\)) for the pre-exponential factor and for the activation factor (Anthony 1975), respectively, in order to overcome any difficulties during setting up the simulation cases and to get optimum agreement with the available physical data.

II-Char oxidation

The char oxidation rate is an important process in pulverized coal combustion. After the devolatilization, the remaining char in the coal particle reacts slowly with the surrounding gases. Therefore, the burnout time of the pulverized coal can be determined in the furnace by this process (Smith 1983).

Due to the complexity of the carbon–oxygen reaction mechanism, in this study, the char combustion is modelled by a global reaction of order unity (global power-law), which
was proposed by Field et al. (1967). The global power-law (one-step) and semi-global (two-step) Langmuir-Hinshelwood models cannot precisely capture the effect of the temperature and oxygen partial pressure dependency on the char combustion kinetics and CO/CO$_2$ production rate (Hurt and Calo 2001). Therefore, Hurt and Calo modelled three-step semi-global kinetics and enhanced three-step semi-global kinetics models for char combustion process to yield intrinsic kinetics data over a range of complex combustion conditions. Nikolopoulos et al. (2011) has recently implemented a three-step semi-global intrinsic kinetic model in the numerical code. They used three different combustion cases: air-fired (reference), partial oxy-fuel, and full oxy-fuel conditions in a large-scale boiler for a low-rank coal (lignite).

In the present heterogeneous reaction, the oxidation rate of the char is governed by the diffusion of oxygen to the particle’s external surface and by the effective char reactivity. Therefore, it is considered as more suitable reactive model with respect to other char oxidation models, especially for low-rank coal that has high porosity and surface area as described in the comprehensive book by Gronhovd (1982). The diffusion rate of oxygen is calculated by $K_d (P_g - P_s)$, where $P_g$ is the partial pressure of oxygen in the bulk phase of the furnace (far from particles boundary layer), $P_s$ is the oxygen partial pressure at the external surface of the particle and $K_d$ is expressed by the following equation (Baum and Street 1971):

$$K_d = \frac{2.53 \times 10^{-7}}{R_p} \left( \frac{T_p + T_g}{2} \right)^{0.75} \frac{P_A}{P}$$  \hspace{1cm} (3.43)

Where: $R_p$ is the radius of the particle, $T_p$ is the temperature of the particle, $T_g$ is the gas temperature in the far field, and $P_A$ and $P$ are the atmospheric and local pressure respectively. While the rate of char oxidation per unit area of the particle surface is described by $K_c P_s$. The kinetic rate is expressed by the following Arrhenius expression:

$$K_c = A_c \exp \left( -\frac{E_c}{T_p} \right)$$  \hspace{1cm} (3.44)
Where: $A_c$ is the pre-exponential factor (kg. m$^{-2}$. s$^{-1}$. (N.m$^{-2}$)) and $E_c$ is the activation energy (J kmol$^{-1}$.K$^{-1}$). Due to the lack of measured char reactivity data, the recommended values by Ref. (Wall 1976) are used for $A_c$ and $E_c$ in this simulation, which are 497 (kg . m$^{-2}$. s$^{-1}$. (N.m$^{-2}$)) and 8540 (J kmol$^{-1}$.K$^{-1}$), respectively. Finally, the rate of the overall char reaction of a particle can also be written as follows

$$\left(\frac{1}{K_d^{-1} + K_c^{-1}}\right) P_A 4\pi R_p^2 \frac{P}{P_A}$$

and can be controlled by the smaller rates of $K_d$ and $K_c$.

### 3.4.4 Heat transfer models

#### 3.4.4.1 Radiative heat transfer

In order to account for the radiative heat transfer in the overall computational domain, the discrete transfer radiation method (DTRM) that is present by Lockwood and Shah (1981) has shown to be a very appropriate method in many industrial applications such as furnaces (Lockwood and Shah 1981), which is used in this work. The radiation transfer equation (RTE) is very convenient to describe the radiation phenomena in participating media (specific internal cells) due to the sum of contribution of all rays crossing the cell. The main assumption of DTRM is that a single ray can approximate the intensity through a solid angle. This is meaning that the number of rays and their directions, which is chosen in (RTE), is solved for each ray on its way from boundary to boundary. The general basis of this method is that the absorption coefficient and the temperature are assumed constant within a single cell (control volume). However, the total radiation intensities at intersections of a ray with control volume faces can be calculated over the entire spectrum as follow (Versteeg and Malalasekera 2007):

$$i_{n+1} = i_n (1 - \varepsilon(T,x_i)) + i_b(T)\varepsilon(T,x_i)$$  \hspace{1cm} (3.45)

where $i_b = \sigma T_g^4 / \pi$ is the directional blackbody emissivity in the control volume, $\sigma$ is the Stephan-Boltzmann constant that is equal to 5.67 $10^{-8}$ W/m$^2$K$^4$, and $\varepsilon(T,x_i)$ represents the emissivity and depends upon the local temperature and gas mixture. Thus
the gas mixture emissivity can be represented through the Weighted Sum of Gray gases Model (WSGGM) (Smith et al. 1982) as given in the following equation:

\[ \varepsilon(T, x_i) = \sum_{j=1}^{i+1} \alpha_{x,i}(T) \left(1 - e^{-a_i p B x_i} \right) \]  (3.46)

where \( \alpha_{x,i}(T) \) is the emissivity weighting factor for the \( i \)th gray gas, \( S \) is the path length, \( a_i \) is the absorption coefficient of the gas mixture, and \( p \) is the sum of the partial pressures (mass concentrations) of absorbing species such as H\(_2\)O and CO\(_2\). The weighting factors are usually given by polynomials of order \( J \) in the following form:

\[ \alpha_{x,i}(T) = \sum_{j=1}^{J} b_{x,i,j} T^{j-1} \]  (3.47)

The absorbing model selected (WSGGM) in this study, for a large-scale furnace, is of great importance for the gas radiation calculation, particularly in oxy-fuel combustion scenarios due to the higher increase of the species concentrations (H\(_2\)O and CO\(_2\)) in the flue gas (Edge et al. 2011; Zhou and Moyeda 2010). The number of gray gases used in this absorbing model was three, and third order polynomials of weighting factors were used.

Nozaki et al. (1997) revealed that the good evaluation of the radiation characteristics of the radiating gas components CO\(_2\) and H\(_2\)O can definitely improve the prediction accuracy, particularly in the centreline of the furnace. Thus, in this study, in lab-scale furnace, the absorption coefficient of the gas phase is assumed to have a uniform value of 0.24 m\(^{-1}\) (Andersson 2007) for air-fired and 0.31 m\(^{-1}\) (Andersson 2007) for oxy-fuel combustion cases instead of using the WSGGM that led to underestimating in the temperature value along the furnace axis. However, these values of the absorption coefficients of gases are evaluated according to the average gas temperature of experimental results (Andersson 2007).

The accuracy of the (DTRM) depends upon surface discretisation and angular discretisation. Therefore, all geometrical information related to the rays and their intersections with control volumes (cells) must be calculated and stored before starting the radiation calculation. Finally, in order to ensure a more accurate solution in the
discrete transfer radiation method and computational cost, the raytracing parameters are selected to be (2) for the number of polar divisions and (8) for the number of Azimuthal divisions in this simulation.

3.4.4.2 Heat and mass transfer

In this section, the additional source term for particle-gas coupling in Eq. (3.39), representing the energy gain or loss between the particles and gases due to the heat transfer processes is explained. The two heat transfer processes: convection and radiation, used to estimate the rate of change of temperature between the particles and gases inside the combustor are explained. The convective heat transfer between the particle and gas is accounted for using the equation:

\[ Q_c = \pi D_p \lambda N_u (T_g - T_p) \]

(3.48)

Where \( D_p \) is the diameter of the particle, \( \lambda \) is the thermal conductivity, \( T_g \) and \( T_p \) are the temperature of the gas and particle, respectively, and \( N_u \) is the Nusselt number given by Ranz and Marshall (1952):

\[ N_u = 2 + 0.6 \text{Re}_p^{0.5} \text{Pr}^{0.33} \]

(3.49)

Where \( \text{Re}_p \) is the particle Reynolds number and \( \text{Pr} \) is the Prandtl number.

While, the radiative heat transfer between the particle and gas is given by the following equation:

\[ Q_r = \varepsilon \sigma \pi D_p^2 \left( T_g^4 - T_p^4 \right) \]

(3.50)

Where \( \varepsilon \) is the particle emissivity.

In CFD studies, the emissivity of particle is an important property for calculating the radiative heat transfer from combustion gases and particles. Several studies (Chui et al. 1993; Rego-Barcena et al. 2007) have been conducted for measuring particle emissivity in a gas-particle medium. These studies revealed that the particle emissivity vary
between the emissivity of unburned carbon (1.0) and fly ash (0.6). As a result, the recommended value of emissivity from Achim et al. (2009) is used in this study, where $\varepsilon = 0.7$. 
3.5 Chemistry reaction mechanisms

In this section, eight species fuel (volatile and char), O2, N2, CO2, CO, H2, and H2O were considered and taken into account in one- (single-), two-, and three-step chemical reactions. Although, there were some good predictions in term of temperature distributions and species concentrations in a single-step reaction, some discrepancies were visible in those numerical results against the experimental data (Al-Abbas et al. 2011). As described previously, those discrepancies in the predicted results might have been caused due to the usage of a single-step chemical reaction. Therefore, it is appropriate to consider these species, especially in the flame envelope zone (hottest region in the furnace) in order to predict the important intermediate species such as CO and H2, and the thermodynamic equilibrium temperature accurately enough. In addition, the one-step chemical mechanism used to describe the fuel conversion cannot capture the CO2/CO ratio and the equilibrium between H2 and H2O (Al-Abbas and Naser 2012). Moreover, regarding the char burn-out, these multi-step chemical reaction mechanisms can provide good information to clarify the connection of the order of reaction of char combustion rate and the CO/CO2 production rate with the temperature and oxygen partial pressure (Hurt and Calo 2001; Nikolopoulos et al. 2011).

3.5.1 Single-step chemical reaction

The one-step irreversible reaction of solid fuel (lignite) with air or O2/CO2 was considered in term of a hydrocarbon fuel (CnHm) and residual char (C_char) for all the combustion cases. For coal combustion, there are two main reaction processes. The first process is homogenous reactions of volatile matter (VM). In this reaction, methane (CH4) is considered as a sample of the hydrocarbon fuel because there are no crucial differences could be distinguished between methane and other released gases during the thermal decomposition process of coal particles (Lockwood et al. 1998). The second process is heterogenous reaction of residual char particles. During the oxy-fuel combustion, the following chemical equations were considered as shown below:
The chemical equation for devolatilized methane burned with oxygen (homogenous phase) can be expressed as follows:

\[ \text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} \] (3.51)

The chemical equation for char burned with oxygen (heterogenous phase) can be expressed as follows:

\[ \text{C}_{\text{char}} + \text{O}_2 \rightarrow \text{CO}_2 \] (3.52)

The heats of combustion (\(\Delta H\)) of the methane and residual char are considered and taken into account of the combustion model that are equal to -802310 kJ/kmol. and -393520 kJ/kmol., respectively.

### 3.5.2 Two-step chemical reaction

Due to the limitation of single-step reaction mechanism on the important intermediate species (CO) and flame temperature, two-step reaction mechanism can be partially provided information on the carbon monoxide (CO) in the hydrocarbon reaction and the char burn-out schemes which are based on the following reactions:

The chemical equation for devolatilized methane burned with oxygen can be expressed in the two chemical reactions:

\[ \text{CH}_4 + 3/2\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2\text{O} \] (3.53)

\[ \text{CO} + 1/2\text{O}_2 \leftrightarrow \text{CO}_2 \] (3.54)

While, the chemical equation for char burned with oxygen can be expressed in the two chemical reactions:

\[ \text{C}_{\text{char}} + 1/2\text{O}_2 \rightarrow \text{CO} \] (3.55)

\[ \text{CO} + 1/2\text{O}_2 \leftrightarrow \text{CO}_2 \] (3.56)
An outcome from this work is that the reverse chemical reactions of Eqs. (3.54) and (3.56) have a significant effect on the equilibrium concentration of CO and the heat release intensity in the flame envelope, which is considered the higher temperature level inside the furnace. The heats of reaction of first and second equations in the two-step reaction scheme are 307880 kJ/kmol and -1110190 kJ/kmol, respectively. These aforementioned chemical reactions have been widely used by a number of numerical simulation Refs. (Choi et al. 2009; Dupont et al. 1993; Frassoldati et al. 2005; Tian et al. 2010).

3.5.3 Three-step chemical reaction

As previously stated, the flame envelope zone is considered the higher temperature region compared to other locations inside the furnace. As a result, the dissociation of the main gaseous product (water vapour and carbon dioxide) into many radical species (carbon monoxide and hydrogen) in the flame region should be taken into account during the numerical modelling of both the homogenous and heterogenous reactions of the pulverized coal particles. Three-step reaction mechanism has the ability to predict well these species (CO and H₂), as well as the aforementioned main species. Therefore, the devolatilized hydrocarbon fuel (methane) and residual char (C_char), in this reaction mechanism, are presented in three-step chemical reaction in order to accurately explain the dissociation processes, as illustrated in the following chemical equations:

The chemical equation for devolatilized methane burned with oxygen can be expressed in the three chemical reactions:

\[ \text{CH}_4 + \text{O}_2 \rightarrow \text{CO} + \text{H}_2 + \text{H}_2\text{O} \]  \hspace{1cm} (3.57)

\[ \text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 \] \hspace{1cm} (3.58)

\[ \text{O}_2 + 2\text{H}_2 \leftrightarrow 2\text{H}_2\text{O} \] \hspace{1cm} (3.59)

The heats of reaction of first, second, and third chemical equations in the three-step reaction scheme are 549710 kJ/kmol, -868360 kJ/kmol, and -483660 kJ/kmol, respectively. Regarding the char burn-out, due to increasing carbon dioxide (CO₂)
concentration (partial pressure) in the flue gas, particularly in oxy-fuel combustion cases, the effect of Boudouard reaction is of great importance under oxy-fuel combustion promoting. Therefore, further char reaction with CO$_2$ should be taken into consideration in the numerical model, as shown in Eq. (3.61) (that represents Boudouard reaction, $\Delta H=172464$kJ/Kmol.). In contrast, Eq. (3.60) is only relevant for air-fired case. Although, the gasification process of coal particles has lower importance on the char reaction (i.e., heat of combustion, $\Delta H=131298$kJ/Kmol.) for both air-fired and oxy-fuel combustion cases, Eq. 3.62 is also presented and taken into consideration in order to increase the certainty of accuracy of the present simulation. Detailed information of the final char reaction (Eq. 3.62) can be found in the recent numerical simulation work of Erfurth et al. (2009).

The chemical equation for char burned with oxygen can be expressed in the three heterogenous chemical reactions:

$$C_{\text{char}} + \frac{1}{2}O_2 \rightarrow CO \quad (3.60)$$

$$C_{\text{char}} + CO_2 \rightarrow 2CO \quad (3.61)$$

$$C_{\text{char}} + H_2O \rightarrow CO + H_2 \quad (3.62)$$

The heats of combustion ($\Delta H$) of the above-mentioned species are taken into account and incorporated as a source term in the enthalpy equation for all combustion cases as separate subroutines, and as was used in the similar simulation effort of Nikolopoulos et al. (2011).
3.6 Nitric oxide (NO\textsubscript{x}) modelling

Generally, the nitric oxide (NO\textsubscript{x}) formation can be simulated via three principal sources: Thermal NO that is formed by the dissociation of the molecular air-nitrogen, Prompt NO that is formed from the attack of hydrocarbon fragments on the air-nitrogen, and Fuel NO that is formed from nitrogen containing components in the coal for both the volatile matter and residual char. In the present study, the only main sources of NO\textsubscript{x} formation (Thermal NO and Fuel NO) were used, whilst the Prompt NO formation was ignored because it is only important at low temperature (below 1000 K), and in fuel-rich mixtures (Díez et al. 2008). For a realistic turbulent combustion model of NO\textsubscript{x} formation in reactive system, a simplified approach of the chemical kinetics is more appropriate than other approaches (i.e. such as detailed chemistry and advanced engineering correlations) due to the complexity of the interacting processes such as turbulence, heterogenous reactions, heat transfer, etc. Therefore, this simplified approach used in the model for NO\textsubscript{x} formation must be considered for complex combustion applications, particularly furnaces, thereby there is no loss in the essential information due to the reduction path (Maas and Pope 1992).

3.6.1 Thermal NO formation

The NO\textsubscript{x} model involved solving three extra transport equations for the mass fraction of NO, HCN, and NH\textsubscript{3} as source term values (kg/m\textsuperscript{3}sec) in Eq. (3.39) as \( S_{NO}, S_{HCN}, \) and \( S_{NH3} \) respectively. Regarding thermal NO formation, the extended Zeldovich mechanism is used and modelled as follows:

\[
\begin{align*}
N_2 + O & \rightleftharpoons NO+N \quad (3.63) \\
N + O_2 & \rightleftharpoons NO+O \quad (3.64) \\
N + OH & \rightleftharpoons NO+H \quad (3.65)
\end{align*}
\]

Thermal NO reaction mechanism is defined based on the chemical equilibrium assumption, which means that only atomic nitrogen (N) is used as an extra intermediate species. Eq. (3.63) and Eq. (3.64) were firstly proposed by Zeldovich and extended later to include Eq. (3.65) in order to take into account the hydrogen radical’s effect on the
nitric oxide formation during the oxidation processes at near-stoichiometric conditions. This reaction mechanism is called the extended Zeldovich mechanism, which is strongly dependent on the flame temperature. The net rate of NO formation via Eqs. (3.63-3.65) can be given as follows:

\[
\frac{dc_{NO}}{dt} = K_{1f} c_O c_{N_2} + K_{2f} c_N c_{O_2} + K_{3f} c_N c_{OH} - K_{1b} c_{NO} c_N - K_{2b} c_{NO} c_O - K_{3b} c_{NO} c_H
\]

(3.66)

where \( c \) is the concentration of the species in mol/m\(^3\), \( K_{1f}, K_{2f}, K_{3f} \) are the kinetic rate constants for the forward reactions and \( K_{1b}, K_{2b}, K_{3b} \) are the kinetic rate constants for the backward (reverse) reactions.

The expressions of the kinetic rate constants (m\(^3\)/kmol. sec) used in the thermal NO formation are given according to Hanson and Salimian (1984) as follows:

\[
K_{1f} = 1.8 \times 10^{11} e^{-319.023917 \times 10^{-6}/RT},
K_{2f} = 1.8 \times 10^{10} e^{-38.914388 \times 10^{-6}/RT},
K_{3f} = 7.1 \times 10^{10} e^{-173.1060162 \times 10^{-6}/RT},
K_{1b} = 3.8 \times 10^{10} e^{-3.53362425 \times 10^{-6}/RT},
K_{2b} = 3.81 \times 10^{10} e^{-173.1060162 \times 10^{-6}/RT},
K_{3b} = 1.7 \times 10^{11} e^{-204.2019096 \times 10^{-6}/RT}
\]

(3.67)

In the fuel-lean zones, a quasi-steady state consumption and formation of free nitrogen atoms can be established, particularly when there is an adequate amount of oxygen in the combustion zones. Therefore, the overall NO formation rate for the three above-mentioned equations (Eqs. 3.63-3.65) can be written as follows:

\[
\frac{dc_{NO}}{dt} = 2 K_{1f} c_O c_N \frac{1 - \frac{K_{1b} K_{2b} c_{NO}^2}{K_{1f} c_{N_2} K_{2f} c_{O_2}}}{1 + \frac{K_{1b} c_{NO}}{K_{2f} c_{O_2} + K_{3f} c_{OH}}}
\]

(3.68)

It could be seen that, in Eq. (3.68), the thermal NO formation is completely independent on the coal as a fuel, but it is strongly dependent on the oxygen atoms (oxygen radicals)
concentrations. Therefore, the precise calculation of the concentration of oxygen atoms is of most importance, particularly with increasing the latter in the combustion zones. All species concentrations in Eq. (3.68), except concentrations of the oxygen atoms, are obtained from the combustion simulation. However, the overall NO formation rate mechanism is slow compared to the fuel oxidation processes (Zeldovich et al. 1947), and as a result the thermal NO is formed after carrying out of combustion process. Therefore, the thermal NO formation mechanism can be decoupled from the fuel oxidation processes, and the concentrations of oxygen atoms can be calculated by either the equilibrium approach or the partial equilibrium approach. The partial equilibrium approach is used, in this simulation, according to the recommended Refs. (Ishii et al. 2000; Peters and Weber 1997), where it was noticed that, in turbulent diffusion flames, the concentrations of oxygen radicals were not in equilibrium with the oxygen molecules. The partial equilibrium oxygen atom concentration can be given by the following expression:

$$c_o = 36.64 \times T^{0.5} \times e^{\frac{271235}{T}}$$  (3.69)

Where all species concentrations are giving in mol. m\(^{-3}\) and T is in Kelvin.

### 3.6.2 Fuel NO formation

The fuel nitrogen (fuel-bound nitrogen-containing compounds) in the coal via both the volatile matter and the char can be contributed to the total NO\(_x\) formed during the reaction pathways. Although, the route leading to the formation/destruction of fuel NO\(_x\) is still under investigating, the conversion of the fuel nitrogen to NO is highly dependent on two main concepts: the initial nitrogen-containing compounds concentration and the local combustion characteristics. Generally, during the devolatilization process of the pulverized coal particles several secondary intermediate nitrogen species are released into the gas phase such as hydrogen cyanide (HCN), ammonia (NH\(_3\)), nitrogen atom (N), etc. The first two aforementioned species (HCN and NH\(_3\)) are commonly considered the most dominant species from the thermal decomposition of the coal particles in the reaction zone. Therefore, the global simplified fuel NO formation/destruction pathways are presented and taken into
consideration in this numerical calculation, as shown in the schematic diagram of Figure 3-3.

As stated earlier, the routes leading to fuel NO formation/destruction are under development, and they are still not completely understood due to the complexity of the reaction, in real life reaction, that might take place through several chemical intermediate routes. However, the following five simplified models of oxidation and reduction processes (R₁-R₅) can sufficiently simulate the NOₓ model, which used in many similar calculation studies (Díez et al. 2008; Nikolopoulos et al. 2011; Stanmore and Visona 2000):

\[
\text{HCN} + 1.25 \text{O}_2 \rightarrow \text{NO} + \text{CO} + 0.5\text{H}_2\text{O} \quad (3.70)
\]

\[
\text{HCN} + 1.5 \text{NO} \rightarrow 1.25\text{N}_2 + \text{CO} + 0.5\text{H}_2\text{O} \quad (3.71)
\]

\[
\text{NH}_3 + 1.25 \text{O}_2 \rightarrow \text{NO} + 1.5\text{H}_2\text{O} \quad (3.72)
\]

\[
\text{NH}_3 + 1.5 \text{NO} \rightarrow 1.5\text{N}_2 + 1.5\text{H}_2\text{O} \quad (3.73)
\]

\[
\text{C}_{\text{char}} + \text{NO} \rightarrow 0.5\text{N}_2 + \text{CO} \quad (3.74)
\]
As for the above reactions mechanism, Eqs. (3.70-3.73) represent the oxidation and reduction processes, and the depletion rates of HCN and NH$_3$ are given below according to De Soete (1975). Whilst Eq. (3.74) represents an additional heterogeneous reduction of NO to N$_2$ due to reacting between the char particles and the nitric oxide, and its reaction rate is approximately equivalent to the carbon consumption rate that is given by Levy et al. (1981):

\[ R_1 = 1.0 \times 10^{10} \times X_{HCN} \times X_{O_2} \times e^{\left(\frac{-33730.829}{T}/F\right)} \]
\[ R_2 = 3.0 \times 10^{12} \times X_{HCN} \times X_{NO} \times e^{\left(\frac{-30206.713}{T}/F\right)} \]
\[ R_3 = 4.0 \times 10^{16} \times X_{NH_3} \times X_{O_2} \times e^{\left(\frac{-16110.247}{T}/F\right)} \]
\[ R_4 = 1.8 \times 10^{08} \times X_{NH_3} \times X_{NO} \times e^{\left(\frac{-13593.021}{T}/F\right)} \]
\[ R_5 = 4.8 \times 10^{04} \times e^{\left(\frac{-3470}{RT}\right)} \times A \times P_{NO} \]  \hspace{1cm} (3.75)

where $R_{1-4}$ are the conversion rates of Eqs. (3.70-3.73) in units equal to s$^{-1}$, $X$ is the mole fraction of the aforementioned species in mol.m$^{-3}$, $R_5$ is the coefficient rate for the NO/char reaction in mol. s$^{-1}$, $A$ is the external surface area of the char, which is equal to about 20.3 m$^2$/gmol in this study, $P_{NO}$ is the bulk pressure of nitric oxide in atmospheric, and $a$ is the oxygen reaction order that is derived based on oxygen mole fraction in the flame as given in the following mathematical expression:

\[ a = \begin{cases} 1.0 & X_{O_2} \leq 4.1 \times 10^{-03} \\ -3.95 - 0.9 \ln X_{O_2} & 4.1 \times 10^{-03} \leq X_{O_2} \leq 1.11 \times 10^{-02} \\ -0.35 - 0.1 \ln X_{O_2} & 1.11 \times 10^{-02} < X_{O_2} < 0.03 \\ 0 & X_{O_2} \geq 0.03 \end{cases} \]  \hspace{1cm} (3.76)

The source terms of NO, HCN, and NH$_3$ must be incorporated in the transport equation for predicting fuel NO formation, as given in the following expressions:

\[ S_{HCN} = S_{HCN,P} + S_{HCN,1b} + S_{HCN,2b} \]
\[ S_{NH_3} = S_{NH_3,P} + S_{NH_3,1b} + S_{NH_3,2b} \]
\[ S_{NO} = S_{char,NO} + S_{NO,1} + S_{NO,2} + S_{NO,3} \]  \hspace{1cm} (3.77)
Based on the literature information of the NO\(_x\) formation mechanism (Díez et al. 2008; Nikolopoulos et al. 2011; Xu et al. 2000), as for the gas-solid reaction, coal-nitrogen is supposed to be equally divided by the volatile matter and the char, and its amount is usually obtained from the proximate analysis of the coal. The nitrogen bound of the char is directly converted to NO; whilst a fraction of nitrogen in volatile is commonly released in a mixture of NH\(_3\) and HCN with a ratio (\(\alpha\)) of 9:1 to NH\(_3\)/HCN. This ratio (\(\alpha\)) of the intermediate nitrogen compounds released in the devolatilization stage is only applicable for low-rank coal, lignite and brown coal in this study. This means that the production level of NH\(_3\) is higher by approximately 10 times than HCN that could provide better numerical results of NO\(_x\) formation. In the subbituminous coals and lignite (brown coal), NH\(_3\) was a dominant species; while HCN was a dominant species from bituminous coal (Zheng 2011). Therefore, the above-mentioned ratio is presented and taken into account in the source terms of production rates of HCN and NH\(_3\) as shown in below:

\[
\begin{align*}
S_{HCN,p} &= \frac{(1-\alpha) \times S_{vol} \times Y_{N,fuel} \times M_{HCN}}{M_N \times \Delta V} + \frac{S_{char} \times Y_{N,fuel} \times M_{HCN}}{M_N \times \Delta V} \\
S_{NH3,p} &= \frac{\alpha \times S_{vol} \times Y_{N,fuel} \times M_{NH3}}{M_N \times \Delta V} + \frac{S_{char} \times Y_{N,fuel} \times M_{NH3}}{M_N \times \Delta V}
\end{align*}
\]

(3.78)

where \(S_{HCN,p}\) and \(S_{NH3,p}\) are the sources of HCN and NH\(_3\) from the thermal decomposition of the coal in kg/m\(^3\).s, \(S_{vol}\) and \(S_{char}\) are the rates of coal devolatilization and char burnout in kg/s, \(Y_{N,fuel}\) is the mass fraction of nitrogen in the coal (see Tables 3.3 and 3.4), \(M_{HCN}\), \(M_{NH3}\), and \(M_N\) present the molecular weight of species HCN, NH\(_3\) and N respectively, and \(\Delta V\) is the control volume in m\(^3\).

For the mass consumption rates of HCN and NH\(_3\), the following expressions are used in this simulation:
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\[ S_{HCN,1b} = - R_1 \frac{M_{HCN} \times P}{R \times T}, \quad S_{HCN,2b} = - R_2 \frac{M_{HCN} \times P}{R \times T} \]

\[ S_{NH_3,1b} = - R_3 \frac{M_{NH_3} \times P}{R \times T}, \quad S_{NH_3,2b} = - R_4 \frac{M_{NH_3} \times P}{R \times T} \]

(3.79)

where \( S_{HCN,1b} \) and \( S_{HCN,2b} \) are the consumption rates of HCN in Eqs. (3.70) and (3.71), \( S_{NH_3,1b} \) and \( S_{NH_3,2b} \) are the consumption rates of \( NH_3 \) in Eqs. (3.72) and (3.73), \( P \) is the pressure, and \( T \) presents the mean temperature.

Finally, as shown in Eq. (3.77) the source term of NO can be accurately calculated via four different terms and can be written as follows:

\[ S_{char,NO} = \frac{S_{char} \times Y_{N_fuel} \times M_{NO}}{M_N \times \Delta V} \]

\[ S_{NO,1} = R_1 \frac{M_{NO} \times P}{R \times T} - R_2 \frac{M_{NO} \times P}{R \times T} \]

\[ S_{NO,2} = R_3 \frac{M_{NO} \times P}{R \times T} - R_4 \frac{M_{NO} \times P}{R \times T} \]

(3.80)

where \( S_{char,NO} \) is the rate of production of NO from the char reaction, \( S_{NO,1} \) and \( S_{NO,2} \) present the production and destruction rates of NO via Eqs. (3.70) and (3.71) for HCN and via Eqs. (3.72) and (3.73) for \( NH_3 \), respectively. While the fourth term of NO ( \( S_{NO,3} \) ) in Eq. (3.77) is the reduction rate of NO due to its reaction with char particles, as explained in Eq. (3.74).
3.7 Summary

The commercial CFD code, AVL Fire ver.2008.2 was used in this thesis to solve the Navier-Stokes equations in modelling 100 kW furnace (Chalmers’ furnace) and 550 MW tangentially-fired boiler (Loy Yang A power plant). The geometries of the furnaces were based on the experimental study of Andersson (2007) and power plants data of Staples and Marshall (2010) in the lab- and large-scale furnaces, respectively. Subroutines required for mathematical models of the gas and coal particles combustions were written and incorporated into the CFD code.
Chapter 4. Modelling of Gas Combustion in Air-fired and Two Oxy-fuel Cases in a 100 kW Furnace
4. Modelling of Gas Combustion in Air-fired and Two Oxy-fuel Cases in a 100 kW Furnace

4.1 Introduction

In this chapter, the first step of modelling and validation strategy of this project has been carried out on both the air-fired and two oxy-fuel combustion cases in a 100 kW down-fired (drop tube) unit of firing propane. An AVL Fire code has been developed, integrating gaseous fuel combustion with associated chemical reactions, radiative heat transfer, gas compositions, and turbulent models in a 3-D hybrid unstructured grid CFD code. A swirl injection system was used to achieve the flame stability of the turbulent non-premixed combustible gases. A modified turbulent combustion of the Eddy Breakup (EBU) model was used with appropriate empirical coefficients for propane reaction, from which the irreversible single-step and reversible multi-step reaction mechanisms were considered. The numerical results were widely validated against the physical data which were collected from experiments (reported in the literature) in order to increase the level of confidence of the numerical results. Therefore, this study was completely focused on the numerical solution in order to provide a good insight of knowledge for both the physical and chemical mechanisms of the oxy-fuel combustion technique. Furthermore, the validation of the numerical results against the experimental data of lab-scale facility unit has been considered a very important stage in this type of research. As a result, the successful selection of mathematical models and their associate coefficients and parameters, in the lab-scale furnace, could successfully be used for the next stage of this investigation.

In the present chapter, gas temperature distributions, chemical species concentrations ($\text{CO}_2$, $\text{CO}$, and $\text{O}_2$), velocity components, and fuel consumptions were numerically calculated under the air-fired and two oxy-fuel combustion environments that referred to as OF21 and OF27. The first oxy-fuel (OF21) combustion case has the same oxygen concentration and volumetric flow rate to those of the air-fired (reference) case. While the second oxy-fuel (OF27) combustion case has different thermodynamic and
aerodynamic conditions compared to the reference combustion case. Full descriptions of geometries of burner and furnace are given in this chapter.

**4.2 Description of the furnace and the combustion scenarios**

A 100 kW oxy-fuel firing test unit (Andersson, 2007) was selected for this simulation study. The furnace is a cylindrical refractory lined drop tube unit with dimensions: 80 (cm) inner diameter and 240 (cm) inner height (see Fig.4-1). The gas-fired burner is composed of three circular separate lances that are: one for fuel (C$_3$H$_8$) in the centre (3.4 cm dia.) and others for primary and secondary swirl registers (air or O$_2$/CO$_2$). The burner exit plane and the furnace ceiling are in line. The primary register (5.2 cm dia.) is swirled with a fin angle of 45°, while the secondary register (9.2 cm dia.) is swirled with a fin angle of 15° as shown in Fig.4-2. Generally, the volumetric flow rates of feed oxidizer gases were 40% for primary register and the remaining part for secondary register. The oxidizers/fuel stoichiometric ratio ($\lambda$) was kept constant (1.15) for all combustion cases. In radiation heat transfer field, the total emissivity of the surface wall and gas absorptivity for air-fired (reference) case were 0.41 and 0.24.
(m⁻¹), respectively at 928 (K), while for oxy-fuel-fired scenarios were 0.52 and 0.31 (m⁻¹), respectively at 953 (K). The initial temperatures for fuel and oxidizers were kept 298.15(K) for all combustion cases. The composition of feed oxidizers gases for the reference (air-fired) case was 21 vol.% O₂ and 79 vol.% N₂, but the challenging (oxy-fuel-fired) cases were 21 vol.% O₂ and 79 vol.% CO₂ for OF21 combustion case, and 27 vol.% O₂ and 73 vol.% CO₂ for OF27 combustion case.

Figure 4-2: Burner of gas combustion (dimensions are not to scale)
4.3 Boundary Conditions

The inlets of fuel and other oxidizers in primary and secondary registers are located in the central position of the top-wall of furnace. A fully developed flow was assumed at the exits of the burner. The initialization information was kept constant for all combustion cases such as an initial temperature (298.15 K) and initial pressure (101325 Pa). The inlet velocities of primary and secondary registers of oxidizers (air or O₂/CO₂) are affected by the fin angles 45° and 15°, respectively in order to stabilize the flame structure of combustion. This swirled effect was numerically configured in the CFD model by taking the effects of normal and angular velocities (ω̃) for each registers at the inlet ports of furnace (see Table 4-1).

Table 4-1. The inlet flow field parameters of three different combustion cases for primary and secondary registers of the burner

<table>
<thead>
<tr>
<th>Inlet Flow Field Parameters</th>
<th>Combustion Scenarios</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Air</td>
</tr>
<tr>
<td>Primary Register</td>
<td></td>
</tr>
<tr>
<td>Volume Flow Rate (m³/h)</td>
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<tr>
<td>Mean Velocity (m/s)</td>
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<tr>
<td>Angular Velocity (rad/s)</td>
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<tr>
<td>Secondary Register</td>
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<tr>
<td>Volume Flow Rate (m³/h)</td>
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</tr>
<tr>
<td>Mean Velocity (m/s)</td>
<td>3.3</td>
</tr>
<tr>
<td>Angular Velocity (rad/s)</td>
<td>27.19</td>
</tr>
</tbody>
</table>

In Table 4-1, the inlet flow parameters of all combustion modes are summarized for the primary and secondary registers of the burner. As mentioned previously, about 60% of the total feed oxidizer gases enter the secondary and the remaining part is delivered to the primary. The input power of propane was 80 kW. The volumetric flow rate of O₂/CO₂ mixture for OF27 case was reduced by around 21.9% relative to the both air-fired and OF21 combustion cases, where the latter two cases were set up to the same value (91 m³/h). In this CFD calculation, the lower heating value of propane was used in
enthalpy subroutine as a source term based on the fuel properties (Andersson, 2007). The turbulent combustion time-scale was around $6.08 \text{ s}^{-1}$ in the combustion model according to the inlet turbulent kinetic energy and its inlet dissipation rate. The ideal gas law equation was used for calculating the densities of chemical species, while the material database of the AVL Fire code was employed for other physical properties.

For accurate numerical calculations, the furnace’s wall was separated into two parts: top-wall and vertical-wall. For both parts of wall, no-slip condition ($u, v, \text{ and } w = 0$) was applied. The wall emissivity for air-fired case and oxy-fuel-fired cases were 0.41 and 0.52, respectively according to the adopted values in the experiments (Andersson, 2007). The temperature value was kept constant for top-wall (925 K) and changeable for vertical-wall. Two second-degree polynomial functions were used for calculating the temperature distributions along the vertical-wall (see Table 4-2) in order to match the real values of experimental data in that region of furnace’s wall. A zero gradient was applied for the outflow of furnace.

**Table 4-2. Temperature distribution equations along the vertical-wall of furnace**

<table>
<thead>
<tr>
<th>Location from burner (m)</th>
<th>Temperature equations (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0 - 0.046</td>
<td>$T(Y) = 925$</td>
</tr>
<tr>
<td>0.046 - 0.553</td>
<td>$T(Y) = 358.88Y^2 - 54.615Y + 925.6$</td>
</tr>
<tr>
<td>0.553 - 1.4</td>
<td>$T(Y) = -567.89Y^2 + 1115.1Y + 564.02$</td>
</tr>
<tr>
<td>1.4 - 2.4</td>
<td>$T(Y) = 953$</td>
</tr>
</tbody>
</table>
4.4 Grid independent test

A Grid independent test was carried out using three different 3-D non-uniform grid systems (224000, 480000, and 595200 grids) for the combustion calculations. The average values of flame temperature distribution at 384 mm downstream of burner exit were used for this purpose. This location includes higher values of flame temperature distributions compared to the other locations. The simulation was started with a coarse mesh which was gradually refined until the changes observed in predicted results are not very significant. The grid independent test indicated that the grid number of 480000 satisfies a good balance between the computational time and calculation accuracy with respect to the other grid systems (see Table 4-3).

Table 4-3. Grid independency test for three different grid systems at 384 mm downstream of burner exit plane

<table>
<thead>
<tr>
<th>Number of cells</th>
<th>T(K)_{mean}</th>
<th>Percentage error of ΔT_{mean}</th>
</tr>
</thead>
<tbody>
<tr>
<td>224000</td>
<td>1404.12</td>
<td>-</td>
</tr>
<tr>
<td>480000</td>
<td>1397.24</td>
<td>0.48</td>
</tr>
<tr>
<td>595200</td>
<td>1400.93</td>
<td>-0.26</td>
</tr>
</tbody>
</table>

In Table 4-3, the percentage error of mean different temperature distributions for the selected grid system was within 1% at that chosen location of furnace. Therefore, the numerical solution was not essentially sensitive to the number of cells for these three different grid systems. The grid used in this study was a 3-D non-uniform structured grid with 480000 cells. In general, a high mesh concentration was used along the centreline axis of furnace in the region between the burner exit plane and the centre of furnace (X, Y, and Z=0.0). While the number of cells is gradually decreased at the near wall and outlet boundaries that represent regions of low flow gradients, as shown in Figure 4-3.
Chapter 4- Modelling of Gas Combustion in Air-fired and Two Oxy-fuel Cases in a 100 kW Furnace

Figure 4-3. Grid system of computational domain, dimensions are not to scale.
4.5 Results and discussion

The compositions of feed oxidizer gases for both primary and secondary registers of oxy-fuel (OF21) combustion case were, as explained earlier in the BCs, composed of 21 vol.% O\textsubscript{2} (similar to air-fired case) and 79 vol.% CO\textsubscript{2}, while that of OF27 combustion case included 27 vol.% O\textsubscript{2} and 73 vol.% CO\textsubscript{2}. This change in combustion media has a significant impact on the combustion characteristics and flame structure. In order to explain the differences and comparisons between air-fired and oxy-fuel-fired scenarios, the results and discussion are divided into sections describing: temperature distributions, velocity, species concentrations and fuel consumption. For temperature distribution, the comparisons were performed at different vertical and horizontal planes of the furnace. The values of species concentrations and propane consumption were compared at the most intense combustion locations near the inlet of the furnace.

4.5.1 Temperature distributions

Figures 4-4 and 4-5 show the comparisons between the gas temperature distributions for the air-fired, oxy-fuel (OF21), and oxy-fuel (OF27) combustion flames on the vertical and horizontal (384 mm from burner exit) planes of the furnace, respectively. It can be clearly seen that both the air-fired and OF27 flames exhibit more bright aspects than the OF21 flame. This luminous appearance of the flame in the OF27 case may be attributed to the higher oxygen concentration in the gas mixture, which resulted in higher flame temperature levels compared to those in the OF21 combustion case. In addition, the increased CO\textsubscript{2} in flue gases absorb more radiation in the latter flame (OF21), leading to reduced flame brightness. Andersson (2007) referred to this aspect of the luminous feature to the soot formation, which was not modelled in this simulation. In Figure 4-4, the flames of both oxy-fuel cases were obviously concentrated in the central position of the furnace compared to the air-fired flame. Spreading of the air-fired flame was evident, especially in the centre of the furnace.
Figure 4-4. Values of temperature distributions (K) for the air-fired flame, OF21 flame, and OF27 flame at the vertical cut (X-Y plane) of the furnace

The peak gas temperature value for the air-fired case was 1955K but decreased to 1822 K and 1518K for the OF27 and OF21 combustion cases, respectively. This temperature drop affected the combustion delay in both the oxy-fuel combustion cases, as shown clearly in Figure 4-4 in the near-burner region. The OF21 flame appears to be affected more than the OF27 flame in terms of temperature level and combustion delay, as shown in Figure 4-5. This can be attributed to the oxygen concentration in the feed gases and also to the reduced volume flow rate adopted in OF27 combustion case. This reduced volume flow rate increased the residence time for combustibles in the
combustion zone, resulting in a higher gas temperature. The differences in the flame structure between the air-fired and oxy-fuel combustion cases are mainly due to the differences in the thermodynamic properties between nitrogen and carbon dioxide and also the radiative properties of the gas mixture. However, these numerical results of combustion delay in oxy-fuel-fired environments were very consistent with the recent experimental study of Moore and Kuo (2008). They conducted over 170 combustion tests in a lab-scale combustion chamber to investigate the effect of switching the primary and secondary gaseous reactant supply (CH\textsubscript{4}/O\textsubscript{2}) in a coaxial injector of a non-premixed flame.

Figure 4-5. Values of temperature distributions (K) for the air-fired flame, OF21 flame, and OF27 flame at the horizontal cut (X-Z plane) of the furnace

Figure 4-6a-c, shows the comparisons of the gas temperature distribution between the experimental and the predicted CFD results on a horizontal cut (X-Z plane) of the furnace at 215 mm from the burner exit plane. It is clear that the amount of soot formed in the combustion zone gradually decreased from the air-fired and OF27 cases to the OF21 combustion case, affecting the illumination of the OF21 flame (Andersson 2007). In addition, the higher concentration of CO\textsubscript{2} in the oxy-fuel combustion cases also affected the illumination as explained earlier. The validation of these three combustion flames revealed that the numerical simulations of the present CFD model can provide confidence on the luminous feature and flame structure at these important locations of the furnace.
Figure 4-6a-c. Comparisons of the gas temperature distributions between the experimental and predicted CFD results for: a) Air-fired case, b) OF21 case, and c) OF27 combustion cases at the horizontal cut (X-Z plane), 215 mm from the burner exit plane.
Figures 4-7 to 4-9 present comparisons between predicted results and experimental data of gas temperatures at four different locations: 384, 553, 800, and 998 mm, respectively from the burner exit plane. A four-step reaction mechanism was implemented for all combustion cases to provide improved predictions with the experiments. For the air-fired (reference) case, reasonably good agreement is attained at the first two locations, whereas a slight over-prediction is observed at the other locations. These expected increases in the gas temperatures occurred in the intense reaction region of the furnace. Also, oxygen purity used in the experiments (Andersson 2007) was 99.5 vol.% (0.5 vol.% minor constituent inert gases such as nitrogen and argon), while the purity of O₂ used in the present study was assumed to be 100 %. This 0.5 % by vol. of impurity would result in marginal decrease in temperature in the experiments (Al-Abbas et al. 2011).

In the numerical simulation, the mixture fraction equation (Eq. 3.23) used in the present study was close to stoichiometric combustion characteristics, which insured a complete consumption between oxygen and fuel, resulting in a higher gas temperature in the flame zone. For the OF21 and OF27 cases, overall agreements of the numerical results were achieved with the experimental data except in the flame region (from 0.0 to 0.1 m in the radial direction). In this intense reaction region, the predicted results had the same over-prediction observed in the air-fired case. The overall deviation between the numerical results and physical data was less than 12%. These deviations may have been due to the numerical schemes and the turbulence model used and/or the uncertainties of experiments.
Figure 4-7a-d. Temperature distribution profiles at: a) 384, b) 553, c) 800, and d) 998 mm from the burner exit plane for the air-fired case.
Figure 4-8a-d. Temperature distribution profiles at: a) 384, b) 553, c) 800, and d) 998 mm from the burner exit plane for the oxy-fuel (OF21) combustion case.
Figure 4-9a-d. Temperature distribution profiles at: a) 384, b) 553, c) 800, and d) 998 mm from the burner exit plane for the oxy-fuel (OF27) combustion case.
4.5.2 Velocity

Figure 4-10 shows the mean velocity vectors of the air-fired, oxy-fuel (OF21), and oxy-fuel (OF27) combustion cases at different horizontal planes of the furnace. Some differences were evident among the mean velocity distributions for the cases examined, particularly at these selected locations: 1.19, 0.816, and 0.647 m from the furnace centre point. In addition to the burner configuration effect on the flow behaviour (see Table 4-4), the aerodynamic and thermodynamic characteristics of reactants (O$_2$/N$_2$ or O$_2$/CO$_2$ mixture) also had important impact on the flame structure. For both oxy-fuel cases, the flames were more intense along the furnace centreline, while the air-fired flame was relatively spread out, as shown in Figure 4-4.

![Figure 4-10. The mean velocity vectors of the air-fired, oxy-fuel (OF21), and oxy-fuel (OF27) combustion cases at different horizontal cuts of the furnace.](image)

Although the air-fired and OF21 combustion cases had the same inlet flow parameters and oxygen concentration, the flame in the latter combustion showed a clear difference in its structure due to the higher heat capacity of CO$_2$ compared to the N$_2$ in the gas mixture. However, with a decreasing volumetric flow rate in the OF27 case, as reported in Table 4-1, the flame structure improved relative to the OF21 flame due to increased
residence time. These predicted results were consistent with the recent experimental study of Boushaki et al. (2007). They used new burner configurations to characterize the influence of burner parameters on flame stability in the turbulent non-premixed oxy-flame.

Figure 4-11 shows the effect of swirl on the flame stability at three different recirculation zones. The recirculation regions of the flow field inside the furnace were divided into three separate zones: internal recirculation zone, reaction zone, and external recirculation zone. Generally, a swirl injection system is used in a furnace to achieve well-mixing conditions in the vicinity of the burner exit plane. The swirl numbers used were 0.79 and 0.21 for primary and secondary registers, respectively. Swirl was introduced to enhance the turbulent mixing between fuel and feed oxidizer gases in the near-burner region. The values of velocity vectors in the reaction zone were higher than those in both the internal and external recirculation zones.

Figure 4-11. The mean velocity vectors (m/s) for three different recirculation zones: internal recirculation zone, reaction zone, and external recirculation zone, along the furnace height.
4.5.3 Species concentration

4.5.3.1 Carbon dioxide concentrations

Figure 4-12 displays carbon dioxide concentrations (kg/kg) on a vertical plane showing the upper part of the furnace (X-Y plane). Due to the elimination of nitrogen from the combustion processes, and the use of a mixture of pure oxygen and recycled flue gas (mainly CO$_2$) as oxidizers, CO$_2$ concentration greatly increased in the flue gas for the OF21 and OF27 cases. The increase was from around 11% kg/kg in the air-fired case to 87% kg/kg in both oxy-fuel cases, which is eight times higher in dry basis, as compared to the reference case. These predicted values were confirmed with the experiments (Andersson 2007). No air leakage is considered, in the present numerical simulation. These higher CO$_2$ concentrations in flue gas in oxy-fuel scenarios are more appropriate for compressing and separating processes. The high purity of CO$_2$ in the flue gas can be practically controlled in the real life combustion systems by using pure oxygen (close to 99.5% or more) and by avoiding air leakages into the firing systems.

Figure 4-12. Carbon dioxide concentrations (kg/kg) at the vertical cut along the upper part of furnace axis for the air-fired, OF21, and OF27 combustion environments, all dimensions are in mm.
Figure 4-13a-c presents the comparison between the experimental data and predicted results for the carbon dioxide mass fraction (kg/kg) profiles at 384 mm from the burner exit plane for the air-fired, oxy-fuel (OF21), and oxy-fuel (OF27) combustion scenarios, respectively obtained with one-step and four-step chemical reactions. This location (384 mm) was chosen for comparison because it represents the most intense combustion location inside the furnace. The simulations were begun by using an irreversible single-step reaction, followed by the four-step reaction mechanism. The subsequent four-step reaction was carried out in order to improve the CFD results. As can be seen in Figure 4-13, the results obtained with single-step reaction show marginal over-prediction. This is not surprising because the one-step reaction mechanism could not capture the CO/CO$_2$ production rate and equilibrium between H$_2$ and H$_2$O in the combustion zone (see Eq. 3.28) (Choi et al. 2009).

In contrast, the four-step reaction mechanism showed improved agreement with the measurements. In Figure 4-13 b and c, the overall agreement was reasonably achieved for both of the oxy-fuel combustion cases at this location of the furnace, but a slight under-prediction can be observed, in Figure 4-13a, for the air-fired (reference) case between 0.0 and 0.1 m in the radial direction (flame zone). As will be discussed in the following paragraph, the dissociation mechanism of major species such as CO$_2$ was largely enhanced in the flame region due to the higher flame temperature, as explained earlier with reference to Eq.3.32.

Table 4-4. The dimensions and geometric configuration data of the burner

<table>
<thead>
<tr>
<th></th>
<th>Fin angle</th>
<th>Swirl number</th>
<th>Outlet diameter (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary register</td>
<td>45°</td>
<td>0.79</td>
<td>52</td>
</tr>
<tr>
<td>Secondary register</td>
<td>15°</td>
<td>0.21</td>
<td>92</td>
</tr>
</tbody>
</table>
Figure 4-13a-c. Carbon dioxide mass fraction (kg/kg) profiles at 384 mm from the burner exit plane for a) the air-fired, b) oxy-fuel (OF21), and c) oxy-fuel (OF27) combustion scenarios in one- and four-step chemical reactions.
4.5.3.2 Oxygen concentrations

Figure 4-14 shows the mass fraction of oxygen concentrations (kg/kg) on a vertical plane showing the upper part of the furnace. These O\textsubscript{2} distributions were obtained with the multi-step reaction mechanism. Although, the O\textsubscript{2} concentration of the OF21 case was similar to that of air-fired case in the gas mixture, the distributions of O\textsubscript{2} concentration inside the furnace were completely different compared to both the air-fired and OF27 combustion cases. On the other hand, the similarity in the oxygen distributions of the air-fired and OF27 cases was evident (Fig. 4-14). The low oxygen concentrations observed in the OF21 case resulted in a drop in the flame temperature. The lower oxygen concentration in OF21 case also leads to the combustion delay mentioned in the previous temperature section; where the ignition point started further down (around 200 mm from the burner exit); in contrast to the ignition point of the other combustion cases which were closer to the burner tips (see Fig. 4-4).

![Figure 4-14. Oxygen concentrations (kg/kg) at the vertical cut along the upper part of furnace axis for the air-fired, OF21, and OF27 combustion environments, all dimensions are in mm.](image-url)
Comparison amongst the numerical results, obtained with one-step and four-step chemical reaction, and the experimental data of oxygen concentrations at 384 mm from the burner exit plane is presented in Figure 4-15a-c. The predicted results of oxygen concentrations are in reasonably good agreement with the experiment. For all cases examined, the predicted results of four-step reaction are in better match with the physical data at the furnace centerline compared to the one-step reaction. This accurate numerical result in the furnace can potentially provide better understanding in regards to the investigation of combustion delay. As seen, oxygen concentrations in the near-burner region have not only a significant influence on the flame characteristics, but also on the fuel consumption as explained in the next sub-section.
Figure 4-15a-c. Oxygen mass fraction (kg/kg) profiles at 384 mm from the burner exit plane for a) the air-fired, b) oxy-fuel (OF21), and d) oxy-fuel (OF27) combustion scenarios in one-, and four-step chemical reactions.
4.5.3.3 Carbon monoxide concentrations

One benefit of the multi-step reaction mechanism used in this study is the capture of CO/CO$_2$ production rates in the flame zone. In Figure 4-16, the distributions of carbon monoxide (CO) concentrations are presented on a vertical plane showing the upper part of furnace. The distributions of CO concentrations, for air-fired and OF27 cases, showed some similarities in the near-burner region. This is due to the similar levels of the flame temperatures in the near-burner region, as already explained with reference to Fig. 4-4. In contrast, the OF21 case shows a low CO concentration relative to the other combustion cases. This decrease in CO concentrations might have happened because of the shortage in the O$_2$ concentration in this oxy-fuel case, which also resulted in a decrease in the combustion temperature. In general, the higher flame temperature leads to enhanced chemical dissociation of main species in the flame envelop zone, and therefore increases the intermediate species concentrations, as recently reported in the outstanding study of Kim et al. (2009). They predicted the structure of natural gas flames in both air-firing and oxy-fuel combustion scenarios by coupling a conditional moment closure reactive model with the flow solver. The detailed chemistry model was used to calculate the intermediate species formed in the flame zone due to the thermal dissociation at the higher temperature region.

Further validation of the present CFD results with the experiments are presented in Figs.4-17a-c and 4-18a-c at 215 and 384 mm, respectively from the burner exit plane for combustion scenarios, respectively. The overall qualitative and quantitative agreements of the predictions of this species (CO) with the experimental data are reasonably achieved at these two combustion intensive locations of the furnace.
Figure 4-16. Carbon monoxide concentrations (kg/kg) at the vertical cut along the upper part of furnace axis for the air-fired, OF21, and OF27 combustion environments, all dimensions are in mm.
Figure 4-17a-c. Carbon monoxide mass fraction (kg/kg) profiles at 215 mm from the burner exit plane for a) the air-fired, b) oxy-fuel (OF21), and c) oxy-fuel (OF27) combustion scenarios.
Figure 4-18a-c. Carbon monoxide mass fraction (kg/kg) profiles at 384 mm from the burner exit plane for a) the air-fired, b) oxy-fuel (OF21), and d) oxy-fuel (OF27) combustion scenarios.
4.5.4 Fuel consumption

Figure 4-19 illustrates the mass fraction distribution (kg/kg) of propane on the vertical plane showing the upper part of the furnace. The fuel burn-out rate of the OF21 case was less than those of the other combustion cases in the vicinity of the burner exit. This could be due to the low O\textsubscript{2} concentration observed in the near-burner region of the furnace (see Fig. 4-14), which also resulted in a decrease in the flame temperature level. In contrast, the higher O\textsubscript{2} concentration and resident time observed in OF27 case led to increased fuel consumption and temperature levels. The fuel consumption in OF27 case was closer to that of the air-fired case than that of OF21 case. However, in the air-fired and OF27 combustion cases the fuel was completely consumed at around 300 mm from the burner exit, while in the OF21 case the unburned fuel existed until 500 mm from the burner.

![Figure 4-19. Mass fraction distribution (kg/kg) of propane at the vertical cut along the upper part of furnace axis for the air-fired, OF21, and OF27 combustion environments, all dimensions are in mm.](image)

In order to display this aspect of fuel consumption for the cases examined, Figure 4-20a and b presents the mass fraction distributions of propane at 215 and 384 mm, respectively from the burner exit plane. At both these locations, the amounts of
unburned fuel, in the air-fired and OF27 cases, was smaller than that of the OF21 case. Moreover, compared to the air-fired case, the oxy-fuel combustion cases have produced much wider zones of propane distributions around the furnace centreline. This indicates that the chemical reaction processes in oxy-fuel cases were affected by the increased CO$_2$ in the flue gas, leading to wider reaction zone. This is clearly shown in Figure 4-20b between 0.0 and 0.12 m from the centreline in the radial direction. This observation was also consistent with the numerical results of Kim et al. (2009) on the oxy-flame structure.

Figure 4-20a and b. Mass fraction distribution (kg/kg) profiles of propane consumption at: a) 215 and b) 384 mm from the burner exit plane for all combustion cases.
4.6 Summary and conclusion

In this chapter, a three-dimensional computational fluid dynamics (CFD) model has been developed to model an air-fired and two different oxy-fuel combustion cases, referred to as OF21 and OF27, in a 100 kW lab-scale furnace. The investigations of the temperature distribution levels, species concentration (CO$_2$, CO, and O$_2$), velocity distributions, and propane consumption were carried out at the most intense combustion locations of the furnace. An efficient turbulent combustion model with the most appropriate empirical coefficients was used in this numerical study. Primary and secondary swirl registers of the burner were employed to enhance an internal recirculation mechanism of flames and to ensure a well-mixing condition for turbulent non-premixed gaseous reactants. A grid independence test and validations of the predicted results with the experiments were conducted; a reasonably good agreement was achieved for the temperature distributions and species concentrations. Slight over-predictions of temperature levels and species concentration levels were observed in the one-step reaction relative to the measurements. These discrepancies were attributed to neglecting the dissociation mechanism of the major species. The prediction accuracy improved with the use of multi-step chemical reaction. The numerical results showed that the flames were concentrated near the burner and along the central axis of the furnace. The oxy-fuel flames showed less radical spreading. The luminous appearance and temperature levels of the OF27 flame were comparable to the air-fired flame. A combustion delay was particularly evident for the oxy-fuel (OF21) case. This delay was partially attributed to the insufficient oxygen concentration in the near-burner region compared to the reference (air-fired) and OF27 cases. The residence time of combustible reactants for the OF27 case was increased due to reduced volumetric flow rate of about 21.9% relative to those of the air-fired and OF21 combustion cases. The reduction in the O$_2$ concentration in the OF21 case affected the amount of unburned fuel and CO formation in the vicinity of the burner. In the next chapter, the second step of this project will comprehensively focus on lignite coal combustion in the same lab-scale furnace using more oxy-fuel combustion conditions.
Chapter 5. Modelling of Lignite Combustion in Air-fired and Three Oxy-fuel Cases in a 100 kW Furnace
5. Modelling of Lignite Combustion in Air-fired and Three Oxy-fuel Cases in a 100 kW Furnace

5.1 Introduction

In this chapter, a comprehensive computational fluid dynamics (CFD) modelling study was undertaken by integrating the combustion of pulverized dry lignite in several combustion environments. Four different cases were investigated: an air-fired case and three different oxy-fuel combustion environments (25 % vol. O\textsubscript{2} concentration (OF25), 27 % vol. O\textsubscript{2} concentration (OF27), and 29 % vol. O\textsubscript{2} concentration (OF29). The chemical reactions (devolatilization and char burnout), convective and radiative heat transfer, fluid and particle flow fields (homogenous and heterogenous processes), and turbulent models were employed in 3-D hybrid unstructured grid CFD simulations. The available experimental results (Andersson 2007) from a lab-scale 100 kW firing lignite unit (Chalmer’s furnace) were selected for the validation of these simulations.

To overcome difficulties in applying the oxy-fuel combustion and make it more appropriate and acceptable in the large-scale furnaces, experimental and modeling studies on the lab-scale or pilot-scale furnaces should initially establish and take their results into consideration during setting up the large-scale furnaces. Therefore, this chapter presents the second step of modelling and validation strategy of this project. Furthermore, the emissions of carbon dioxide (CO\textsubscript{2}) and other pollutants from the existing coal-fired power plants are higher compared to the gas-fired power plants. As a result, it is important in this stage of investigation to address these toxic emissions levels in coal-firing facility units as well.

A good understanding of oxy-fuel combustion with recycled flue gas (RFG) and their effect on boiler thermal performance can increase the potential for CO\textsubscript{2} capture and provide key parameters to the necessary modifications of the conventional boiler upstream such as a flue gas recycle system and an air separation unit. Therefore, numerical simulation methods may provide a wide range of information in furnace and burner design and their operation. In the present study, validation and comparison of all
combustion cases with the experimental data were made by using the temperature distribution profiles and species concentration (O₂, CO, CO₂, and H₂O) profiles at the most intense combustion locations of the furnace. The aerodynamic effect of primary and secondary registers of the burner was included through swirl at the burner inlet in order to achieve the flame stability inside the furnace. In addition, the devolatilized hydrocarbon gas consumption and char residual oxidation were presented.

### 5.2 A review of experimental setup of Andersson

Chalmers 100 kW test facility has been designed to burn both gaseous and pulverized fuels. In order to enable coal-fired in both combustion environments (air-fired and oxy-fuel cases), some necessary equipments were added to the design of unit, which is explained in chapter 4, as follows: a fabric filter, a soot-blowing system, and a gravimetric coal feeder. According to these modifications on the test unit, the pulverized coal was continuously delivered from the pneumatic feed system to pass through the burner. In order to reach to the practical operations of the testing unit, the dried recycled flue gas (RFG) was applied by passing the flue gas through the flue gas cooler, the fabric filter and the flue gas condenser, respectively. As shown in Figure 5-1, this process was before recycling and mixing with pure oxygen. This process (dry RFG) is also important to detect the effect of radiant emission and absorption from the carbon dioxide on the gaseous mixture and furnace wall (Andersson 2007).
The geometrical information of the furnace and burner is repeated again in this section for convenience. The combustor is a down-fired cylindrical refractory lined unit that measures 80 cm inner diameter and 240 cm inner height. The burner configuration composes of three circular separate lances that are: one for fuel (German lignite) in the centre (34 mm dia.) and others for primary and secondary swirl registers (air or O\textsubscript{2}/CO\textsubscript{2}) consequently (see Fig. 4-2). The burner exit plane and the combustor ceiling are in line. Three different oxy-fuel combustion cases are used as follows: OF25 (25% vol O\textsubscript{2} and 72% vol CO\textsubscript{2}), OF27 (27% vol O\textsubscript{2} and 71% vol CO\textsubscript{2}), and OF29 (29% vol O\textsubscript{2} and 69% vol CO\textsubscript{2}). The carrier gas in the air-fired case, which is used to inject the coal, is air with a volumetric flow rate of 83.3*10\textsuperscript{-5} (m\textsuperscript{3} per sec). While the carrier gas in oxy-fuel combustion cases is recycled flue gas (RGF) with a volumetric flow rate of 66.6*10\textsuperscript{-5} (m\textsuperscript{3} per sec.) that has the same oxygen concentration (30% vol dry) and recycled flue gas (68% vol dry) for all oxy-fuel combustion cases. The primary register (52 mm dia.) was equipped with swirl producing fin at an angle of 45\textdegree, whereas the secondary
register (92 mm dia.) was equipped with swirl producing fin at an angle of 15°. Generally, the volumetric flow rates of feed oxidizer gases (air or dry RFG for oxy-fuel combustion cases) were 30% for primary register and the rest were through secondary register. The volumetric flow rates of air or RFG through the primary and secondary registers of the burner were decreased gradually by 17%, 23%, and 28% in the OF25, OF27, and OF29, respectively with respect to the air-fired case. The oxidizers / fuel stoichiometric ratio ($\lambda$) was kept constant (1.18) for all combustion cases. The initial inlet temperature of dry flue gas at the inlet of burner was around 298.15 K for all combustion tests. The combustor is initially fired by using gas (propane) as a pilot-fuel to start up the combusting process before switching to coal (Andersson 2007).

### 5.3 Computational method descriptions

The commercial CFD package, AVL Fire ver.2008.2, was used to solve the 3-D governing equations of turbulent flows, combustion and heat transfer using the finite-volume technique in an unstructured grid system. The semi-implicit method for pressure linked equations (SIMPLE) algorithm was used for calculating the pressure and velocity. In the convergence criterion, the normalised absolute residuals for all the variables in each cell were limited to be less than $10^{-4}$. In all the simulation cases, the overall convergence was achieved after about 35000-40000 time-step with 0.0025 (s) for each time-step. The initial temperature condition for the domain was set to 298K. This value was selected based on the inlet temperature boundary conditions. The strategy of this simulation was dependent upon the experimental procedures, i.e. the simulation was started, in transient mode, calculating combustion of the gas (propane) only until the stable temperature was reached. Then the injection of coal particles was started. Under initial simulation start up, the time step was restricted to 0.0005 (sec.) to allow for the temperature profile to stabilize and then the time step was gradually increased to 0.0025 (sec.), a value allowed by the numerical stability. Transient simulations were run until reasonable flame stability was achieved. However as was observed in the experiments of Andersson (2007), the flame was found to show some unsteadiness. Simulations were run under transient mode, and results were averaged.
over the final 10000 time-steps in the line with the averaging procedure adopted in the experiments (Andersson 2007).

The main aim in the discretisation of the convective-diffusion equations is the calculation of the value of transport property (\( \phi \)) at cell faces and its convective flux over these boundaries (Versteeg and Malalasekera 2007). The central differencing approximation scheme with second order accuracy is used for continuity equation, which uses a linear interpolation to compute the cell face values for the convective term of the convection-diffusion equations. However, the central differencing scheme is unable to identify flow direction because of its lack in transportiveness and unrealistic solution at high value of the Peclet number (Pe). As a result, a first order upwind scheme is employed for other equations such as momentum, turbulent, and energy equations as Peclet number is high (Pe \( \geq 2 \)) and because it is highly stable. The size of the inlet particle is kept constant in this simulation with a mean diameter of 50(µm). The physical properties (proximate and ultimate analysis) of coal particle (German Lignite), used in the present study are summarized in Table 3-3.

### 5.4 Grid independency test

A grid independency was used as a scaling test to determine minimum grid resolution required to generate a solution, which is independent of the grid used. Three different non-uniform smaller cell sizes (136000, 224000, and 480000) were successively used for the calculations in the air-fired combustion case. The mean values of flame temperature profile at port 1 (see Table 5-1) were used for this purpose. The results of grid independence test are presented in Figure 5-2.

Table 5-1 Port numbers at different locations in the furnace.

<table>
<thead>
<tr>
<th>Port number</th>
<th>Distance from burner exit (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Port 1</td>
<td>215</td>
</tr>
<tr>
<td>Port 2</td>
<td>384</td>
</tr>
<tr>
<td>Port 3</td>
<td>553</td>
</tr>
<tr>
<td>Port 4</td>
<td>800</td>
</tr>
</tbody>
</table>
There are some changes in the predicted profiles with each successive refinement. The flame temperature distribution for the 480000-grid system was slightly higher than the experiment from 0.1 m to the wall in the radial direction. In contrast, the flame temperature level for 136000-grid system was slightly higher than the experiment from the centreline of the furnace to 0.08 m. As further grid independency test, the two higher grid systems (224000 and 480000 cells) have been compared again in another location of the furnace (port 2). The differences between the predicted temperatures and the experimental data were very marginal (see Figure 5-3). In addition, the percentage error in the mean temperature distribution for these two grid systems was within 1 %. Thus the numerical solution was essentially not sensitive to the number of cells and both the grid systems can provide same results. Therefore, the 224000-grid system was selected to validate the numerical results with the experiments.
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Figure 5-3: Temperature distribution profiles of the air-fired combustion case at port 2 for grid independence test.

Table 5-2 shows the percentage error of the mean temperature for the selected grid system is within 1% at that challenging location of the furnace (port 1). In general, a high mesh concentration was used along the centreline of the furnace in the region between the burner exit plane (top-wall of furnace) and the centre of the furnace, while the mesh size was gradually increased away from the centre as shown in Figure 5-4.

Table 5-2 Grid independency test.

<table>
<thead>
<tr>
<th>Number of Cells</th>
<th>$T \text{ (K)}_{\text{mean}}$</th>
<th>Percentage Error of $\Delta T_{\text{mean}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>136000</td>
<td>1560.36</td>
<td>-</td>
</tr>
<tr>
<td>224000</td>
<td>1548.62</td>
<td>0.75</td>
</tr>
<tr>
<td>480000</td>
<td>1572.39</td>
<td>-1.53</td>
</tr>
</tbody>
</table>
5.5 Boundary conditions

The good selections of boundary conditions can definitely play a significant effect on the accuracy of the numerical results in comparison with the physical data of the combustion media. Therefore, the computational domain of the present furnace is divided into three main boundaries: the inlet, the wall, and the outlet. For all the used simulation cases, the following fundamental boundary conditions are being considered.

5.5.1 The inlet boundary condition

The fuel (German Lignite) inlet and other oxidizers (air or O₂/CO₂) in primary and secondary registers of the burner are located in the central position of the top-wall of the furnace (see Fig. 5-4). The control volumes (cells) were concentrated in this region of furnace in order to resolve the flame structure inside the furnace. As stated previously, approximately 70% of the total feed-gas oxidizers enter the secondary and the rest...
through the primary. For oxy-fuel, the volumetric flow rates through the primary and secondary registers of the burner were reduced by fixed ratios. Furthermore, the mean and angular velocities were calculated to account for the effects of fin angles of the burner (swirl no. of primary and secondary registers were 0.79 and 0.21 respectively) and the stoichiometric ratio ($\lambda = 1.18$) of combustion. The inlet flow field parameters at the primary and secondary registers of the burner, for all the combustion cases, are summarized in Table 5-3.

Table 5-3: The inlet flow field parameters of all combustion cases for primary and secondary registers of the burner.

<table>
<thead>
<tr>
<th>Inlet Flow Field Parameters</th>
<th>Air</th>
<th>OF25</th>
<th>OF27</th>
<th>OF29</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Primary Register</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Volume Flow Rate (m$^3$/h)</td>
<td>34.87</td>
<td>28.94</td>
<td>26.85</td>
<td>25.11</td>
</tr>
<tr>
<td>Mean Velocity (m/s)</td>
<td>7.966</td>
<td>6.612</td>
<td>6.134</td>
<td>5.737</td>
</tr>
<tr>
<td>Angular Velocity (rad/s)</td>
<td>433.293</td>
<td>359.615</td>
<td>333.645</td>
<td>312.052</td>
</tr>
<tr>
<td><strong>Secondary Register</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Volume Flow Rate (m$^3$/h)</td>
<td>81.37</td>
<td>67.54</td>
<td>62.65</td>
<td>58.59</td>
</tr>
<tr>
<td>Mean Velocity (m/s)</td>
<td>4.995</td>
<td>4.146</td>
<td>3.845</td>
<td>3.596</td>
</tr>
<tr>
<td>Angular Velocity (rad/s)</td>
<td>41.14</td>
<td>34.152</td>
<td>31.673</td>
<td>29.608</td>
</tr>
</tbody>
</table>

The fuel input power of coal was 76 kW and the particle (pulverized lignite) mass flow rate was 13.1 (kg/h) for all the simulation cases. The composition of feed gases and fuel carrier gases for air-fired and oxy-fuel combustion cases at the inlet boundaries are summarized in Table 5-4. The initial conditions were kept constant for all combustion cases with: initial temperature (298.15 K) and initial pressure (101325 Pa). The densities of reactants and products were calculated by ideal gas law equation, while the other physical properties information such as specific heat, molecular weight, viscosity, thermal conductivity, and diffusion coefficient were taken from the material database that given by AVL Fire ver.2008.2 code.
Table 5-4: The composition of feed gases and fuel carrier gases of air-fired and oxy-fuel combustion cases at the inlet flow boundary conditions.

<table>
<thead>
<tr>
<th>Feed Gas Composition</th>
<th>Inlet Gases concentration (vol. %)</th>
<th>Combustion Media</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>O₂ Concentration</td>
<td>Air</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td>CO₂ Concentration</td>
<td>0</td>
</tr>
<tr>
<td>Fuel Carrier Gas Composition</td>
<td>O₂ Concentration</td>
<td>21</td>
</tr>
<tr>
<td></td>
<td>CO₂ Concentration</td>
<td>0</td>
</tr>
</tbody>
</table>

5.5.2 The wall boundary condition

For mean momentum and energy equation, the wall functions based on the assumed logarithmic velocity and temperature distributions were used (Versteeg and Malalasekera 2007). For turbulent mean velocity, the following wall function was used:

\[ U^+ = \frac{1}{k} \ln(E y^+) \text{, } y^+ > 11.63 \]  \hspace{1cm} (5-1)

Where, k = 0.41 is Von Karman constant and E = 9.0 is a constant in the law of the wall.

For mean temperature, the following mathematical expression was used:

\[ T^+ = \sigma_r \left[ \frac{1}{K} \ln(E y^+) + Y \right] \]  \hspace{1cm} (5-2)

Where, Y is a function of (Pr) Prandtl number and (\(\sigma_r\)) turbulent Prandtl/ Schmidt number, 0.9 is used for these calculations.

For precise modelling, the wall of the furnace was divided into two parts: top-wall and vertical-wall. No-slip condition \((u, v, \text{ and } w = 0)\) and wall emissivity were applied for
both parts. The adopted value of emissivity was $\varepsilon = 0.52$ for oxy-fuel conditions, in contrast to the value of $\varepsilon = 0.41$ for air-fired combustion conditions (Andersson 2007). The top-wall and the vertical-wall were kept at constant temperatures of 873 (K) and 923 (K) respectively as described in the experimental work (Andersson 2007). A non-elastic spherical collision model was used to control the interaction between the particles and the wall. The magnitude of the perpendicular momentum of particles was reduced by the coefficient of compensation value of 0.9.

### 5.5.3 The outlet boundary condition

At the outlet boundary condition of the furnace, a zero gradient ($\frac{\partial \phi}{\partial X_j} = 0$) was applied for all variables. This condition was specified from the Von Neumann condition but the continuity equation was enforced as it is more appropriated for the compressible flow problems.
5.6 Results and discussion

In this section, the results and discussion of four different combustion cases are presented. The differences and comparisons for these combustion environments are based on the composition and the amount of the feed gas (air or O₂/CO₂) as oxidizers (see Table 5-3). The volume flow rate of the fuel inlet (coal particles) is kept constant for all the combustion environments. These four combustion environments were considered because of their perfect combustion conditions. For instance, combustion case (21% vol. O₂, and 79% vol. CO₂) was not considered because this case led to flame stability problems. For the same trend, due to the technical problems of ash melting point, combustion case (≥ 30% vol. O₂, and ≤ 65% vol. CO₂) was also not considered (Andersson 2007). The findings of these different combustion environments are analysed and discussed in four separate sections: temperature distribution, velocity, species concentration, and particles consumption. Experimental data for all variables were not available at all measurements locations. Hence comparisons were carried out for variables at locations when experimental data were available. For the temperature distribution, the comparisons are performed at the most intense combustion locations of the furnace (port 1, 2, and 3), as well as, along the furnace axis (see Table 5-1 for port locations). For the velocity, the mean velocity distribution and the recirculation zones are presented in the areas close to the burner exit plane, which represents the strong turbulent mixing zones of the furnace. The species (O₂, CO₂, and H₂O) concentration values are compared with the experiments at ports 1, 2, 3, and 4. Most of these selected locations are within the flame envelop, which is the most important locations in the furnace. Finally, the particle consumption or burning are divided into the hydrocarbon gas concentration (due to devolatilization process) and char oxidation at the same previous mentioned locations. In order to compare with the experimental data, all the temperatures and species concentrations presented in this chapter were time-averaged over the final 10000 time-steps (25 sec.) in the line with the averaging procedure adopted in the experiments of Andersson (2007).
5.6.1 Temperature distribution:

Figure 5-5 shows the temperature distributions on a vertical plane through the middle of the furnace. The left hand sides of each image show the air-fired case as the reference. The three different oxy-fuel combustion cases are presented on the right hand sides. The main purpose of this figure is to visualize the overall flame temperature in this axisymmetric furnace.

Figure 5-5. Flame temperature distributions (K) at the vertical cut along the furnace axis for the reference air-fired case (left hand sides) and oxy-fuel combustion environments OF25, OF27, and OF29 (right hand sides), respectively.
The flame started at the burner exit and extended up to the middle of the furnace for the reference air-fired case. The near-burner flame temperature distribution of oxy-fuel combustion (OF25) is closer to that of the air-fired case. Whereas, the near-burner flame temperature of oxy-fuel (OF27) is higher, and the length of the flame is shorter and more confined in the burner exit region. For the OF29 case, the flame temperature distribution is similar to that of OF27 case with marginally higher flame diameter in the near burner region. The peak flame temperature values of the air-fired and OF25 cases were 1603.3 (K), and 1577.5 (K) respectively. While the peak flame temperature values for OF27 and OF29 were 1666.2 (K) and 1699.1 (K), respectively. These peak flame temperature values are very consistent with the experimental result values (Andersson 2007). It is clear that when the oxygen concentration in the feed gas stream is increased and the recycled flue gas (RFG) is decreased in the oxy-fuel combustion environments, the flame temperature increases and the shape of the flame is more confined and close to the inlet flow field tip. This phenomenon can be attributed to the higher oxygen content in the near burner reaction zone and higher residence time for the coal due to lower velocity that gives more time to burn. Furthermore, the decreased amount of recycled flue gas (CO$_2$) will absorb less heat released by combustion, thereby increasing the flame temperature.

In short, inlet temperature, resident time, stoichiometry (oxygen to fuel ratio), and recycled flue gas rates can be used as parameters to optimize the oxy-fuel combustion processes to bring it close air-fired (conventional) combustion in order to minimize the retrofitting processes, as described in References (Boushaki et al. 2007; Andersson et al. 2008b).

Figures from 5-6 to 5-9 present comparisons between measured and numerical values of temperature for air-fired (reference), OF25, OF27 and OF29 combustion environments, respectively at three different locations (ports 1, 2 and 3 given in Table 5-1). For the air-fired case, reasonably good agreement is achieved at port 1 and 2, but a slight over-prediction is evident at port 3 between 0.02 (m) and 0.1 (m) in the radial direction. This
discrepancy could have been caused due to sensitivity of the combustion reaction to the purity of oxygen. In the real life experiments (Andersson 2007), the purity of oxygen was 99.5 % vol., and the remaining part in the bottled oxygen included some argon and nitrogen. This 0.5 % vol. of oxygen impurity has a significant effect on the flame temperature level, and thereby reduces the thermal efficiency of the boiler as reported by Baukal (1998). However, in the numerical simulation, the purity of oxygen was assumed to be 100 % vol. in both feed and carrier gases leading to this increase in flame temperature, especially in the flame envelope.

The comparisons of three oxy-fuel combustion cases (OF25), (OF27), and (OF29) with the physical data are widely achieved in the first two challenging locations (ports 1 and 2), but port 3 still has the same over-prediction observed in the reference air-fired case. Peak temperature occurred between central point of the furnace and 0.1 (m) in the radial direction, which is the flame zone. In case of oxy-fuel combustion cases, the high concentration of oxygen in the near burner region of the furnace leads to consume a large amount of fuel and thereby increases the flame temperature level. The discrepancies observed in the comparisons can also be attributed to the usage of constant values of absorption coefficients which made the gas radiation model independent of the temperature distribution and species concentration (H$_2$O and CO$_2$). Furthermore, neglecting the two and the three-step chemical combustion mechanisms definitely affected the species concentration inside the furnace (i.e. the one-step reaction used did not have the ability to consider the effect of species such as CO, OH, and H$_2$ on the radiation heat transfer). The maximum deviations between the measured and predicted temperatures were: 9.6%, 10.4%, 10.7%, and 9.8% for air-fired, OF25, OF27, and OF29, respectively. Even though the maximum percentage error is not high, it is generally observed that the overall qualitative agreement was reasonably achieved.
Figure 5-6 a-c. Temperature distribution profile at ports: (a) 1, (b) 2, and (c) 3 of the furnace for the air-fired case.
Figure 5-7 a-c. Temperature distribution profile at ports: (a) 1, (b) 2 and (c) 3 of the furnace for the oxy-fuel (OF25) combustion case.
Figure 5-8 a-c. Temperature distribution profile at ports: (a) 1, (b) 2 and (c) 3 of the furnace for the oxy-fuel (OF27) combustion case.
Figure 5-9 a-c. Temperature distribution profile at ports: (a) 1, (b) 2 and (c) 3 of the furnace for the oxy-fuel (OF29) combustion case.
5.6.2 Velocity:

In Figure 5-10, the velocity vectors at the primary and secondary swirl registers, located at the tip of the burner. The differences in the directions of velocity vectors between the primary and secondary registers are related to the values of swirl numbers at the same combustion case as mentioned in section 2 of this chapter. The values of the velocity vectors for both inlet registers are different for different combustion cases and are dependent upon the inlet flow conditions as reported in Table 5-3. A swirl injection system is widely used in the burning systems in order to increase the mixing and give enough time for oxidizers to burn maximum amount of fuel in that critical zone of the furnace thereby avoid incomplete combustion. The swirl effect, in this study, is certainly used to enhance the turbulent mixing and thereby leads to stabilize the structure of the flame.

Figure 5-10. The velocity vectors (m/s) of the primary (A) and secondary (B) swirl registers of the burner in the inlet flow tip of the furnace.
Figure 5-11(a-c) shows the mean velocity vectors for air-fired, OF25, and OF29 combustion cases, at the upper part of the furnace (up to 400 mm from the burner exit plane). According to the burner configuration, the oxidizers and fuel (coal particles) are fed into the combustion chamber from separate lances. The effect of swirl on the flow field is evident. The combustion region is divided into three different zones: internal recirculation zone (the inner), reaction zone (in the middle), and external recirculation zone (the outer). Although the burner configuration has a clear effect on the mixing of the reactants, the geometry of the recirculation zones is essentially dependent upon the volumetric flow rates of the recycled flue gas (RFG). As mentioned earlier, it can be seen that the velocity of oxidizer stream is gradually decreased from air-fired case to until OF29 combustion case. However, this decrease in the feed gas velocities ensured more residence time for coal particles, particularly in the near-burner reaction zone and improved the ignition conditions of oxy-fuel combustion cases. Some differences in the mean velocity are clearly noticed between the air-fired case and oxy-fuel combustion cases near the upper region of the furnace. This can also be attributed to the differences in thermodynamic properties between nitrogen and carbon dioxide, which affect the flow behavior of the reactants. The lower velocities in the oxy-fuel combustion cases are associated with the flames which are shorter and more intensified in the near burner region. Furthermore, it can be seen that the flow field in the side ways of the entrained jet is not symmetric, particularly in the air-fired combustion case (Fig. 5-11a). The changes in the combustion conditions such as the feed gases composition and mass flow rates of oxidizers have not only affected the combustion characteristics, but also the regularity of flow field behaviours of the gases and coal particles. The reduction in the mass flow rates of oxidizers substantially depressed the swirl, which pushes the coal particles away from the centreline in an irregular way (i.e. at high mass flow rate value). The weak swirl gives the coal particles an increased residence time in the combustion region and improves the combustion characteristics in the near burner region, as shown in Fig. 5-5. Finally, the three-recirculation zones certainly pointed out to the most important aspects of the flame structure and the intensive heat transfer from the high flame temperature to the surrounding regions inside the furnace.
Figure 5-11 a-c. The mean velocity vectors of a) the air-fired, b) the oxy-fuel (OF25) and c) the oxy-fuel (OF29) combustion cases from the burner exit plane to 400 (mm) over cross-section of the furnace.
5.6.3 Species concentration:

5.6.3.1 Oxygen concentration

The oxygen concentrations (mass fraction, kg/kg) on a vertical plane through the middle of the furnace are shown in Figure 5-12. In this figure, the left hand sides of the images are for the reference air-fired case, while the right hand sides are for OF25, OF27, and OF29 respectively. The oxygen concentrations in the air-fired case and OF25 case are approximately similar. These two cases show a delay in the consumption of \( O_2 \) in the upper part of the furnace, especially along the centerline of the furnace, compared to OF27 and OF29 cases. The similarity in \( O_2 \) consumption between air-fired and oxy-fuel cases is approximately coupled to the flame temperature levels described in Fig. 5-5. In both the OF27 and OF29 cases, the \( O_2 \) consumption starts early due to improved ignition conditions and faster combustion leading to the flame to be closer to the burner tip. These results of oxygen concentrations are very similar to that obtained in experiments (Andersson 2007).
Figure 5-12. Oxygen mass fraction (kg/kg) in the upper part of the combustor for the reference air-fired case (left hand sides) and oxy-fuel combustion cases OF25, OF27, and OF29 (right hand sides), respectively.
Figure 5-13 a and b presents the comparisons of oxygen mass fraction with experimental data at port 1 for air-fired and OF25 cases respectively. As already explained, oxygen concentrations in the near burner region have a significant impact on the fuel consumption and the flame characteristics. There is some over prediction in the numerical results of oxygen concentration at 0.05 (m) from the center and from 0.2 (m) to the wall of the furnace. Figure 5-13 c and d shows the comparisons of $O_2$ concentrations with the experimental data at port 1 for the OF27 and OF29, respectively. Although, there are some deviations in the $O_2$ concentration profile near the wall of the furnace in the OF29 case, the numerical results predicted the overall qualitative trend very well given the complex combustion environments. The deviations observed can be partially attributed the usage of: one-step combustion model and the 100% pure oxygen in the present study as compared to 99.5% pure oxygen used in the experiments (Andersson 2007).
Figure 5-13 a-d. Oxygen mass fraction (kg/kg) profiles at port 1 of the furnace for (a) air-fired, (b) oxy-fuel (OF25), (c) oxy-fuel (OF27) and (d) oxy-fuel (OF29) combustion cases.
5.6.3.2 Carbon dioxide concentration

Figure 5-14 a-c displays the comparisons of the mass fraction distributions (kg/kg) of carbon dioxide with the experiments for air-fired, OF25, and OF29 combustion cases, respectively at port 2 of the furnace. The usage of flue gas (mainly CO₂) instead of air in the oxy-fuel cases was increased the carbon dioxide concentration from approximately 18% (kg/kg) to 90% (kg/kg). This result reveals that the carbon dioxide concentration (partial pressure) generally increases by around 5 times in the oxy-fuel cases compared to air-fired case. A good comparison with experimental data is noticed for the air-fired while the oxy-fuel fired cases show slightly over-prediction. This discrepancy could have been caused due to the air leakage in the combustor that led to increase in the nitrogen concentration and thereby reduces the carbon dioxide concentration in the experiments.

In order to increase the validation exercise, comparisons were carried out inside the combustor at port 4 and presented in Figure 5-15 a-c. It can be seen that the numerical result compared well with the experiment for air-fired case, but for oxy-fuel cases show over-prediction due to air-leakage as already mentioned. The increase in the carbon dioxide concentration in the oxy-fuel combustion environments has important benefit in protecting the furnace wall by absorbing more heat due to its high specific heat with respect to the nitrogen.
Figure 5-14 a-c. Carbon dioxide mass fraction (kg/kg) profiles at port 2 of the furnace for (a) the air-fired, (b) oxy-fuel (OF25) and (c) oxy-fuel (OF29) combustion cases.
Figure 5-15 a-c. Carbon dioxide mass fraction (kg/kg) profiles at port 4 of the furnace for (a) the air-fired, (b) oxy-fuel (OF25) and (c) oxy-fuel (OF29) combustion cases.
5.6.3.3 Water vapor concentration

Although the same moisture (H$_2$O) content was used at burner inlet for all combustion cases (see Table 3.3), it can be seen in Figure 5-16 a and b that the water vapor concentration in OF29 is slightly higher than the air-fired case. Due to similarities in the H$_2$O concentration in all the oxy-fuel cases (not mentioned in this chapter for brevity), only OF29 is selected for validations and comparisons with the reference air-fired case. This slight increase in the water content in OF29 case can be attributed to higher content of oxygen in the feed oxidizer gases compared to the reference case. There is some over-prediction in the flame envelop (from the centerline of the furnace to 0.1 (m) in the radial direction) zone in both Fig. 5-16 a and b. The flame envelop a high temperature zone, where the dissociation of the main combustion products such as CO$_2$ and H$_2$O, into many unstable radicals such as CO, H$_2$, OH, and O takes place. The one-step combustion mechanism, used in this chapter, neglects this dissociation and hence the existence of unstable radicals, leading to small over-prediction in the water content in the flame envelop (Choi et al. 2009).

Due to the assumption of constant values of absorption coefficients in the gas radiation model (used in this chapter), their dependency on temperature and species concentration was ignored. This may also have contributed to the over predictions in the numerical results, particularly in the oxy-fuel combustion cases. However, the overall agreement of the predictions of this species with the experimental data is qualitatively and quantitatively achieved with reasonable accuracy.
Figure 5-16 a and b. Water mass fraction (kg/kg) profiles at port 4 of the furnace for (a) the air-fired and (b) oxy-fuel (OF29) combustion cases, respectively.
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5.6.4 Particles consumption:

In this section of discussion, the coal particles consumption is divided into two parts: the hydrocarbon gas consumption and char residual oxidation. The total hydrocarbon gas is considered as methane (CH$_4$) equivalent in this calculation as previously used by Lockwood et al. (1998). It is selected because there are no crucial differences between methane and the gaseous product obtained from devolatilization of coal used.

5.6.4.1 Hydrocarbon gas consumption

Figure 5-17 a and b illustrates the mass fraction of hydrocarbon gas concentration for air-fired, OF25, OF27, and OF29 combustion cases at two ports 1 and 3, respectively. It is clear that the hydrocarbon gas concentration in OF29 is higher in the flame envelope zone (from centerline of the furnace to 0.1 m in the radial direction) compared to the other combustion cases at port 1 (Fig. 5-17 a). As shown in Table 5-3, the volume flow rate is gradually reduced from the air-fired case to OF29 combustion case. This reduction in volume flow rate through the burner increased the residence time and hence the release of hydrocarbon gas from coal particles in the reaction zones. However, at port 3 (Fig. 5-17 b) the consumption of hydrocarbon gas is faster for the OF27 and OF29 cases than the air-fired and OF25 cases. A similar trend was observed in the experiments by Andersson (2007).

![Figure 5-17 a and b](image-url) Mass fraction of hydrocarbon gas concentrations (kg/kg) for the air-fired, OF25, OF27, and OF29 combustion cases at ports: (a) 1 and (b) 3 of the furnace.
5.6.4.2 Char residual oxidation

The rapid reduction of oxygen concentration in the near burner region, due to burning of larger amounts of volatile in the OF27 and OF29 cases, negatively affected the oxidation of the residual char in the remaining part of the furnace. Figure 5-18 a shows the char content of coal particles (%) for the air-fired (A) and OF25 (B) combustion cases in the top half of the furnace. Availability of sufficient oxygen led to burn out of residual char by about 900 (mm) into the furnace. Figure 5-18 b demonstrates the residual char for OF27 (C) and OF29 (D) cases. Shortage of the oxygen content led to reduced char burnout, particularly in the OF29 combustion case. The exclusion of the carbon monoxide (CO) as chemical species in the combustion process (i.e. ignoring the Boudouard reaction) of coal, especially in the flame envelop zone (higher temperature region) may have resulted in lower char burnout in the OF27 and OF29 cases. However, these results certainly confirm that the burning out of hydrocarbon gas is faster and low char burnout is achieved at high O₂ concentration of the oxy-fuel combustion cases as reported in the previous findings (Liu et al. 2005; Tan et al. 2006; Zhang et al. 2010a; Chui et al 2004). As a result, there will be some differences in the total radiation intensities inside the combustor between the reference air-fired case and oxy-fuel combustion case at high O₂ content, especially with high CO₂ concentration in the flue gas.
Chapter 5- Modelling of Lignite Combustion in Air-fired and Three Oxy-fuel Cases in a 100 kW Furnace

Figure 5-18 a. Char content of coal particles (%) for the air-fired (A) and OF25 (B) combustion cases over a cross-section of the upper half of the furnace.

Figure 5-18 b. Char content of coal particles (%) for the OF27 (C) and OF29 (D) combustion cases over a cross-section of the upper half of the furnace.
5.7 Summary and conclusion

The 3 D numerical simulations of pulverized dry lignite in a 100 kW test facility were conducted to simulate four different combustion environments (air-fired, OF25, OF27, and OF29) and to investigate the temperature distribution levels, species concentrations, velocity, and particles consumption in the furnace. The commercial computational fluid dynamics (CFD), AVL Fire ver. 2008.2 was used to model and analyze all the combustion media. Several mathematical models with the appropriate related constants and parameters were employed for lignite coal combustion. The combustion conditions of oxy-fuel combustion cases were satisfied by modifying the following factors: oxygen concentrations in the feed gas and carrier gas, and recycled flue gas rates. The aerodynamic effects of primary and secondary registers of the burner were used to enhance the flame stability. The predicted results of all combustion cases showed a reasonably good agreement against the measured results in terms of temperature distribution levels and species concentrations at the most important locations of the furnace. The numerical results showed that the flame temperature distribution and O$_2$ concentration of oxy-fuel (OF25) combustion case are similar to the air-fired case. Whereas, the flame temperatures of OF27 and OF29 are higher, and the flame structure is shorter and more confined to the region of the burner exit plane because of the higher oxygen consumption. The carbon dioxide concentrations in the oxy-fuel combustion environments were increased by approximately 5 times with respect to the reference combustion case due to using dry RFG (mainly CO$_2$) as feed oxidizer gases instead of air. Due to the usage of a one-step chemical reaction mechanism in these simulations, over-prediction in the moisture content was noticed in the flame envelope zone. The one-step chemical reaction mechanism neglects the dissociation of main combustion products CO$_2$ and H$_2$O into several unstable radicals such as CO, O, H$_2$, and OH. In the air-fired and OF25 combustion cases, the hydrocarbon gas consumption was relatively faster than the OF27 and OF29 cases at port 3. This led to a shortage in oxygen concentration in the near burner regions and therefore more unburned char in OF27 and OF29 cases at port 3. The present study provides the confidence to predict the combustion of coal particles in oxy-fuel conditions. This is important for future simulation, particularly in modeling of a large brown coal oxy-fuel tangentially fired furnace.
Chapter 6. Modelling of Multi-step Reaction and Nitric Oxides Formation
6. Modelling of Multi-step Reaction and Nitric Oxides Formation

6.1 Introduction

The precise investigations on the combustion characteristics of O₂/CO₂ furnaces are of great importance due to the significant increase in the partial pressures of CO₂ and H₂O, and the noticeable decrease of NOₓ in the flue gas recycling. As the oxy-fuel combustion campaign was started in the last decade, several experimental and numerical studies have been conducted on the different coal types in lab-scale and pilot-scale furnaces. These studies could provide relevant information to maintain the similar combustion characteristics to those of the conventional combustion case. Thereby the cost-effective basis can be achieved for retrofitting the equipments of existing power plant or to build a new power plant unit under oxy-fuel combustion conditions. As a result, investigations, development, innovation and research in this approach are significantly important in order to provide confidence and operational experience in a lab-scale and pilot-scale, and then gradually proceed to a large-scale oxy-fuel power plant.

The coal combustion is considered as a complex process with respect to the combustion of liquid and gaseous fuels because it includes several complex physical and chemical processes. During the thermal decomposition of the pulverized coal particles the volatile matter (VM) and moisture content (MC) are released, and the char is stayed as a solid fuel in this pyrolysis process. As a result, in the gas-phase process, several radical species can be formed in the reaction zone such as THC (total hydrocarbon), HCN (hydrogen cyanide), NH₃ (ammonia), N, CO, H₂ etc. In order to be more close to the real reaction mechanisms and achieve an accurate reaction modelling, these intermediate species need to special treatments in the combustion zone. This can be practically performed by applying multi-steps chemical reaction mechanism on these aforementioned species and residual char in order to predict the important species and the thermodynamic equilibrium temperature accurately enough.
Chapter 6- Modelling of Multi-step Reaction and Nitric Oxides Formation

The gaseous and solid phase chemistry mechanisms are presented and discussed in this chapter. Multi-steps chemical reaction mechanisms and nitric oxides formation mechanisms were performed in four different combustion scenarios on a lab-scale 100 kW firing lignite unit (Chalmers’ furnace). Air-fired (reference combustion case) and three different oxy-fuel combustion cases (known as OF25, OF27, and OF29) were modelled again by using AVL Fire ver.2008.2 CFD code, as the solver, and writing the subroutines required for coal devolatilization and coal combustion, and NO\textsubscript{x} models. The temperature distributions and species concentrations inside the furnace were presented and validated against the measurements.

6.2 Numerical description of the furnace

The commercial CFD code, AVL Fire ver. 2008.2 has been used to simulate the combustion, gases and particles flow, heat and mass transfer using the finite-volume technique in an unstructured grid system, inside the furnace as a first step of calculation. SIMPLE algorithm was used for calculating the combination between the velocity and the pressure. For the convergence criterion, the numerical calculations are repeated for all variables in each cell until the accepted convergence limit was achieved with less than $10^{-4}$. Detailed information of the numerical description can be found in a previous chapter. Regarding the NO\textsubscript{x} model calculation, the final step of calculation has been executed after achieving the convergent solutions for all the variables in the main CFD calculations. This means that NO\textsubscript{x} formation processes can be decoupled from the fuel reactions mechanism. Therefore, the transport equations for NO, HCN, and NH\textsubscript{3} have been solved for both Thermal and Fuel NO\textsubscript{x} formation at the end of this simulation. However, in the present study the NO\textsubscript{x} formation process was also carried out together with the fuel reaction mechanism. This means that the transport equations for NO, HCN, and NH\textsubscript{3} have been solved during the simulation simultaneously with the fuel reaction mechanism. But, the two methods of NO\textsubscript{x} calculation produced exactly the same result. In all the simulation cases, the overall convergences for both the combustion mechanism and NO\textsubscript{x} formation are achieved after about 40000-50000 time-step with 0.0025 (s) for each time-step.
6.3 Results and discussion

The numerical results of four different combustion scenarios are presented and discussed in four separate sections: temperature distribution, species concentration, NO\textsubscript{x} formation, and wall radiative heat transfer. The validations of the predicted results were carried out against the experimental data (Andersson 2007) at four different ports (see Table 5-1 for port locations) from the burner exit plane. For the temperature distribution, the comparisons are performed at the most intense combustion locations of the furnace (ports 1, 2, 3 and 4), as well as, along the furnace axis. The species concentrations of O\textsubscript{2}, CO\textsubscript{2}, CO, H\textsubscript{2}O, and H\textsubscript{2} are compared and validated with the measured data at ports 1, 2, 3, and 4 based on the single-, two-, and three-step chemical reactions modelling of the pulverized lignite particles firing. The NO\textsubscript{x} concentrations are presented and compared in term of Thermal and Fuel NO mechanisms at the vertical cut of the furnace axis for the reference, OF27, and OF29 combustion scenarios, while the validation was carried out at port 1 of the furnace for all combustion cases. Finally, the distributions of radiative heat transfer were conducted at the top and vertical walls of the furnace for all combustion scenarios. In order to be in line with the averaging procedure adopting in the experiments of Andersson (2007), all the predicted results presented in this simulation work were time-averaged over the final 10000 time-steps.
6.3.1 Temperature distribution

Figure 6-1 a-d presents the comparison of the temperature distributions (K) at port 1 of the furnace using one-, two-, and three-step chemical reactions for the air-fired, oxy-fuel (OF25), oxy-fuel (OF27), and oxy-fuel (OF29) combustion scenarios, respectively. As stated in section 5 of chapter three, in one- (single) step reaction model, the pulverized lignite particles used in this reaction are simplified to directly convert to $\text{H}_2\text{O}$ and $\text{CO}_2$ as final gas products. This simplified reaction model used does not have the ability to predict well the thermodynamic equilibrium temperature, particularly in the flame envelope zone. This is because it does not include the formation of CO and $\text{H}_2$ species in the combustion zone. As a result, further chemistry reaction steps such as two-step and three-step reaction models are used in this simulation in order to correct any over-predictions of the heat released during the reaction processes.

As shown in Fig. 6-1 a-d, compared to the single-step reaction results, the two- and three-step reaction schemes yield better predictions of temperature profiles close to the boundary walls. The reasons for this an improvement can be explained as follows: First this region (from 200 to 400 mm, in the radial direction) is also showed an improvement of the $\text{O}_2$ concentration profiles for multi-step reactions, as shown in the next subsection of species concentrations (i.e. it showed a good improvement in the combustion conditions in this region). Secondly, the aforementioned region of the furnace is relatively less aerodynamic effect (swirl effect) by the primary and secondary registers than the central axis in the near-burner region. It is also evident in the OF29 scenario (Fig. 6-1 d), in two-step and three-step models, some slight differences in the temperature distributions comparing to the measured data in the region close to the furnace centreline. This discrepancy is probably caused due to sensitivity of combustion to the higher oxygen content in the near-burner reaction region and higher residence time for the coal that leads to increased flame width. These improvements in the temperature distributions of the last two reaction schemes could be caused due to the formation of CO and $\text{H}_2$ as intermediate species. Therefore, the combustion heat is slowly released causing a drop in the maximum flame temperature.
Figure 6-1 a-d. Temperature distribution (K) profile at port 1 of the furnace in one, two, and three-step chemical reactions for (a) the air-fired, (b) oxy-fuel (OF25), (c) oxy-fuel (OF27), and (d) oxy-fuel (OF29) combustion scenarios, respectively.
The flame envelop zone is practically considered the region of higher dissociation to the intermediate species. As mentioned earlier, the dissociation of the main combustion products (H₂O and CO₂) into several intermediate species leads to reduce the peak flame temperature. Therefore, port 3 of the furnace should show the effect of chemical dissociation phenomenon on the temperature distribution inside the flame envelop zone, given in Figure 6-2a-d. The three-step scheme achieved improved agreement with the experiments, particularly in region between the centreline of the furnace and 0.1 m in the radial direction. But, over-prediction is evident in Fig. 6-2a and b for the same aforementioned region in case of two-step reaction scheme. This discrepancy could be due to ignoring water vapour dissociation to H₂ formation, as given in Eqs. (3.58, 3.59, and 3.62) and used in three-step scheme for both the homogenous and heterogenous coal reactions, which led to an increase in peak flame temperature in the furnace. The maximum deviations between the measured and predicted temperatures in the two-step scheme were: 10.06% and 10.38% for the air-fired and OF25 cases, respectively (see Fig. 6-2a and b). However, it is generally observed that the overall qualitative agreement was practically satisfied. Furthermore, in oxy-fuel combustion scenarios, the absorption model used in the radiative heat transfer calculation is of great importance to improve the predicted results because the gas radiation model is highly dependent upon the temperature distribution and species partial pressures (H₂O and CO₂) in the flue gas, as recently explained in similar simulation works (Nikolopoulos et al. 2011; Al-Abbas et al. 2011).
Figure 6-2 a-d. Temperature distribution (K) profile at port 3 of the furnace in one, two, and three-step chemical reactions for (a) the air-fired, (b) oxy-fuel (OF25), (c) oxy-fuel (OF27), and (d) oxy-fuel (OF29) combustion scenarios, respectively.
6.3.2 Species concentrations

This subsection describes the effect of multi-step reaction mechanisms on the main (CO$_2$, O$_2$ and H$_2$O) and intermediate species (CO and H$_2$) concentrations at different locations (ports 1, 2, 3, and 4) inside the furnace for all combustion scenarios.

6.3.2.1 Oxygen concentration

Figure 6-3 a-d. shows the comparisons of oxygen mass fraction (kg/kg) profiles at port 1 of the furnace for the air-fired, oxy-fuel (OF25), oxy-fuel (OF27) and oxy-fuel (OF29) combustion scenarios, respectively for one-, two-, and three-step chemical reactions. In the near-burner region (close to port 1), the oxygen concentrations have an important influence on the combustion characteristics, especially on the ignition conditions and fuel consumption. Therefore, two- and three-step reaction schemes are highly recommended in order to achieve better numerical results at that challenging location of furnace. In Fig. 6-3 a-d, there is an improved agreement between the results of two- and three-step models and experimental data. The improvements are due to O$_2$ reaction with CO and H$_2$ as extra intermediate reactions in the both phases of coal particle combustion.
Figure 6-3 a-d. Oxygen mass fraction (kg/kg) profiles at port 1 of the furnace for (a) air-fired, (b) oxy-fuel (OF25), (c) oxy-fuel (OF27) and (d) oxy-fuel (OF29) combustion scenarios in one, two, and three-step chemical reactions.
6.3.2.2 Carbon dioxide concentration

The fundamental concept of oxy-fuel combustion technique is mainly to increase carbon dioxide concentration in the flue gas. This technique can be applied, as previously mentioned, by using a mixture of pure oxygen and part of RFG as feed oxidizer gases instead of air to burn with fuel. Therefore, in this study, Figure 6-4 is clearly showed the increase in CO$_2$ concentration for all oxy-fuel combustion scenarios (OF25, OF27, and OF29) with respect to the air-fired case. These results were obtained with three-step chemistry mechanism. As seen, the maximum mass fraction value of CO$_2$ concentration was about 17.21 % (kg/kg) for air-firing, while for oxy-fuel cases was, in general, about 90.11 % (kg/kg) due to usage of dry flue gas recycled, as implemented in experimental work of Andersson (2007). However, the purity of oxygen (99.5% pure oxygen used in the experiments) and leakage in the furnace are relevant parameters to decrease CO$_2$ concentration, and therefore they should be taken into consideration in design any oxy-fuel combustion boiler.

Regarding the validation of the numerical results with the experiments and the comparisons amongst the multi-step reaction schemes, ports 2 and 4 are used for this purpose. In Figure 6-5 a-d, the carbon dioxide mass fraction (kg/kg) profiles are presented at port 2 of the furnace for all the combustion scenarios, and chemical reaction mechanism. A good comparison with the experimental data is achieved for two- and three-step reactions in all combustion scenarios. One-step scheme showed some over-prediction, particularly in oxy-fuel cases. This discrepancy, in the one-step reaction, could have been caused due to increase oxygen concentrations in the feed gas oxidizers of the oxy-fuel cases. However, in the heterogeneous reaction of the three-step scheme, the production of carbon dioxide on the carbon surface is ignored because the CO/CO$_2$ production rate is highly increased with the temperature (flame temperature is greater than 1500 k, in this study) and oxygen concentration (Hurt and Calo 2001; Lee 1995). Hence, in three-step numerical model, most CO$_2$ concentrations are supposed coming from the gas-phase reactions (homogeneous reaction).

At port 4 of the furnace, Figure 6-6 a-d shows further investigation on the carbon dioxide mass fraction (kg/kg) profiles for the air-fired, OF25, OF27 and, OF29
combustion scenarios, respectively in one-, two-, and three-step reactions schemes. It can be seen that the numerical result compared well with the experimental data for the two- and three-step numerical models in all combustion scenarios, but one-step scheme shows over-prediction due to increased oxygen concentrations as previously mentioned. It is interesting to note that the Boudouard reaction used in the three heterogenous chemistry model (Eq. 3.61) was improved the three-step numerical results, especially in oxy-fuel cases. On this base the three-step chemistry mechanism model has been used to visualize the carbon dioxide concentration, as already shown in Fig. 6-4.

![Fig. 6-4. Carbon dioxide concentration (kg/kg) at the vertical cut along the furnace axis for the reference air-fired case (left hand sides) and oxy-fuel combustion environments OF25, OF27, and OF29 (right hand sides) respectively, all dimensions are in mm.](image-url)
Figure 6-5 a-d. Carbon dioxide mass fraction (kg/kg) profiles at port 2 of the furnace for (a) the air-fired, (b) oxy-fuel (OF25), (c) oxy-fuel (OF27) and (d) oxy-fuel (OF29) combustion scenarios, respectively in one-, two-, and three-step chemical reactions.
Figure 6-6 a-d. Carbon dioxide mass fraction (kg/kg) profiles at port 4 of the furnace for (a) the air-fired, (b) oxy-fuel (OF25), (c) oxy-fuel (OF27) and (d) oxy-fuel (OF29) combustion scenarios, respectively in one-, two-, and three-step chemical reactions.
6.3.2.3 Carbon monoxide concentration

The distributions of carbon monoxide (CO) concentrations are presented in Fig. 6-7 on a vertical plane through the furnace axis for the reference air-fired case (left hand sides) and oxy-fuel combustion scenarios OF25, OF27, and OF29 (right hand sides), respectively. As seen, for the air-fired and OF25 cases, the distributions of CO concentrations showed some similarities in the near-burner region. This similar trend of distribution between the two aforementioned combustion cases is definitely caused due to the similar distributions of the flame temperatures in the upper part of the furnace, as already shown in Fig. 5-5. In contrast, OF27 and OF29 cases show higher CO concentration compared to the reference firing and OF25 cases, particularly near the furnace centreline. This increase in CO concentrations might be due to increase in the O$_2$ concentration in the feed oxidizer gases and residence time, in OF27 and OF29 cases, which also leads to increase the combustion temperature. The higher flame temperature in general leads to enhance the chemical dissociation of main species in the flame envelop zone, and therefore increases the intermediate species concentrations, as recently investigated by Kim et al. (2009). They predicted the structure of natural gas flames in both air-firing and oxy-fuel combustion scenarios by coupling a conditional moment closure reactive model with the flow solver. The detailed chemistry model was used to precisely calculate the intermediate species formed due to thermal dissociation at higher temperature.
Figure 6-7. Carbon monoxide concentration (kg/kg, dry) on a vertical plane through the furnace axis for the reference air-fired case (left hand sides) and oxy-fuel combustion environments OF25, OF27, and OF29 (right hand sides) respectively, all dimensions are in mm.
Fig. 6-8 a-d shows the carbon monoxide (CO) mass fraction (kg/kg) profiles at port 1 of the furnace for the air-fired, OF25, OF27, and OF29 combustion scenarios, respectively in two- and three-step chemistry mechanisms. For all combustion cases, a good agreement is achieved between the physical data and predicted results for both the two- and three-step reaction schemes. As previously stated in sections 3.5.2 and 3.5.3 of chapter 3, Eqs. (3.54), (3.56), and (3.58) are strongly showed the clear connection between the CO concentration and CO$_2$ in the reverse reactions. This means that the two- and three-step reaction schemes used to describe the coal conversion can highly capture the equilibrium between CO and CO$_2$ in the flame zone. A slight over-prediction, in Fig. 6-8d, is observed close to the furnace centreline, which is representing the rich-fuel mixture region in the furnace. This discrepancy might be caused due to an increase in the CO/CO$_2$ production rate in OF29. This combustion case has the higher residence time for burning coal particles comparing to the other combustion cases (see Table 5-3). As a result, the thermal dissociation of the main species is largely enhanced in that region of furnace to produce a high amount of CO. In addition, the higher O$_2$ concentration in OF29 could also have contributed to this increase in CO concentration.
Figure 6-8 a-d. Carbon monoxide mass fraction (kg/kg) profiles at port 1 of the furnace for (a) the air-fired, (b) oxy-fuel (OF25), (c) oxy-fuel (OF27) and (d) oxy-fuel (OF29) combustion scenarios, respectively in two and three-step chemical reactions.
6.3.2.4 Water vapour concentration

Fig. 6-9 a and b presents the water vapour mass fraction (kg/kg) profiles at port 4 of the furnace for the air-fired and oxy-fuel (OF29) combustion scenarios, respectively in one-, two-, and three-step reaction schemes. The numerical results obtained with the three-step scheme are closer to the experimental data for both combustion cases, while the one- and two-step results showed over-prediction. The improved predicted results for the three-step scheme are due to using further chemistry reactions in both the combustion phases. In the homogeneous gas-phase reaction, two reverse reactions (Eqs. 3.58 and 3.59) participated to improve the balance between H$_2$O and H$_2$ in the near-burner region for both the air-fired and OF29 cases. In addition, compared to the one- and two-step reaction results, a clear reduction in the water vapour is achieved in the three-step scheme due to the reaction of available H$_2$O with the residual char particles, as displayed in the gasification process (Eq. 3.62) of the heterogenous solid-phase reaction.

![Figure 6-9 a and b. Water vapour mass fraction (kg/kg) profiles at port 4 of the furnace for (a) the air-fired and (b) oxy-fuel (OF29) combustion scenarios, respectively in one-, two-, and three-step chemical reactions.](image-url)
6.3.2.5 Hydrogen concentration

To elaborate improvements in the main and intermediate species in the three-step chemistry mechanism, hydrogen concentration (kg/kg) profiles at port 1 of the furnace for the air-fired, OF25, OF27 and OF29 combustion scenarios are presented in Fig. 6-10. It can be observed that the H$_2$ concentration is higher in the fuel-rich mixture for all combustion cases. As expected, there is an increase in H$_2$ concentration for the OF27 and OF29 cases, but the air-fired and OF25 cases showed less production level of H$_2$, and the two latter cases have approximately a similar distribution trend. This result has been given a clear explanation to the connection between the O$_2$ concentration and production rates of intermediate species, especially the related H$_2$ and CO formation, as previously illustrated in the hot flame zone. Although, the numerical results of these species are in reasonable qualitative and quantitative agreement with the experimental data, further chemistry reaction schemes are required in order to describe the thermal pyrolysis of coal particles and the related intermediate species more precisely.

![Figure 6-10. Hydrogen concentration (kg/kg) profiles at port 1 of the furnace for the air-fired, oxy-fuel (OF25), oxy-fuel (OF27) and oxy-fuel (OF29) combustion scenarios at three-step reaction scheme.](image)
6.3.3 NO\textsubscript{x} concentrations

The NO\textsubscript{x} emissions distribution is presented on a vertical cut through the furnace axis for the air-fired, OF27, and OF29 combustion cases as shown in Fig. 6-11. The images of the figure show full width of the furnace (i.e. from -400 mm to +400 mm), whilst the height is limited to the axial distance: 0.0 to 1200 mm from the burner exit plane. The highest predicted values of NO\textsubscript{x} concentration inside the furnace were 455 ppm, 374 ppm, and 421 ppm for the air-fired, OF27, and OF29 cases, respectively. As seen in Fig. 6-11, the distribution of the NO\textsubscript{x} concentration inside the furnace was noticeably different between the air-fired and oxy-fuel (OF27 and OF29) cases. The NO\textsubscript{x} emissions distribution of OF25 combustion case was not presented because it is approximately similar to the reference (air-fired) case. For the air-fired case, the concentration of NO\textsubscript{x} emissions started at about 400 mm in the axial distance from the burner exit plane. In contrary to the air-fired case, the concentrations of NO\textsubscript{x} emissions for OF27 and OF29 cases were initiated further downstream in which the predicted emissions of NO\textsubscript{x} was started at about 800 mm and 900 mm from the burner exit plane for OF27 and OF29 cases, respectively.

In addition, there is another difference in the NO\textsubscript{x} distribution between the reference case and oxy-fuel combustion cases. In the air-fired case, a very high concentration of NO\textsubscript{x} along the furnace centreline, especially in the region close to the near-burner region was observed. This higher value of nitric oxides may be caused due to the activation of thermal mechanism of NO formation, which is completely dependent on the flame temperature and oxygen concentration (Bowman 1975; Miller and Bowman 1989). In fact, the thermal NO formation is strongly dependent on the temperature distributions and O\textsubscript{2} concentration (see Fig. 5-5). In contrast, it can be seen that, in OF27 and OF29 cases, the concentration of NO\textsubscript{x} emissions is very low in the vicinity of the burner compared to other locations inside the furnace. This is due to ignoring the thermal NO, i.e. there is no atomic nitrogen (N) entering the furnace except that from the air leakage. The above-mentioned region showed low O\textsubscript{2} concentrations in the oxy-fuel combustion scenarios, as stated in Ref. of Al-Abbas et al. 2011.
On the same trend of connection between NO$_x$ and O$_2$ in the furnace, for oxy-fuel cases, there is an elevated concentration of NO$_x$ near the wall compared to the air-fired case. This aspect can be attributed to the higher concentration of oxygen in that region of furnace, and as a result the conversion of fuel nitrogen to NO is increased. In fact, this process of conversion to NO is strongly dependent on the local combustion characteristics, as well as the nitrogen-bound compounds of the coal. However, from these numerical results of all combustion cases, it can be noticed that the concentration of NO$_x$ emissions for the air-fired case is commonly higher than those of oxy-fuel cases because there is no production to the thermal NO in oxy-fuel scenarios. The overall reduction ratios of the NO$_x$ emissions for the oxy-fuel cases compared with the air-fired case were around 18% and 9%, in total, for OF27 and OF29 cases, respectively. The increase of the NO$_x$ concentrations in the OF29 case compared to the OF27 case was probably due to the higher O$_2$ concentration in the combustion environment, and thus enhanced the conversion of fuel nitrogen to NO. These findings are very consistent with the previous experimental (Tan et al. 2006) and numerical works (Nikolopoulos et al. 2011; Chui et al. 2003).

Figure 6-11. NO$_x$ emissions (ppm) on a vertical cut through the upper part of the furnace axis for the air-fired, oxy-fuel (OF27), and oxy-fuel (OF29) combustion scenarios, all dimensions are in mm.
Fig. 6-12a-d presents the comparisons and validations of the NO\textsubscript{x} emissions between the predicted results and measured data at port 1 for all combustion scenarios. Generally, the predicted results of the NO\textsubscript{x} were in a good agreement with the measured data for all combustion cases. As was discussed in the species concentration subsection, in the air-fired and OF25 cases, the O\textsubscript{2} concentration was higher than those of OF27 and OF29 cases along the centreline of the furnace. This higher value of oxygen affected the NO\textsubscript{x} emissions in that region of the furnace. As seen in Fig. 6-12a and b, the concentrations of NO\textsubscript{x} were higher at the centreline of the furnace compared to the other locations along the port 1. In contrast, the higher values of NO\textsubscript{x} in OF27 and OF29 cases, were far from the centreline of furnace at port 1, as showed in Fig. 6-12c and d. In the latter two combustion cases, the maximum predicted values of NO\textsubscript{x} emissions were noticed from 200 mm away from the centre, measured in the radial direction, which also were the region of higher oxygen concentration (see Fig. 6-3). In OF29 case, there was over-prediction in the numerical results of NO\textsubscript{x} emission with respect to the experimental data in the aforementioned region (i.e. from 200 mm away from the centre, measured in the radial direction). This over-prediction could be caused due to the rapid reaction of oxygen with the intermediate species HCN and NH\textsubscript{3} (see Eqs. 3.70 and 3.72) during the oxidation process that leads to form the higher fuel NO concentrations in that location of the furnace. In contrast to this discrepancy, it can be seen that there was a good agreement of the numerical results with the measured data at the centreline of the furnace (Fig. 6-12 d). Although, there was over-prediction in OF29, the numerical results for all cases have maintained the same trend with the experimental data at that critical port. The maximum deviation of the predicted results with the measured data at port 1 were around 14\%, 7\%, 13\%, and 8\% for air-fired, OF25, OF27, and OF29 cases, respectively. These numerical deviations from the measured data can also be partially attributed to the uncertainties of measured data and/or to the lack of measurements calibration. Therefore, the numerical deviation values can be accepted up to 20\% from the experimental data as described in Nikolopoulos et al. (2011). Finally, the predicted results of the present modelling study could capture the main qualitative and quantitative aspects of the measured data in all combustion environments, especially at that given location (port 1) of the furnace.
Figure 6-12 a-d. NO\textsubscript{x} concentration (ppm) profiles at port 1 of the furnace for (a) the air-fired, (b) oxy-fuel (OF25), (c) oxy-fuel (OF27) and (d) oxy-fuel (OF29) combustion scenarios, respectively.
6.3.4 Wall radiative heat transfer

In this subsection of discussion the radiative heat transfer on the furnace wall is presented for all combustion scenarios, as shown in Fig. 6-13. As already observed in the species concentrations section, CO$_2$ and H$_2$O concentrations in the flue gas increased in all oxy-fuel combustion cases. Under this specific condition of oxy-fuel combustion characteristics the effect of gas mixture on the calculation of the radiative heat transfer should be considered. The change in the radiative properties of the gas-mixture under oxy-fuel conditions is taken into account in the present study. The specific heat capacity of CO$_2$, which is dominant in the gas-mixture of oxy-fuel combustion, is high with respect to that of N$_2$.

The WSGGM used in this study accounted for the effect of higher CO$_2$ and H$_2$O concentrations in the calculation of gas absorption coefficient for the radiative heat transfer model used. In their recent study Zhou and Moyeda (2010) used WSGGM for the oxy-fuel combustion purpose. As seen in Fig. 6-13, there is a slight increase in the radiative heat transfer on the furnace wall in the oxy-fuel cases compared to the air-fired case at the same fuel input power (76 kW). Furnace temperature and radiative properties of gas mixture are the main reasons for that increase on the furnace wall under oxy-fuel conditions. The net radiative heat fluxes on the furnace wall were 70.77, 70.2, 74.55, and 77.91 kW for the air-fired, OF25, OF27, and OF29 cases, respectively. Similar investigations (Nikolopoulos et al. 2011; Erfurth et al. 2010) are confirmed with the trend of the present predicted results. Although, higher CO$_2$ concentration observed in the OF25 with respect to the air-firing, a similar radiative heat transfer value is achieved for both the aforementioned combustion cases. This is due to the flames temperature similarity, as shown in Fig. 5-5. It can also be seen that the radiative heat flux values of OF27 and OF29 are not too far from the air-firing values. This may be due to the reduction in the flue gas velocity which has significant influence on the heat transfer distribution of the furnace wall (see Table 5-3 for more details about the inlet flue gas velocities for different combustion cases). However, the oxygen concentrations in the feed oxidizer gases and the flue gas volume rates are also other relevant parameters, in oxy-fuel cases, that could be used to match the corresponding heat flux of the air-fired...
combustion. This is of a great importance in design of the boiler material under oxy-fuel combustion conditions, as investigated experimentally by Tan et al. (2006).

Figure 6-13. Wall radiative heat flux for air-fired, oxy-fuel (OF25), oxy-fuel (OF27), and oxy-fuel (OF29) combustion scenarios.
6.4 Summary and conclusion

The commercial computational fluid dynamics (CFD), AVL Fire ver. 2008.2 was used to predict and analyze four different combustion scenarios (air-fired, OF25, OF27, and OF29), simulating the experiments on a 100 kW Chalmers’ lab-scale furnace. The temperature distributions, species concentrations (O₂, CO₂, CO, H₂O, and H₂), NOₓ emission concentrations were investigated at different locations inside the furnace, as well as, the radiation heat transfer on the furnace wall. The multi-step chemical reaction mechanisms were carried out on the homogenous and heterogeneous reactions of the pulverized lignite particles in terms of single-, two-, and three-step reaction models. The appropriate mathematical models with the related constants and kinetics parameters were used to increase the certainty of predicted results against the measured data, particularly under oxy-fuel combustion conditions. The simplified approach of the chemical kinetics has been modelled to calculate the Fuel and Thermal NO formation, decoupled from the main fluid flow computations.

The present simulation results showed a very reasonable agreement with the measured results for all combustion scenarios, especially with the three-step reaction model. Generally, the predicted results of the three-step chemistry reaction mechanism illustrated improved agreement compared to those of the one-step and two-step reaction schemes. The improvements were particularly observed in the flame envelope zone in terms of the temperature distributions and species concentrations. This is due to the adoption of thermal dissociation of chemical species in the three-step reaction scheme. Furthermore, the three-step chemical reaction mechanism used to describe the fuel conversion can precisely capture the CO/CO₂ production rate and equilibrium between H₂ and H₂O in the near-burner region (fuel-rich zone). A clear difference was observed in the NOₓ distribution between the reference case and oxy-fuel (OF27 and OF29) combustion cases at the centreline of the furnace in the near-burner region. This is principally due to absence of thermal NO formation under oxy-fuel combustion conditions, i.e. there is no dissociation process used to the air-nitrogen and only the conversion of the nitrogen-bound compounds of the coal to fuel NO was adopted during oxy-fuel scenarios. Finally, the elevated values in the flame temperatures and CO₂ and H₂O concentrations under oxy-fuel combustion cases led to increased radiation heat flux.
on the furnace wall. This is important and should be taken into consideration during design the new oxy-fuel tangentially fired furnace.
Chapter 7. Modelling of Brown Coal Combustion in a Full-scale Tangentially-fired Furnace
7. Modelling of Brown Coal Combustion in a Full-scale Tangentially-fired Furnace

7.1 Introduction

In order to design such efficient, clean, and economical brown coal combustion systems, the understanding of the brown coal reactivity and behaviour under several combustion conditions is required. Generally, brown coal has a number of advantages such as abundance, low-cost, high reactivity, and low sulphur content. In despite of these benefits, a high moisture content (about 60-70 wt %) is the major disadvantage of brown coal. However, in the existing pulverised brown coal (PC) tangentially-fired boiler, a large amount of the hot exit flue gas, typically 50% of the total flue gas generated, is reused to dry the brown coal within the mill-duct system (Dodds et al. 2011; Achim et al. 2009; Ahmed and Naser 2011). During that drying process by the hot gas off-takes (HGOTs), a large amount of water vapour is reproduced as well. In order to avoid any flame stability problems inside the combustion chamber, due to that evaporated steam, a fuel-rich mixture (mainly pulverised coal) is passed through the main burner ducts. Whilst a fuel-lean mixture, including water vapour, inert gases, and remaining of PC, is delivered to the inert burner ducts (upper burners). This distribution of the PC and inert gases into the firing system is favourable, particularly in this type of combustion technology.

This chapter focuses on the numerical investigation of a large-scale oxy-fuel furnace. Therefore, the objective of this study is to simulate the brown coal combustion in the large-scale tangentially-fired furnace under several operating conditions. A computational fluid dynamics (CFD) code, AVL Fire ver.2008.2, was used to model and analyse four different combustion environments. A conventional PC combustion and three oxy-fuel combustion scenarios, are known as OF25, OF27, and OF29, were simulated. The subroutines required for the PC devolatilization, char burnout, multi-step chemical reactions, mass and heat transfer, carbon in fly-ash, and nitric oxidizes formation/destruction have been written and incorporated into the CFD code, as user-
defined functions (UDFs). The validation of the CFD results with the power plant data has been conducted in the air-fired combustion. Four parameters: flue gas composition, gas temperatures, carbon in fly-ash, and HGOT mass flow were compared. Results, for all combustion cases investigated, are compared. The species concentrations, temperature distributions, gas-phase velocity fields, char burnout, NO\textsubscript{x} emissions, and radiative heat transfer obtained for all combustion cases were compared.

### 7.2 Boiler description and operating conditions

The tangentially-fired Victorian brown coal 550 MW\textsubscript{e} boilers located in the Latrobe Valley mine, Victoria/Australia was used in this simulation study. The geometric description of the CFD model for the boiler, unit 1 at Loy Yang A, is shown in Fig. 7-1. Under maximum continuous rating (MCR) of operating conditions, the unit produces 430 kg/s of steam flow through the main steam piping at 16.8 MPa and 540 °C. The computational domain illustrated in Fig. 7-1 was extended from the furnace hopper up to the top of the tower, passing through the transition of round duct to before the bifurcation at the inlet to the air heaters. In this CFD model, the complex geometric dimensions of the simulated boiler were 98.84 m (height), 17.82 m (width), and 17.82 m (depth), having a net simulated volume of 35,894 m\textsuperscript{3} up to the bifurcation point to the air heaters.

The tangentially-fired furnace used in this study consists of eight mill-duct systems, two on each side face of the four-sided furnace. For each mill-duct system, there are six separate burners, including three inert burners and three main burners, as well as a hot gas off-take (HGOT) that dries the brown coal. The mill-duct systems were designed for the following purposes: grinding the raw coal into pulverised coal (PC) in the mill, removing the moisture content (62% wt) from the brown coal through the drying shaft, and transporting and distributing the PC. The centrifugal separation system is used to deliver pulverised coal from the grinding mill to the inert and main burners of the furnace. The distribution of PC at both the burner mouths was accompanied by the inert flue gas and water vapour from the drying process in the mill. Approximately 82% of
the PC and 34% of the gases is delivered to the main burner (PC burner) and the remaining 18% of pulverised coal and 66% of the gases is transported to the inert burner (vapour burner). This distribution of fuel and gases (fuel-rich mixture) to the main burners is required to maintain combustion stability in the furnace burning Victorian brown coal.

Figure 7-1. The geometric description of the CFD model for the boiler, unit 1 at Loy Yang A power station.
Regarding the operating conditions, only five mills (1, 2, 5, 6, and 8 mills) are in service (in operation) and the remaining mills are out of service (3, 4, and 7 mills), as shown in Fig. 7-3. Therefore, under full load operation, approximately 81.3 kg/s of PC and 422.8 kg/s of gas mixture are passed through both the inert and main burners of the furnace at different flow distribution ratios. Table 7-1 shows the mass flow distribution of PC and mill gas at each inlet port of the burner ducts. The overall number of vapour and PC burners was 48, while 18 of the total burners were practically out of service, i.e. no fuel is introduced in the latter burners. In the furnace zone, the burners' arrangements on the furnace wall surface were as follows from top to bottom: upper inert burner (UIB), intermediate inert burner (IIB), lower inert burner (LIB), upper main burner (UMB), intermediate main burner (IMB), and lower main burner (LMB).

Table 7-1. The mass flow rates and the distribution ratios for PC and mill gas at each inlet port of the burner ducts.

<table>
<thead>
<tr>
<th>Burner duct</th>
<th>PC flow (as receive.)</th>
<th>Gas flow</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mass flow rate (kg/s)</td>
<td>Distribution ratio (%)</td>
</tr>
<tr>
<td>UIB</td>
<td>0.93</td>
<td>5.7</td>
</tr>
<tr>
<td>IIB</td>
<td>0.54</td>
<td>3.3</td>
</tr>
<tr>
<td>LIB</td>
<td>1.57</td>
<td>9.4</td>
</tr>
<tr>
<td>UMB</td>
<td>4.82</td>
<td>29.7</td>
</tr>
<tr>
<td>IMB</td>
<td>2.78</td>
<td>17.2</td>
</tr>
<tr>
<td>LMB</td>
<td>5.62</td>
<td>34.7</td>
</tr>
<tr>
<td>Total</td>
<td>16.26</td>
<td></td>
</tr>
</tbody>
</table>

The locations, reference levels (R.L.), of the above-mentioned burners are based on the original ground level of the power plant, as shown in Fig. 7-2. The secondary air port ducts were set up above and below each burner in order to improve combustion characteristics. A schematic demonstration of the secondary air ports, in the inert burners, was as follows from top to bottom: upper inert secondary air duct (UISAD), upper intermediate inert secondary air duct (UIISAD), lower intermediate inert secondary air duct (LIISAD), lower inert secondary air duct (LISAD). While in the main burner, the schematic demonstration of the secondary air ports was shown as follows: upper main secondary air ducts 1 and 2 (UMSAD1& 2), intermediate main secondary air ducts 1 and 2 (IMSAD1& 2), and lower main secondary airducts1 and 2.
In order to control the air flow distribution in the central zone of the main burners, a core air duct is installed in the middle of each PC burner, i.e. upper, intermediate, and lower core secondary air ducts (UCSAD, ICSAD, and LCSAD). It is designed as a series of round holes in a crucifix shape for dividing the PC burner duct into four small ports, as illustrated in Fig. 7-2. Regarding the burner configuration, each burner port 1, 3, 5, and 7 were inclined 24° with the perpendicular line to the furnace face, while each the remaining burner ports 2, 4, 6, and 8 were inclined by 30°. This configuration of the burner’s set up was mostly used in this type of tangentially-fired furnace in order to improve flame stability inside the furnace, as schematically plotted in Fig. 7-3.
In representing the convection zone, eight different sources of heat sinks were implemented above the location of hot gas off-takes (HGOTs), i.e. above R.L.=168.0 m, more details about heat sink sources can be found in the wall boundary conditions subsection (4-2-2). Geometric details beyond the bifurcation of air heaters and the mill-duct system have not been included in the present CFD model. Previous numerical study (Dodds et al. 2011) of the PC distribution in this mill-duct system has investigated the coal flow, flue gas velocity, and temperature distribution. The present study mainly focussed on the brown coal combustion in the furnace.
Chapter 7- Modelling of Brown Coal Combustion in a Full-scale Tangentially-fired Furnace

7.3 Computational methodology

7.3.1 Numerical description

The commercial CFD code, AVL Fire ver.2008.2, has been employed to model the brown coal combustion in a 3-D large-scale boiler model. The geometric model was accurately constructed using the CAD tool, and the dimensions of model geometry were taken from the power plant drawings. The first step of this simulation has been carried out solving of the 3-D governing equations of combustion, heat and mass transfer, and turbulent flow under transient mode. The numerical solutions are repeated for all variables in each control volume until the usual convergence limit was achieved with less than $10^{-4}$; the code is based on the finite-volume approach. However, for the convergence criteria, simulations were run up to 48,000 time-steps until the stable quasi steady state was reached. Then, the CFD results were averaged over the final 8,000 time-steps. After the converged solution was achieved for the two-phase (gases and particles) flow, the second step of the simulation was subsequently implemented for the NO$_x$ formation/destruction models. This means that the transport equations for NO, HCN, and NH$_3$ have been solved at the end of this simulation, decoupling from the main CFD calculations following the approach of Nikolopoulos et al. (2011). The combination of velocity and pressure in Navier-stokes equations was solved by using the standard SIMPLE algorithm. A Lagrangian/Eulerian approach was used for gas-solid two-phase flow. Under the initial simulation set up, the time-step used in this simulation was limited to 0.0005 (s) in order to allow for the temperature profile to stabilize. As soon as the simulation results become more stable, the time-step is increased up to 0.0025 (s), an appropriate value by the numerical stability. The total number of particles used in this simulation was 50,000 particles, and the share of each in service mill-duct system was 10,000 particles. The distribution of brown coal particles through each burner ports was based on the distribution ratio of the PC (see Table 7-1). In the convection zone of the furnace, heat absorption sources for the water tube wall and convective tube banks were simulated as heat transfer sink terms (user defined sinks) in the enthalpy equation.
7.3.2 Boundary conditions

The modelling of the brown coal combustion used in the present large-scale utility boiler was required a special concentration on the boundary conditions of the furnace. Therefore, in this study, a large effort has been made on the boiler boundary conditions. The boundary conditions of the present simulated furnace were divided into three main categories: the inlet, the wall, and the outlet.

7.3.2.1 The inlet boundary condition

The fuel (Victorian brown coal) and the other oxidizers and gases such as inert flue gas, water vapour, air, or/and O₂/CO₂ are injected into the furnace from the mill-duct systems to several inlet ports located on the wall surface of the furnace. During the injection process, each firing group system (burners and secondary air ducts) receives the same amount of fuel and oxidizers. The mass flow rate of the PC and gas, in each burner, is set to receive 16.26 kg/s and 84.56 kg/s, respectively under full load operation. Furthermore, each inlet port of the burner ducts is set to obtain a fixed distribution ratio of the PC and gas, as summarized in Table 7-1. It was also supposed that the gas mixture has been fine-tuned in mixing after the mill, and as a result all burners of the furnace are received the same composition of gases. The inlet temperature of the PC and gas is set to 397K. The secondary air was also supposed to be equally distributed across each mill-duct group. The total amount of air mass flow rate and air inlet temperature to each mill group is set to be 120.79 kg/s. and 473K, respectively.

The main sources of leakage air in the boiler are supposed to be in the mill-duct system, firing group system, and hopper region. The effects of the first two sources are taken into account in this simulation through the gas composition and its temperature, as previously investigated in the similar numerical study (Nikolopoulos et al. 2011). Whilst the third source was not included. However, the boiler was assumed to operate under a slight negative pressure in order to avoid or minimize the egress of pollutants through the ports. Generally, this assumption is particularly important for oxy-fuel combustion because of increasing CO₂ concentrations and other harmful gases in the
flue gas. On the furnace wall surface, the effect of upstream burner geometry was partially taken into consideration in this modelling. However, the effect of modelling the boiler with upstream mill ducting is of great importance in establishing the efficient mixing and the flow patterns within the furnace (Achim et al. 2009).

In the upper main burner, the measured data of the particle size distributions were validated with the Rosin-Rammler (RR) distributions function, as shown in Fig. 7-4. The RR distribution is a common method and extensively applied to calculate the particle size distribution of different types and sizes of powders. Therefore, the values of the latter distributions function are used, in this CFD study, to describe the particle size distribution (PSD) of particles generated by grinding the raw brown coal in the mill-duct system.

![Figure 7-4. Validation of the PC size distributions between the measured data and the Rosin-Rammler (RR) distributions function.](image-url)
Detailed theoretical information of the RR distribution function can be found in Djamarani and Clark (1997), and the related parameters used in this work are summarized in Table 7-2 for all inlet ports of the inert and the main burners. For the gas inlet flow, the turbulent kinetic energy is set to be $0.01 \text{ m}^2\text{s}^{-2}$; whilst its dissipation rate is set according to the length scale, which is equal to 0.042 m and 0.039 m for the inert burners and the main burners, respectively. However, the outlet boundary conditions of the previous numerical effort (Dodds et al. 2011), which used to describe the PC distribution in this mill-duct system of the Loy Yang power station, are used as inlets to the furnace in the present study.

Table 7-2. The Rosin-Rammler (RR) distribution parameters for the PC used in this study at each inlet port of the burner ducts (dry basis).

<table>
<thead>
<tr>
<th>Burner duct</th>
<th>RR distribution parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Min. particle size (m)</td>
</tr>
<tr>
<td>UIB</td>
<td>1.0E-05</td>
</tr>
<tr>
<td>IIB</td>
<td>1.0E-05</td>
</tr>
<tr>
<td>LIB</td>
<td>1.0E-05</td>
</tr>
<tr>
<td>UMB</td>
<td>1.0E-05</td>
</tr>
<tr>
<td>IMB</td>
<td>1.0E-05</td>
</tr>
<tr>
<td>LMB</td>
<td>1.0E-05</td>
</tr>
</tbody>
</table>

7.3.2.2 The wall boundary condition

Due to the complexity in the boiler design, the furnace wall was modelled by dividing it into four different boundaries, as follows: furnace zone wall, water tube wall, convection zone wall, and round duct wall. These divisions of the furnace wall parts are appropriate for the heat transfer wall model. Generally, for the gas phase, a non-slip condition ($u, v, \text{ and } w=0$) is applied for the entire wall surface. For the solid phase, a non-elastic spherical collision model was employed to control the interaction between the wall and particles. Hence, the parallel momentum of the particles to the wall is retained and the value of the perpendicular momentum is reduced by means of the compensation coefficient of 0.9. For the wall function calculations, a hybrid wall treatment is implemented on the wall boundary to certify a gradual change between
laminar and turbulent part of the boundary layers. The temperature and the emissivity of the wall surfaces are set to be 973K and 0.71, respectively.

In order to precisely match the power plant data with these simulation boundary conditions, the effect of heat sink in the convection zone (convective tube banks) and water tube wall region of the furnace are taken into account as a cell selection in the computational domain. The convective tubes are penetrated in a perpendicular direction to the flue gas flow inside the convection zone. The top-bottom sequence of the convective tubes is: economiser, reheater 1a, superheater 2, reheater 1b, superheater 3, reheater 2, superheater 4, and superheater 1, as shown in Fig. 7-1. In the water tube wall, the tubes were set up in a parallel direction to the flue gas flow. They were limited by the region between R.L. =152.940 m and R.L. =162.0 m around the four sides of the furnace wall surface. Based on the power plant data, the values of heat absorption in the convective tube banks and water wall are summarised in Table 7-3 and incorporated as a separate subroutine (user defined) in enthalpy equation.

Table 7-3. The heat absorption values (MW) by the convective tube banks and water tube wall of the power plant.

<table>
<thead>
<tr>
<th>Convective tube banks</th>
<th>heat absorption values (MW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Economiser</td>
<td>100.20</td>
</tr>
<tr>
<td>Reheater 1a</td>
<td>121.98</td>
</tr>
<tr>
<td>Superheater 2</td>
<td>151.74</td>
</tr>
<tr>
<td>Reheater 1b</td>
<td>121.98</td>
</tr>
<tr>
<td>Superheater 3</td>
<td>192.12</td>
</tr>
<tr>
<td>Reheater 2</td>
<td>98.48</td>
</tr>
<tr>
<td>Superheater 4</td>
<td>52.27</td>
</tr>
<tr>
<td>Superheater 1</td>
<td>68.44</td>
</tr>
<tr>
<td>Water wall</td>
<td>458.75</td>
</tr>
</tbody>
</table>
7.3.2.3 The outlet boundary condition

In this category of boundary condition, there are two different types of outlets for the simulated furnace. One boundary was in the bifurcation at the inlet to the air heaters, while the other was represented by the HGOTs. A zero gradient was applied for all variables in the bifurcation boundary. In contrast, and based on the power plant data, a negative value of flue gas flow rate (-61.0 kg/s) was applied at each exit port of the HGOTs, except for those out of service. This value was taken from the power plant data. In addition, the gas composition and its temperature were also taken into account in this boundary condition.

7.3.3 Cases studies set up

For this numerical study, four different combustion scenarios have been selected in order to estimate the performances of the 550 MWₑ large-scale boilers under different firing conditions. In the first simulation case, the chemical and physical set up of the boiler operations were completely based on the station data (Staples and Marshall 2010). This first case represents a reference (air-fired) case in investigating the behaviour of brown coal combustion and the boiler performance for the three challenging oxy-fuel combustion scenarios. For the proposed (retrofitted) oxy-fuel combustion scenarios, the thermodynamics set up of the lab-scale oxy-fuel furnace (Andersson 2007), conducted at Chalmers University, was selected in terms of the gas compositions and volumetric flow rates of feed oxidizer gases. The retrofitted oxy-fuel combustion cases are defined as follows: OF25 (25 vol.% O₂ and 75 vol.% CO₂), OF27 (27 vol.% O₂ and 73 vol.% CO₂), and OF29 (29 vol.% O₂ and 71 vol.% CO₂). Detailed information about the Chalmers’ furnace and the combustion conditions can also be found in the previous simulation studies (Al-Abbas et al. 2011; Al-Abbas and Naser 2012).

For oxy-fuel combustion scenarios, efforts were made to reduce as much retrofits as possible to the existing industrial power plant. However, under the operating conditions of the furnace, the total mass flow rates of the feed oxidizer gases (mostly O₂ and CO₂),
in secondary ducts, were gradually decreased to maintain same combustion temperatures to the corresponding reference case. However, the reduction in the volumetric flow rates of RFG, in the retrofitted oxy-fuel cases, were 17%, 23%, and 28% in the OF25, OF27, and OF29, respectively with respect to the reference case, using the same approach to that of the Chalmers’ furnace. Although, there was a comparative reduction in the total gas flow rates, the distribution ratios were kept constant in each port of the secondary ducts, as summarized in Table 7-4 for all combustion cases. The temperatures of feed oxidizer gases (O$_2$/N$_2$ or O$_2$/CO$_2$) are fixed to 200 °C.

Table 7-4. The mass flow rates (kg/s) of air (O$_2$/N$_2$) and O$_2$/CO$_2$ for the reference (air-fired) and oxy-fuel combustion scenarios, respectively at each secondary air duct.

<table>
<thead>
<tr>
<th>Secondary air duct</th>
<th>Distribution ratio (%)</th>
<th>Combustion scenarios</th>
<th>Mass flow (kg/s)</th>
<th>Mass flow (kg/s)</th>
<th>Mass flow (kg/s)</th>
<th>Mass flow (kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Air</td>
<td>OF25</td>
<td>OF27</td>
<td>OF29</td>
<td></td>
</tr>
<tr>
<td>Upper inert</td>
<td>5.0%</td>
<td>6.89</td>
<td>5.71</td>
<td>5.3</td>
<td>4.96</td>
<td></td>
</tr>
<tr>
<td>Upper intermediate inert</td>
<td>5.0%</td>
<td>6.89</td>
<td>5.71</td>
<td>5.3</td>
<td>4.96</td>
<td></td>
</tr>
<tr>
<td>Lower intermediate inert</td>
<td>5.0%</td>
<td>6.89</td>
<td>5.71</td>
<td>5.3</td>
<td>4.96</td>
<td></td>
</tr>
<tr>
<td>Lower inert</td>
<td>5.0%</td>
<td>6.89</td>
<td>5.71</td>
<td>5.3</td>
<td>4.96</td>
<td></td>
</tr>
<tr>
<td>Upper main</td>
<td>20.0%</td>
<td>27.55</td>
<td>22.87</td>
<td>21.21</td>
<td>19.84</td>
<td></td>
</tr>
<tr>
<td>Upper core</td>
<td>6.67%</td>
<td>9.19</td>
<td>7.62</td>
<td>7.07</td>
<td>6.61</td>
<td></td>
</tr>
<tr>
<td>Intermediate main</td>
<td>20.0%</td>
<td>27.55</td>
<td>22.87</td>
<td>21.21</td>
<td>19.84</td>
<td></td>
</tr>
<tr>
<td>Intermediate core</td>
<td>6.67%</td>
<td>9.19</td>
<td>7.62</td>
<td>7.07</td>
<td>6.61</td>
<td></td>
</tr>
<tr>
<td>Lower main</td>
<td>20.0%</td>
<td>27.55</td>
<td>22.87</td>
<td>21.21</td>
<td>19.84</td>
<td></td>
</tr>
<tr>
<td>Lower core</td>
<td>6.67%</td>
<td>9.19</td>
<td>7.62</td>
<td>7.07</td>
<td>6.61</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>137.78</td>
<td>114.35</td>
<td>106.09</td>
<td>99.2</td>
<td></td>
</tr>
</tbody>
</table>

For all cases examined, the same quality and quantity of raw coal are supplied. The proximate and ultimate analysis of the brown coal particle for the Loy Yang A power station is summarized in Table 3-4. The coal properties were based on samples taken from operating open cuts. The same amount of gases is taken from the HGOTs. The oxidizers/fuel stoichiometric ratio (\( \lambda \)) was kept constant (1.18), based on the present operating conditions of the power plant for all combustion cases investigated.
In the drying shaft, a high energy is required to evaporate the M.C. of the brown coal. The evaporated steam was added to the feed gas compositions. This means that the water vapour concentration was increased in the burner ducts. On the other hand, effect of RFG, in the core ducts, was also added to the gas mixture that led to decrease of water vapour in the main burners compared to the inert burners, as shown in Table 7-5 for all combustion cases. For the retrofitted oxy-fuel cases, the gas mixture was also supposed to be evenly distributed across each mill-duct group.

Table 7-5 a. The compositions of feed gases through the duct surfaces of inert and main burners for the air-fired and OF25 combustion scenarios.

<table>
<thead>
<tr>
<th>Burner surface</th>
<th>Species concentrations of air-fired case (wt %)</th>
<th>Species concentrations of OF25 case (wt %)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$O_2$</td>
<td>$N_2$</td>
</tr>
<tr>
<td>UIB</td>
<td>7.00</td>
<td>49.24</td>
</tr>
<tr>
<td>IIB</td>
<td>7.00</td>
<td>49.24</td>
</tr>
<tr>
<td>LIB</td>
<td>7.00</td>
<td>49.24</td>
</tr>
<tr>
<td>UMB + UC</td>
<td>14.02</td>
<td>61.42</td>
</tr>
<tr>
<td>IMB + IC</td>
<td>14.41</td>
<td>62.09</td>
</tr>
<tr>
<td>LMB + LC</td>
<td>14.22</td>
<td>61.76</td>
</tr>
</tbody>
</table>

Table 7-5 b. The compositions of feed gases through the duct surfaces of inert and main burners for the OF27 and OF29 combustion scenarios.

<table>
<thead>
<tr>
<th>Burner surface</th>
<th>Species concentrations of OF27 case (wt %)</th>
<th>Species concentrations of OF29 case (wt %)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$O_2$</td>
<td>$N_2$</td>
</tr>
<tr>
<td>UIB</td>
<td>2.0</td>
<td>6.16</td>
</tr>
<tr>
<td>IIB</td>
<td>2.0</td>
<td>6.16</td>
</tr>
<tr>
<td>LIB</td>
<td>2.0</td>
<td>6.16</td>
</tr>
<tr>
<td>UMB + UC</td>
<td>11.06</td>
<td>3.31</td>
</tr>
<tr>
<td>IMB + IC</td>
<td>11.52</td>
<td>3.17</td>
</tr>
<tr>
<td>LMB + LC</td>
<td>11.31</td>
<td>3.23</td>
</tr>
</tbody>
</table>
7.3.4 Grid independence test and validation

In this section, a grid independence test of CFD model was carried out for the air-fired case. In order to make a balance between the computational accuracy and computing cost, three different non-uniform grid systems were successfully tested. Due to the complexities in an industrial furnace design and the combustion phenomena of Victorian brown coal, a coarse grid (292,897 cells) was initially used in this simulation. Then, the grid system was increasingly refined to reproduce two higher grids with 559,006 and 1,072,000 cells. The refinements of the latter two meshes were mainly concentrated in the burners’ region and outlets that represent regions of high flow gradients. This is important for increasing the level of computational accuracy in the present CFD model. However, for testing these three grid systems, temperature distributions and gas velocity component w (flue gas flow direction) values are selected in both the UMB plane and along the centreline of the furnace zone. In Figure 7-5a and b and Figure 7-6a and b, the comparisons of gas temperatures and gas velocity values, respectively are conducted for the three grid systems. It can be seen that the higher (1,072,000 cells) and medium (559,006 cells) grid systems produce highly similar results compared to the low (292,897 cells) grid system. In addition, for all grid systems, the percentage error of the mean temperature distribution at the centreline of the furnace zone and along the UMB plane was within 1% (see Table 7-6). Therefore, the 559,006-grid system was selected to validate the numerical results with the power station data and for the other oxy-fuel combustion simulations.

Table 7-6. Grid independency test for the average temperature distributions at the furnace zone centreline and the UMB plane.

<table>
<thead>
<tr>
<th>Number of cells</th>
<th>T (K)mean</th>
<th>Percentage error of ΔTmean</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Furnace zone centreline</td>
<td>UMB plane</td>
</tr>
<tr>
<td>292,897</td>
<td>1692.125</td>
<td>1636.081</td>
</tr>
<tr>
<td>559,006</td>
<td>1688.983</td>
<td>1621.915</td>
</tr>
<tr>
<td>1,072,000</td>
<td>1694.876</td>
<td>1615.483</td>
</tr>
</tbody>
</table>
Chapter 7 - Modelling of Brown Coal Combustion in a Full-scale Tangentially-fired Furnace

Figure 7-5a and b. The comparisons of gas temperatures for three grid systems, (a) along the furnace zone centreline, and (b) along UMB plane.
Figure 7-6a and b. The comparisons of gas velocity values for three grid systems, (a) along the furnace zone centreline, and (b) along UMB plane.
In order to verify the predictions of the present CFD model against the measured data, four different validation parameters were used for this purpose (see Table 7-7 for validation results). The validation of these predicted results was based on the boiler test data obtained in October 2009 on Unit 1 from Loy Yang A power station. The flue gas compositions and the carbon in fly-ash were measured at a final exit plane (Staples and Marshall 2010). Regarding the flue gas temperatures, furnace zone exit, economiser exit, and final exit plane were used to check the values of predicted gas temperatures. The total gas flow rate through the HGOTs was calculated and validated with the real plant data by taking the effect of evaporated steam of brown coal at each mill-duct system. As shown in Table 7-7, the CFD predictions closely match the measured data. This good agreement with the boiler test data provided a level of confidence in the present CFD study for investigating different operating conditions, particularly under oxy-fuel combustion on the same boiler. In addition, the present CFD model has been successfully tested on a 100 kW lab-scale furnace under several operating conditions of combustion, air-fired and three oxy-fuel cases, and reasonable overall agreement with the measurements was obtained (Al-Abbas et al. 2011). As a result, the simulation of the retrofitted oxy-fuel combustion cases for the 550 MW large-scale boilers can be conducted with the present CFD model.

Table 7-7. Validation results of CFD model against the station test data for the air-fired (conventional) scenario.

<table>
<thead>
<tr>
<th>Validation parameters</th>
<th>CFD results</th>
<th>Measured data</th>
</tr>
</thead>
<tbody>
<tr>
<td>1- Flue gas composition at a final exit</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \text{O}_2 ) (wt %)</td>
<td>4.03</td>
<td>3.93</td>
</tr>
<tr>
<td>( \text{CO}_2 ) (wt %)</td>
<td>18.84</td>
<td>19.3</td>
</tr>
<tr>
<td>( \text{CO} ) (ppm)</td>
<td>34.8</td>
<td>33.0</td>
</tr>
<tr>
<td>( \text{H}_2\text{O} ) (wt %)</td>
<td>14.87</td>
<td>15.0</td>
</tr>
<tr>
<td>( \text{N}_2 ) (wt %)</td>
<td>62.16</td>
<td>61.67</td>
</tr>
<tr>
<td>NO (ppm)</td>
<td>218.58</td>
<td>201.0</td>
</tr>
<tr>
<td>2- Gas temperature (K)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Furnace exit temperature</td>
<td>1416.51</td>
<td>1404.0</td>
</tr>
<tr>
<td>Economiser exit temperature</td>
<td>638.64</td>
<td>637.7</td>
</tr>
<tr>
<td>Final gas temperature</td>
<td>635.35</td>
<td>633.0</td>
</tr>
<tr>
<td>3- Carbon in fly-ash (%)</td>
<td>2.05</td>
<td>1.7</td>
</tr>
<tr>
<td>4- HGOT mass flow (kg/s)</td>
<td>305</td>
<td>297</td>
</tr>
</tbody>
</table>
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7.4 Results and discussion

7.4.1 Temperature distribution

In Figure 7-7, the distributions of flue gas temperatures are presented along the height of the furnace at the mid cut of X-Z plane for the air-fired, OF25, OF27, and OF29 combustion cases. As illustrated earlier, the inlet flow temperatures of gases in the secondary air flows and in the burner gas flows were 473 and 397 K, respectively. Once the reaction processes between PC and oxidizer gases have been started the flame temperature is progressively increased to be at a peak value in the furnace zone as follows: 1864.37 K for air-fired, 1752.0 K for OF25, 1813.3 K for OF27, and 1865.0 K for OF29. It is clearly seen that a reduction in the levels of the gas temperature when the N\textsubscript{2} is replaced by the CO\textsubscript{2} in the secondary air ducts, particularly in the OF25 and OF27 cases examined. That obvious decrease in the gas temperature was mainly due to the higher volumetric heat capacity of CO\textsubscript{2} compared to N\textsubscript{2} in the gas mixture. On the other hand, the maximum gas temperatures between air-fired and OF29 combustion cases were approximately identical. That improvement on the gas temperature of the latter oxy-fuel case was because of increasing O\textsubscript{2} concentration in the feed oxidizer gases. Furthermore, in this study, the oxygen concentration was not only the dominant factor to control on the flame temperature inside the furnace, but also the resident time of coal combustion. However, the inlet flow fields of feed oxidizer gases (O\textsubscript{2}/CO\textsubscript{2}), in all oxy-fuel cases, were reduced in proportion to the volumetric flow rates by fixed ratios: 83\%, 77\%, and 72\% for OF25, OF27, and OF29, respectively with respect to the conventional firing case, as summarized in Table 7-4. The reduction in the volumetric flow rates of O\textsubscript{2}/CO\textsubscript{2} cases is given a sufficient time to burn more coal particles in the combustion zone. Additional three similar oxy-fuel combustion cases, not shown in this study, have been examined where the same boundary conditions (BCs) as of the air-fired case were maintained, i.e. without reducing the volumetric flow rates of O\textsubscript{2}/CO\textsubscript{2} in the secondary air duct. Values of the maximum average gas temperature of the latter oxy-fuel cases were, in contrast, less than the values of the oxy-fuel combustion cases presented in this study. Those values were 1667 K for OF25, 1718 K for OF27, and 1753 K for OF29 combustion cases. However, according to the Chalmers’ approach (Andersson 2007), the reduction in the volumetric feed-gas flow rates through the
secondary air ducts of the furnace is an efficient method to stabilize and increase the flame temperatures.

![Figure 7-7. Distributions of the flue gas temperature (K) along the height of the furnace at the mid cut (X-Z plane) for air-fired, OF25, OF27, and OF29 combustion cases.](image)

Because of the complexity of brown coal combustion, changing bulk oxidizer gases from 21% O\(_2\)/79% N\(_2\) to 25% O\(_2\)/75% CO\(_2\) in the gas mixture led to the delay in the ignition mechanism of PC. This undesirable phenomenon occurred because of the higher moisture content in the raw coal and the higher concentration of CO\(_2\) in the gas mixture, i.e. the volumetric heat capacities of H\(_2\)O and CO\(_2\) are relatively higher than that of N\(_2\), which are equal to 1.3 and 1.7 times, respectively. Furthermore, the higher CO\(_2\) partial pressure in the feed oxidizer gases led to increased in accelerating brown coal pyrolysis prior to ignition process (Zhang et al. 2010; Durie 1991). As the O\(_2\) partial pressure increased in 27% O\(_2\)/73% CO\(_2\) and 29% O\(_2\)/71% CO\(_2\), the combustion of the volatile matter (VM) took place earlier, and the oxygen is highly consumed in the flame zone, and low char burn out is noticed in this region of the furnace. However, an increase in the O\(_2\) concentration in the gas mixture, in general, leads to reducing the ignition delay time due to increased reaction rate between the volatile released and
oxidizer gases. It is also noticed that, in all oxy-fuel cases, the flame temperature distributions were more confined and concentrated in the furnace zone, as seen in Fig. 7-7. In contrast, in the conventional combustion case, the distributions of flame temperature were more spread. The homogeneous distribution of gas temperature inside the furnace is of great importance for the heat transfer processes (convection and radiation), in particular, to the water wall region. Regarding the heat transfer in the convection zone, i.e. in the upper boiler, the convective tube banks are taken the heat from the hot elevated flue gases, for all cases investigated in this CFD study. The final gas temperatures of $O_2/CO_2$ combustion cases, at the bifurcation to the air heaters, closely matched the temperature of the reference combustion case. The values were as follows: 635.35 K for air-fired, 623.81 K for OF25, 628.27 K for OF27, and 631.4 K for OF29 combustion cases.

In Figure 7-8, the distributions of flue gas temperature are presented in different cross-sections of the furnace, at the UMB plane, at the UIB plane, and at the HGOTs plane, for all cases examined. The gas temperatures at the UMB plane, for all combustion cases, were comparatively higher than that in the UIB plane. This can be attributed to the fact that the mass flow rates of PC in the main burners were relatively high and accompanied by low gas flow rates compared to the inert burners (see Table 7-1). In addition, the core air ducts in the PC burners effectively participated to increase oxygen concentrations, and therefore raise the combustion temperatures. As the hot flue gases rise up inside the furnace, a large amount of heat is transferred towards the water walls. The heat transfer processes between the flue gases and furnace water walls resulted in reducing in the gas temperatures. However, due to the higher moisture content in brown coal, a part of hot gases is recycled through the HGOT pipes for drying the PC before transporting it towards the burner mouths.
Figure 7-8. Distributions of the flue gas temperature (K) in different cross-sections: a) at the UMB plane (lower X-Y plane in the figure), b) at the UIB plane, c) at the HGOT pipes plane in the air-fired, OF25, OF27, and OF29 combustion cases.

Based on the present boiler design, the convective tube banks are located above the eight HGOTs location (see Fig. 7-1). This location is of great importance regarding the slagging and fouling formation problems in the PC tangentially-fired boiler. The temperatures of flue gases beneath the first convective tube bank (superheater 1) were 1416.5, 1206.5, 1317.8, and 1387.08 K for the air-fired, OF25, OF27, and OF29 combustion scenarios, respectively. In general, an ash deposit on the above-mentioned tubes reduces the heat exchange processes, and as a result decreases the overall boiler efficiency. For that reason, Akiyama et al. (2011) conducted experimental investigations on the 145 MW coal combustion boiler to evaluate the ash deposition behaviour for low-rank coal such as brown coal. The results showed that the ash melting temperature for brown coal is 1523 K, and the molten slag fraction can reach to around 90% in this undesirable temperature at the exit furnace zone. However, all the values of the exit furnace temperature reported in this simulation study were below the ash melting temperature mentioned. Therefore, there is no concern regarding this practical problem on heat exchanger tubes of the boiler under the present conditions of the oxy-fuel firing.
Figure 7-9 presents the average flue gas temperature profiles along the furnace centreline, from bottom of the hopper up to the convective tube banks’ location, for all combustion scenarios. As seen in the hopper region (level Z=0 m to level Z=14 m), the gas temperatures are low for all O$_2$/CO$_2$ cases compared to that of the conventional firing case. This phenomenon might be due to the availability of oxygen, in this region of the furnace, in the air-fired case. In contrast, no air leakage is considered in all O$_2$/CO$_2$ cases, and thus nearly no combustion occurs in the hopper zone. In Fig. 7-9, two peak gas temperatures exist in the furnace zone. The first peaks appear in the zone close to the main (PC) burners, which considered the fuel-rich mixture region in the furnace. Whilst the second peak values were approximately in the inert burner region, around level Z=28 m. These higher gas temperatures resulted in the reaction between the volatile matters released from the coal and the surrounding oxygen, and thus a high amount of heat is generated. After the increase of the gas temperature in the burners’ region, the value gradually falls due to the heat absorption sinks of the furnace water wall and heat exchanger tubes at the upper zone of the boiler. The values of heat absorption sources were kept same for all cases examined in this study in order to maintain similar outputs to the boiler power (see Table 7-3).

Also seen in Fig. 7-9 is that despite similarities in the distributions of gas temperatures, the 25% O$_2$/75% CO$_2$ mixture case showed lower temperature values than other cases, in particular in the furnace zone. While as the oxygen concentrations and the resident time of coal combustion are increased in the 27% O$_2$/73% CO$_2$ and 29% O$_2$/71% CO$_2$ cases, higher temperature profiles are evident, which is beneficial for char burnout. In short, the overall agreement of the gas temperatures between the air-fired case and the OF29 combustion case was achieved in two important regions, the furnace zone and the bifurcation to the air heaters zone, as was shown in Fig. 7-7.
Figure 7-9. Profiles of the mean flue gas temperature (K) along the furnace centreline (from bottom of the hopper up to the water wall’s location) for all combustion scenarios.
7.4.2 Velocity distribution

In the tangentially-fired furnace, the aerodynamic effects are of great importance on the PC combustion characteristics. This importance arises from using a swirl injection system, which largely increases the mixing flow conditions between the PC and feed oxidizer gases, especially in this type of furnaces. To fully understand how this aerodynamic system works, it is necessary to investigate the flow field behaviour in the furnace. Figure 7-10 shows the distributions of mean velocity vectors for the feed oxidizer gases (O$_2$/N$_2$ or O$_2$/CO$_2$) at the upper main duct (UMD) of the secondary air, in X-Y plane, for the air-fired, OF25, OF27, and OF29 combustion scenarios. Ducts 3, 4, and 7 were kept out of service, in all cases, based on the reference BCs of boiler operations; while the remaining ducts were in service. Due to the inlet burners configuration, a strong recirculation zone is constructed in the furnace’s core for all cases. This enhances the turbulent mixing conditions, and concentrates the combustion flame in that zone. For all oxy-fuel cases, a significant reduction of the gas flow is evident due to the decrease of the gas flow rates entering the combustion chamber. Although, the secondary to primary flow ratios were kept fixed, the total amounts of feed oxidizer gases received were gradually reduced based on the Chalmers’ approach adopted (OF25: 114.35 kg/s, OF27: 106.09 kg/s, and OF29: 99.2 kg/s). A similar strategy of gas velocity reduction was also adopted in recent oxy-fuel combustion study (Nikolopoulos et al. 2011). However, the reduction in gas mixture used in that study led to increase the combustion temperatures because of increased residence time of coal particles in the combustion zone.

Moreover, as shown in Fig. 7-10, a small part of the upstream mill ducting was included in order to closely reproduce the effects of upstream flow fields, and thus provides better flow pattern predictions in the furnace zone. This configuration is also important for the oxy-fuel combustion cases due to increasing the CO$_2$ concentration that leads to enhance the pyrolysis process of coal particles prior to ignition mechanism, as investigated experimentally by Zhang et al. (2010).
Figure 7-10. Distributions of the mean velocity vectors (m/s) at the upper main duct (UMD) of the secondary air, X-Y plane, for the air-fired, OF25, OF27, and OF29 combustion scenarios.
In Figure 7-11, the profiles of mean Z-velocity component are presented along the furnace centreline, from the bottom of the hopper up to the convective tube banks’ location, for all the cases examined. As seen in all oxy-fuel cases, the negative values of the average Z-velocity component, in the hopper region, were less than that of the air-fired case. Fig. 7-9 that showed low gas temperatures for oxy-fuel cases compared to the reference case in the same region of furnace, this velocity component has a significant effect on burning process. This means that some coal particles are forced to travel down and then to burn with the available oxygen at the bottom of the furnace. In the burner zone, the maximum value of the average velocity component for air-fired, OF25, OF27, and OF29 cases are 18.02, 16.23, 15.08, and 13.01 m/s, respectively. However, the decrease of the mean Z-velocity component values is evident for all oxy-fuel cases investigated, which is due to the decrease of flow BCs adopted in this study. In addition, a sharp decrease of the average Z-velocity component is predicted, for all cases, after level Z= 50 m that can be attributed to the HGOTs effect.

![Figure 7-11. Profiles of mean Z-velocity component (m/s) along the furnace centreline (from bottom of the hopper up to the convective tube banks’ location) for all cases investigated.](image-url)
7.4.3 Species concentrations

7.4.3.1 Oxygen concentration
The distributions of oxygen mass fraction (kg/kg) along the height of the hopper and furnace zone at the mid cut of X-Z plane for all cases examined are showed in Figure 7-12. In general, the $O_2$ distributions are relatively different at all cases investigated. The differences were a result of the $O_2$ concentrations injected in both the burner ducts and secondary air ducts. It can be seen that the highest values of $O_2$ concentrations are observed in vicinity to the burners region; while the lowest values are predicted in the central zone of the furnace, the region of the higher flame temperatures (see Fig. 7-7). It is interesting to note that for the air-fired case, the higher $O_2$ concentrations are predicted in the hopper region compared to the oxy-fuel cases. This can be attributed to ignoring the air-leakage in that region. The sequence increase in the gas temperatures of the OF25, OF27, and OF29 cases were strongly coupled with the $O_2$ concentrations used in the secondary air ducts, which are equal to 25%vol. $O_2$, 27%vol. $O_2$, and 29%vol. $O_2$, respectively.

Due to the complexity of the brown coal combustion process, specifically in homogeneous combustion, the combustion of VM takes place first, and then $O_2$ is completely consumed in the flame region, as seen in Fig. 7-12. In contrast, in the heterogeneous combustion, the available $O_2$ will directly attack on the residual char at low particle temperatures, as described in the comprehensive book of Chun-Zhu Li (2004). Due to decreasing volumetric flow rates of feed gases, the $O_2$ concentrations are highly decreased in the upper burners region resulting in higher gas temperatures in all oxy-fuel cases.
Due to the importance of the O$_2$ concentrations in the burners region, the distributions of oxygen mass fraction (kg/kg) were also presented at the UMB plane (lower X-Y plane in the figure) and at the UIB plane for all cases examined, as shown in Figure 7-13. As can be seen, despite the higher O$_2$ concentrations used in the oxy-fuel cases, lower oxygen is predicted in both the planes compared to the reference combustion case. This is due to the increased residence time of coal particles adopted in oxy-fuel cases, and therefore led to the consumption of large amounts of oxygen in the combustion zones.

Fig. 7-13 also shows that the O$_2$ concentrations in the UIB plane were relatively lower than that in the UMB plane, for all cases examined. This is due to the differences in the compositions of circulated gases that are taken from the RFG ports, as well as, the effect of core secondary air ducts installed in the three main burners (see Table 7-5). However, the O$_2$ concentrations in both the above-mentioned planes were significantly affected by the gas temperature levels, as showed earlier in Fig. 7-8. This obvious consumption of oxygen in the combustion zones, in the middle zone of the furnace, was also observed in the previous simulation studies of Nikolopoulos et al. (2011).
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Figure 7-13. Distributions of oxygen mass fraction (kg/kg) at the UMB plane (lower X-Y plane in the figure) and at the UIB plane for all cases examined.

7.4.3.2 Carbon dioxide concentration

Figure 7-14 shows the distributions of carbon dioxide concentration (kg/kg) along the height of the furnace at the mid cut of the X-Z plane for all cases examined. The recycled flue gas (RFG) (mainly CO$_2$) used in the oxy-fuel cases has increased the CO$_2$ concentrations in the flue gases. The differences in the CO$_2$ concentrations between the conventional combustion case and the oxy-fuel cases are evident due to adopting the Chalmers’ approach in this study. Around five times higher CO$_2$ is achieved for all oxy-fuel combustion scenarios compared to the air-fired case. This increase of the CO$_2$ concentrations was also observed in the combined studies of the experimental investigations of Andersson (2007) and numerical modelling of Al-Abbas et al. (2011) which was conducted on the lab-scale 100 kW firing lignite furnace. The concentrations of CO$_2$ mass fractions at the furnace exit were equal to 18.84, 85.76, 85.01, and 84.18 wt% for the air-fired, OF25, OF27, and OF29, respectively. Due to the higher capability of carbon dioxide to absorb the combustion heat, this elevated CO$_2$ in the oxy-fuel cases can potentially increase the protection of the furnace wall against the hot flue gases.
The three-step reaction mechanism was applied in this study, as is illustrated in the homogeneous and heterogeneous reactions of Eqs. 3.57-3.62. Figure 7-15 demonstrates the profiles of carbon dioxide mass fraction (kg/kg) along the furnace centreline (from bottom of the hopper up to the convective tube banks’ location) for all cases examined. For all oxy-fuel cases, the values of the CO$_2$ concentrations were approximately similar along the furnace centreline. Additionally, the thermal dissociation mechanism of CO$_2$ adopted is evidently noticed in the furnace zone (level Z=14 m to level Z=25 m), especially in the air-fired case.
Figure 7-15. Profiles of carbon dioxide mass fraction (kg/kg) along the furnace centreline (from bottom of the hopper up to the convective tube banks' location) for all cases examined.

7.4.3.3 Carbon monoxide concentration

Figure 7-16 shows the distributions of CO mass fraction (kg/kg) in the hopper and furnace zone on the mid-cut plane. The highest CO concentrations are predicted in both the air-fired and OF29 cases; while the lowest values are in the OF25 and OF27 cases. The decrease in the CO concentrations of the latter two cases was likely due to the lower gas temperature of these combustion cases. The gas temperature levels in the air-fired and OF29 cases affected the CO concentrations in the flame regions. In addition, the highest CO values predicted in the flame region were accompanied by the lowest CO$_2$ values (Fig. 7-14) for all cases examined. The higher CO$_2$ concentration has a clear effect on the char burnout leading to an increase in the CO concentrations in the hot
furnace zone and the heat released from this gasification process, as explained in Eq. 3.61 of Boudouard reaction.

![Figure 7-16. Distributions of carbon monoxide concentration (kg/kg) along the height of the hopper and furnace zone at the mid cut for all cases investigated.](image)

### 7.4.3.4 Concentrations of water vapour and hydrogen

In Figures 7-17 and 7-18, the distributions of water vapour (H\textsubscript{2}O) and hydrogen (H\textsubscript{2}) mass fractions (kg/kg) are shown at the UMB plane (lower X-Y plane in the figures) and at the UIB plane for all cases. As seen, the highest values of H\textsubscript{2}O concentrations are predicted near the upper inert burners. This is due to the higher water vapour injected through these burners (see table 7-5). In the UMB plane, the concentrations decreased, especially in the central zone of the plane because of the chemical reaction processes. Due to adopting the multi-step homogeneous reactions and the gasification process of char (see Eq. 3.62) in the heterogeneous reaction, there was an obvious link between the H\textsubscript{2}O and H\textsubscript{2} concentrations. The lowest values of H\textsubscript{2} concentrations are predicted in the near-burner regions at the UIB plane, accompanied by higher H\textsubscript{2}O concentrations, and vice versa for both concentrations at the UMB plane. The O\textsubscript{2} concentrations on these planes were (see Fig. 7-13). However, the elevated H\textsubscript{2}O concentrations will tend to enhance the oxygen diffusion to the char surface at the higher gas temperatures (in this
study, >1750 K at all) due to the higher thermal conductivity of water vapour in the gas mixture, and thus affect the char burning rate at the UIB plane, as shown in next section.

Figure 7-17. Distributions of water vapour mass fraction (kg/kg) at the UMB plane (lower X-Y plane in the figure) and at the UIB plane for all cases examined.

Figure 7-18. Distributions of hydrogen mass fraction (kg/kg) at the UMB plane (lower X-Y plane in the figure) and at the UIB plane for all cases examined.
7.4.4 Char consumption

Figure 7-19 shows the char content of brown coal particles (%) for all cases at the hopper and furnace zones. It is clear that the char burnout varied with changing the conditions of combustion media. A significant decrease in the char burnout is evident for oxy-fuel cases. This decrease resulted in an increase in the content of carbon in fly-ash at the final furnace exit, from about 2.05% for the air-fired case to be 9.74, 7.04, and 5.49% for the OF25, OF27, and OF29 cases, respectively. This can be firstly explained due to a significant decrease in the gas temperatures of the oxy-fuel cases resulting from the higher heat capacities of CO\(_2\) and H\(_2\)O, especially for the OF25 and OF27 scenarios, as showed in Fig. 7-7. This was also confirmed by the experimental measurements conducted on the coal combustion in both the O\(_2\)/N\(_2\) and various O\(_2\)/CO\(_2\) mixtures by Liu et al. (2005). Secondly, because of persisting bulky volatile cloud produced from the brown coal pyrolysis in higher CO\(_2\) concentrations on the char surface. This phenomena leads to oxygen exhaustion on the char surface, as recently reported by the experimental investigations on the brown coal combustion of Zhang et al. (2010). This means that the ignition mechanism under the rich-CO\(_2\) conditions does not happen for a single particle, but takes place for an accumulated volatile cloud.

Figure 7-19. Char content of brown coal particles (%) for the air-fired, OF25, OF27, and OF29 combustion cases at the hopper and furnace zone of the boiler.
However, as the oxygen concentrations increased in the feed gases for the oxy-fuel cases, the carbon in fly-ash decreased. In the hopper zone, the char content is negligible for the air-fired case due to the availability of O$_2$ (see Fig. 7-12). Whereas in oxy-fuel cases, significant amounts of char are evident in the bottom of furnace.

In general, the volatile matter oxidation and char burnout rate of brown coal is controlled by the chemical reactions and pore diffusion (Li 2007). Therefore, the gasification process and the Boudouard reaction of coal particles, adopted in this study (Eqs. 3.61 and 3.62), showed better prediction results, in particular, for the oxy-fuel cases.

7.4.5 NO$_x$ emissions

The required subroutines for the NO$_x$ model in terms of Thermal NO and Fuel NO were written and incorporated into the CFD calculations through the source terms of NO, NH$_3$, and HCN in the transport equations. The validation of the present NO$_x$ model with the power plant data is conducted under air-fired condition at the final exit plane and a good agreement was achieved (Table 7-7). The recycled flue gas (RFG) used in the retrofitted oxy-fuel combustion scenarios was without recycled NO, only dry RFG (mainly carbon dioxide) is considered.

The low-NO$_x$ burner, higher moisture contents and low nitrogen contents in the brown coal tangentially-fired furnace are additional advantageous factors for NO$_x$ reduction in oxy-fuel firing mode. Figure 7-20 presents the distributions of NO$_x$ (ppm) at the UMB plane and at the UIB plane for all cases. As expected there is a remarkable decrease in NO$_x$ formation in oxy-fuel cases compared to the air-fired case. This reduction can be attributed into two main reasons: (1) due to a decrease in the gas temperatures in the combustion zone; and (2) due to the suppression of the thermal NO mechanism, no nitrogen is assumed in all oxy-fuel cases. As seen in Fig. 7-20 for the oxy-fuel cases, the conversion rates of coal-N to NO$_x$ are slightly increased with oxygen concentrations in the feed gases. The maximum NO$_x$ are at the UIB plane for all cases examined due to the elevated gas temperatures in that region. These concentrations were 375, 180, 240,
and 280 ppm, under dry basis, for the air-fired, OF25, OF27, and OF29 cases, respectively.

In the Fuel NO formation mechanism adopted in this study, once the coal particles are heated up, the fuel-N is evenly distributed between volatile (Vol-N) and char (Char-N). The main N-containing products from the pyrolysis process of coal are HCN and NH₃. The concentrations of these intermediate nitrogenous species under oxy-fuel conditions are higher than those of air-fired case, as is recently verified by the numerical study of Cao et al. (2010). They stated that, in O₂/CO₂ mixture, the higher concentrations of N-containing products are favourable in terms of NOₓ emissions. In addition, more NH₃ concentrations than HCN were formed from brown coal, as a low-rank coal, relative to the bituminous coal (Li 2004; Nikolopoulos et al. 2011). Therefore, effects of the concentrations of nitrogen intermediate species are modelled and taken into account in this CFD study, and as illustrated in a schematic diagram (Fig. 3-3). Phong-Anant et al. (1985) conducted an experimental study on the drop-tube furnace to investigate NOₓ formation from Australian brown coal under different modes of heating. Their results showed that the conversion rate of char-N to NOₓ is principally dependent on the combustion temperatures and char burnout. As was shown in Fig. 7-19, the char burnout

Figure 7-20. Distributions of NOₓ (ppm) at the UMB plane (lower X-Y plane in the figure) and at the UIB plane for all cases investigated.

In the Fuel NO formation mechanism adopted in this study, once the coal particles are heated up, the fuel-N is evenly distributed between volatile (Vol-N) and char (Char-N). The main N-containing products from the pyrolysis process of coal are HCN and NH₃. The concentrations of these intermediate nitrogenous species under oxy-fuel conditions are higher than those of air-fired case, as is recently verified by the numerical study of Cao et al. (2010). They stated that, in O₂/CO₂ mixture, the higher concentrations of N-containing products are favourable in terms of NOₓ emissions. In addition, more NH₃ concentrations than HCN were formed from brown coal, as a low-rank coal, relative to the bituminous coal (Li 2004; Nikolopoulos et al. 2011). Therefore, effects of the concentrations of nitrogen intermediate species are modelled and taken into account in this CFD study, and as illustrated in a schematic diagram (Fig. 3-3). Phong-Anant et al. (1985) conducted an experimental study on the drop-tube furnace to investigate NOₓ formation from Australian brown coal under different modes of heating. Their results showed that the conversion rate of char-N to NOₓ is principally dependent on the combustion temperatures and char burnout. As was shown in Fig. 7-19, the char burnout
is increased with the $O_2$ concentrations in the feed gases; hence the destruction process of NO is significantly affected with decreasing char burnout rates (Eq. 3.74). The NO$_x$ concentrations in Fig. 7-20 confirmed the results of the present NO$_x$ model.

The comparisons of the NO$_x$ concentrations amongst all combustion cases investigated were carried out at the final furnace exit, and are summarized in Table 7-8. Comparing to the air-fired case, it can be seen that the 29%vol. $O_2$ and 71%vol. CO$_2$ mixture can provide approximately similar gas temperature levels and less carbon in fly-ash relative to the other oxy-fuel cases. Furthermore, the NO$_x$ formation is drastically decreased to around half as compared to the conventional combustion case. The conversion rate of coal-N to NO$_x$ is also decreased with increasing the resident time of coal combustion adopted in all oxy-fuel cases compared to the air-fired case, and as is confirmed by the experimental measurements of Liu et al. (2005). Finally, more research is required to fully understand the complex reaction processes involved in the conversion of fuel-N to NO$_x$ formation/destruction mechanisms.

Table 7-8. Main predicted CFD results of all combustion cases examined at the final exit plane, and the net radiative heat flux on the furnace wall.

<table>
<thead>
<tr>
<th>Combustion Media</th>
<th>Temp. (K)</th>
<th>CO$_2$ (wt %)</th>
<th>Net Rad. Heat Flux (MW)</th>
<th>Carbon in Fly-Ash (%)</th>
<th>NO$_x$ (ppm, dry)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air-Fired (conventional)</td>
<td>635.35</td>
<td>18.84</td>
<td>778.76</td>
<td>2.05</td>
<td>218.58</td>
</tr>
<tr>
<td>Oxy-Fuel (OF25)</td>
<td>623.81</td>
<td>85.76</td>
<td>534.3</td>
<td>9.74</td>
<td>96.31</td>
</tr>
<tr>
<td>Oxy-Fuel (OF27)</td>
<td>628.27</td>
<td>85.01</td>
<td>596.37</td>
<td>7.04</td>
<td>103.2</td>
</tr>
<tr>
<td>Oxy-Fuel (OF29)</td>
<td>631.4</td>
<td>84.18</td>
<td>685.7</td>
<td>5.49</td>
<td>120.0</td>
</tr>
</tbody>
</table>
7.4.6 Radiation heat transfer

For all cases investigated in this study, the mass flow rates of coal particles are kept constant (Table 7-1). The same heat input to the combustion chamber, and the convection and radiation heat transfer of the furnace wall are considered (Nikolopoulos et al. 2011; Tan et al. 2006).

The increases in the gas temperatures and combustion product’s emissivity, due to higher concentrations of CO$_2$ and H$_2$O in the flue gas as well as particulate matter, for oxy-fuel cases, lead to significant differences in the incident heat flux of furnace wall. Figure 7-21 shows the predicted wall incident heat flux on the radiation region (hopper, furnace zone, and water wall) of the south furnace wall for all cases investigated. The total net radiative heat flux gradually increased for the oxy-fuel cases, as follows: 778.76, 534.31, 596.37, and 685.72 MW for the air-fired, OF25, OF27, and OF29, respectively.

![Figure 7-21. Predicted wall incident heat flux on the radiation region (hopper, furnace zone, and water wall) of the south furnace wall for all cases examined.](image)
Chapter 7- Modelling of Brown Coal Combustion in a Full-scale Tangentially-fired Furnace

The increased $O_2$ concentrations and the reduction in the volumetric flow rates adopted in the oxy-fuel firing cases are predominantly considered the key parameters for that increase. Therefore, these parameters can play an important role to control the heat flux and gas temperature under oxy-fuel conditions, as was experimentally investigated by Tan et al. (2006). They carried out several oxy-combustion tests on three different coals (bituminous, sub-bituminous, and lignite) by using a 0.3 MW utility boiler. Their main results showed that the heat flux and gas temperature levels of 28% vol. $O_2$ case were lower than those of air-fired (reference) case; while with 35% vol. $O_2$ in the feed gas, the results were slightly high. However, in the present study, both the values of the radiative heat flux and flue gas temperature profiles of OF29 case were closest to the air-fired case compared with the remaining oxy-fuel combustion cases, as seen in Figs. 7-21 and 7-7. This means that the heat transfer distributions from combustion products to the boiler water wall and convective tube banks are approximately similar between the OF29 and conventional air combustion case, which in turn is expected to keep the same furnace thermal efficiency. Thus, in this boiler tested, no change to the furnace wall materials has to be taken into consideration under these heat transfer characteristics of oxy-fuel-fired conditions.

As seen in Fig. 7-21, the heat transfer processes between the elevated gas temperatures and the water wall of the furnace are evident in all cases investigated. In addition, it is noticed that, in the hopper region, the incident heat flux of air-fired case is slightly higher than that of OF25 and OF27 cases. This increase is likely to have resulted from the higher gas temperature. Furthermore, in the OF25 and OF27 cases examined, the increased carbon dioxide in the flue gas (Fig. 7-14) can give another explanation to that reduction in the incident heat flux; where the $CO_2$ has a larger heat absorption capability than $N_2$. On the other hand, the OF29 case was somewhat similar to the air-fired case in the bottom of the furnace. This similarity might have occurred due to decreasing the volumetric flow rate of RFG (mainly $CO_2$); a slight reduction in the $CO_2$ concentrations of OF29 is observed in the hopper region compared with the OF25 and OF27 cases. Moreover, the higher $O_2$ concentrations and low carbon in fly-ash observed are also other parameters for that resemblance. However, the heat transfer to the furnace wall for the air-fired and retrofitted OF29 combustion case is technically conformed through
two intrinsic aspects: First the gas temperature distributions (in the furnace zone and at furnace exit, see Table 7-8), and secondly the wall heat flux in difference furnace wall locations.

As far as the gaseous radiative properties model is concerned, under oxy-fuel combustion modelling, the gray gaseous model (WSGGM) of Smith et al. (1981) is used. As previously stated, this model can consistently give better numerical results, in particular, for the higher concentrations of H\textsubscript{2}O and CO\textsubscript{2} in the flue gas. More recent, Yin et al. (2011) developed a new gaseous radiative properties (WSGGM) model and implemented it to the CFD calculations of oxy-natural gas combustion in order to make a comparison with the Smith et al. model. The new model made a slight difference from the old model in the predicted absorption coefficient; while no significant differences were observed in the calculated temperature, radiation source term, or oxygen concentration profiles.

In short, the characteristics of oxy-fuel combustion are likely to be different from those of the conventional firing. For the retrofitted oxy-fuel firing systems, the ignition properties, gas temperature levels, flame stability, radiative heat transfer, and char combustion can relatively be matched with the corresponding conventional combustion characteristics via adopting the residence time of coal particles and O\textsubscript{2} enrichments in the gas mixture. Therefore, further research is needed to obtain optimal results.
7.5 Summary and conclusion

The oxy-fuel combustion mode can potentially provide significant opportunities for near-zero emissions from the existing and newly-built power plants. In this study, a commercial CFD code, AVL Fire ver.2008.2, has been modified to investigate the Victorian brown coal combustion in a 550 MW tangentially-fired boiler under different combustion media. Several mathematical models such as coal devolatilization, char burnout, combustion chemistry, convection and radiation heat transfer processes, carbon in fly-ash, and thermal and fuel nitric oxides models were developed through subroutines and added to the CFD calculations. The available experimental data (Staples and Marshall 2010) were used to validate the predicted results under air-fired condition, a good agreement was achieved. The oxy-fuel combustion approach adopted in a 100 kW facility unit (Chalmers’ furnace) was applied to the present large-scale furnace in three $O_2/CO_2$ mixture conditions, namely OF25, OF27, and OF29.

As the compositions of feed oxidizer gases are replaced from $O_2/N_2$ to $O_2/CO_2$ mixtures, significant changes in the combustion characteristics are observed. In the OF25 and OF27 combustion scenarios, a clear reduction in the gas temperatures was noticed compared to the reference firing case. In contrast, OF29 case showed similar gas temperature levels and radiative heat transfer to that of the air-fired case. This is due to augmenting the residence time of coal particles and oxygen concentrations in the gas mixture. For all oxy-fuel combustion cases examined, lower gas temperatures levels were observed in the hopper region compared to the air-fired case due to availability of $O_2$ in the latter combustion case, which also led to increased burning rate of residual char. The higher $CO_2$ concentrations in the oxy-fuel cases significantly affected the pyrolysis process of coal particles and thus resulted in an increase in the carbon in fly-ash. A remarkable decrease in the $NO_x$ formation was observed because of the elimination of thermal NO process from the oxy-fuel combustion scenarios, as well as low nitrogen content and higher $H_2O$ concentrations in the raw brown coal. In the furnace zone, the CO concentrations in oxy-fuel cases gradually increased with oxygen concentrations, and made a chemical equilibrium with $CO_2$ based on the multi-step chemistry mechanism adopted in these investigations. Finally, the aerodynamic and
thermodynamic conditions of OF29 combustion case are favourable, and closely match the conventional combustion characteristics in several important areas in comparison with the other oxy-fuel-fired conditions.
Chapter 8. Conclusions and Recommendations
Chapter 8- Conclusions and Recommendations

8 Conclusions and Recommendations

8.1 Conclusions

In this thesis a computational fluid dynamics (CFD) tool has been developed and validated to numerical turbulent combustion models of gaseous and solid fuels in different furnaces. The numerical investigations of the air-fired and several oxy-fuel combustion environments have been carried out based on the available experimental data. The observations of this research project can provide useful information for improving the combustion characteristics and heat transfer performance of the tangentially-fired boiler under using oxy-fuel combustion conditions.

The objectives of this research work were mentioned in section 1.3 of chapter one of this thesis. There were four main objectives of this research program, and the following conclusion will individually discuss the most interesting findings of each objective.

The first objective was to perform a CFD modelling investigation of propane combustion with associated chemical reaction, radiative heat transfer and turbulence models. The three different combustion cases that were adopted experimentally in a 100 kW drop tube firing unit were examined. One air-fired (reference) and two oxy-fuel combustion cases (OF21 and OF27) were investigated.

In chapter 4, the commercially available CFD code, AVL Fire ver.2008.2, was used as a first stage of this research project to model the experimental work of Andersson (2007) in regards to the propane reaction. The numerical investigations of the temperature distribution levels, species concentration (CO₂, CO, and O₂), velocity distributions, and propane consumption were carried out at the most intense combustion locations of the furnace. One-step and four-step chemical reaction mechanisms were performed and compared in this numerical investigation.

A swirl injection system was used to achieve the flame stability of the turbulent non-premixed combustible gases. A modified Eddy Breakup (EBU) model was modelled
with appropriate empirical coefficients for propane combustion reaction. Since the empirical coefficients are dependent on the flow turbulence and fuel parameters, several allowable values were tested in this investigation to adjust the appropriate values with the physical data.

A grid independence test and validations of the predicted results with the measured data were conducted for all combustion cases examined. A reasonably good agreement was achieved for the gas temperature levels and species concentrations (CO₂, CO, and O₂). In the one-step (irreversible) reaction, the temperature distributions and species concentration levels were slightly over-predicted compared to the measured data. These discrepancies might be happened due to neglecting the dissociation mechanism of the major species in particular to the flame zone. But, the prediction accuracy improved with the use of four-step reaction scheme.

In addition, the predicted results showed that the flame envelopes of all combustion cases were concentrated along the central axis (Y-axis) of the furnace. However, the oxy-fuel flames showed less radical spreading than the air-fired flame. Compared to the OF21 flame, the luminous appearance and temperature distributions of the OF27 flame were comparable to the air-fired flame. That was due to reduced volumetric flow rate and increased in the oxygen concentration of the OF27 case. Due to the insufficient O₂ concentration in the OF21 case, a combustion delay was evident in the vicinity of the burner compared to the air-fired and OF27 combustion cases. The concentrations of CO₂ for the both oxy-fuel combustion cases were around eight times higher than that of the reference case. Also the reduction in the O₂ concentration in the OF21 case affected the amount of unburned fuel and CO formation in the near-burner region.

The second research objective was to conduct a three dimensional numerical simulation of pulverized dry lignite in a 100 kW test facility in order to provide the confidence to predict the combustion of coal particles in oxy-fuel conditions. The purpose of this study was to simulate four different combustion environments (air-fired, OF25, OF27,
and OF29) and to investigate the gas temperature distributions, species concentrations (CO$_2$, H$_2$O, and O$_2$), velocity, and particles consumed in the furnace.

In chapter 5, the commercial CFD code, which is based on the finite volume method, was used as a second stage of this research project to model and analyze all the combustion media that were conducted experimentally by Andersson (2007) regarding lignite coal reaction. Several mathematical models with the appropriate related constants and parameters were employed for lignite coal combustion by writing the subroutines required for coal devolatilization and coal combustion. Oxygen concentrations in the feed gas and carrier gas, and recycled flue gas rates were key aspects in the combustion conditions of oxy-fuel combustion environments.

The numerical results of all combustion cases examined were reasonably in a good agreement with the experimental data in terms of gas temperature distributions and species concentrations. For the OF25 combustion case, the flame temperature distributions and O$_2$ concentrations in the furnace were similar to the air-fired case. But, the flame temperatures of OF27 and OF29 were higher, and the flame structure was shorter and more confined to the near-burner region because of the high oxygen consumption. In all oxy-fuel combustion cases, the CO$_2$ concentrations were increased by around five times with respect to the air-fired case due to using dry RFG as feed oxidizer gases and carrier gases instead of air. The burner configuration and the reduction in the volumetric flow rates of the RFG (from air-fired to until OF29) have a significant effect on the mixing of the reactants. This decrease in the gas velocities ensured more residence time for PC and led as a result to improve the ignition conditions of oxy-fuel-fired cases in the near-burner reaction zone.

The one-step chemical reaction mechanism adopted in these simulations led to over-predict in the moisture content, particularly in the flame envelope zone. This reaction scheme neglects the dissociation of main combustion products CO$_2$ and H$_2$O into several unstable radicals such as CO, O, H$_2$, and OH. In the reference and OF25 combustion cases, the hydrocarbon gas (volatile matter released) consumption was
relatively faster than the OF27 and OF29 cases at port 3. This led to a shortage in oxygen concentration in the near burner reaction zones and therefore more unburned char in OF27 and OF29 cases at port 3.

The third research objective was to conduct a CFD modelling investigation of gaseous and solid phase chemistry mechanisms for lignite coal as a third stage of this project. The purpose of this study was to perform multi-steps reaction schemes and nitric oxides (NO\textsubscript{x}) formation/destruction mechanisms in the same combustion scenarios on a 100 kW firing unit. This numerical investigation is considered as an attempt to improve the predicted results with the physical data and to be a basis for the brown coal oxy-fuel tangentially-fired boiler.

In chapter 6, the simplified approach of the chemical kinetics has been modelled to calculate the Fuel and Thermal NO formation, decoupled from the main fluid flow computations. An assumption of the chemical equilibrium model was carried out on the homogeneous and heterogeneous reactions of the pulverized lignite particles in terms of single-, two-, and three-step reaction schemes. The temperature distributions, species concentrations (O\textsubscript{2}, CO\textsubscript{2}, CO, H\textsubscript{2}O, and H\textsubscript{2}), NO\textsubscript{x} emission concentrations were investigated and compared at different locations inside the furnace, as well as, the radiation heat transfer on the furnace wall.

The numerical results showed a very reasonable agreement with the experimental data for all the combustion scenarios examined, especially with the three-step reaction scheme. The results of the three-step chemistry reaction mechanism illustrated improved agreement compared to those of the one-step and two-step reaction models. The improvements were particularly observed in the flame envelope zone in terms of the gas temperature levels and the species concentrations. This is obviously due to the adoption of thermal dissociation of chemical species in three-step reaction mechanism.
In addition, the three-step chemistry mechanism used to describe the fuel conversion can precisely capture the CO/CO\textsubscript{2} production rate and equilibrium between H\textsubscript{2} and H\textsubscript{2}O in the near-burner reaction zone. There was a clear difference in the NO\textsubscript{x} distribution between the air-fired case and the oxy-fuel (OF27 and OF29) combustion cases in the near-burner region. This was mainly due to absence of thermal NO formation under oxy-fuel combustion conditions. Finally, the elevated values in the flame temperatures and CO\textsubscript{2} and H\textsubscript{2}O concentrations under oxy-fuel combustion led to the increased radiation heat flux on the furnace wall.

The final research objective was to simulate the Victorian brown coal combustion in a 550 MW tangentially-fired boiler under different combustion media. This study focussed on the numerical investigation of a large-scale oxy-fuel furnace. The available power plant data (Staples and Marshall 2010) were used to validate the predicted results under the air-fired condition. Four parameters: flue gas composition, gas temperatures, carbon in fly-ash, and HGOT mass flow were compared. A reasonably good agreement was achieved. The Chalmers’ approach in a 100 kW facility unit (Andersson 2007) was selected to the present large-scale furnace in three O\textsubscript{2}/CO\textsubscript{2} mixture conditions, referred to as OF25, OF27, and OF29, in terms of aerodynamic conditions and thermodynamic properties.

Several mathematical models such as coal devolatilization, char burnout, combustion chemistry, convection and radiation heat transfer processes, carbon in fly-ash, and thermal and fuel nitric oxides models were developed through subroutines and added to the CFD calculations. The temperature distributions, species concentrations (CO\textsubscript{2}, CO, O\textsubscript{2}, H\textsubscript{2}O, and H\textsubscript{2}), gas-phase velocity fields, char burnout, NO\textsubscript{x} emissions, and radiative heat transfer obtained for all combustion cases were computed and compared.

The findings of chapter 7 confirmed that the combustion characteristics and heat transfer processes of oxy-fuel-fired cases can essentially be matched the conventional combustion characteristics if the appropriate amounts of oxygen and RFG are to be optimised. Compared to the OF25 and OF27 combustion scenarios, the OF29 case
showed similar gas temperature levels and radiative heat transfer to that of the air-fired case. This was due to increasing the residence time of coal particles and \( \text{O}_2 \) concentrations in the gas mixture. It was also noticed that the higher \( \text{CO}_2 \) concentrations in the oxy-fuel cases significantly affected the pyrolysis process of coal particles and thus resulted in an increase in the carbon in fly-ash. A remarkable decrease in the \( \text{NO}_x \) formation was observed because of the elimination of thermal NO process from the oxy-fuel combustion scenarios, as well as low nitrogen content and higher \( \text{H}_2\text{O} \) concentrations in the raw brown coal used. Finally, it can be concluded that the aerodynamic and thermodynamic conditions of OF29 combustion case were favourable, and closely matched the conventional combustion characteristics in several important areas in comparison with the other oxy-fuel-fired conditions.
8.2 Recommendations for further research

Several recommendations are now made for future work to extend the completed research. These recommendations aim to create better understanding of the development and validation of the combustion models in tangentially-fired oxy-fuel furnaces. The recommendations are summarized below:

- The char combustion was modelled in this investigation by a global reaction of order unity due to the complexity of carbon-oxygen reaction scheme. This model can not accurately capture the effect of the temperature and O₂ partial pressure dependency on the CO/CO₂ production rate and char reaction kinetics. The enhanced three-step semi-global kinetics model (n-th order) is important and needs to be used to yield intrinsic kinetics data over a range of complex oxy-fuel combustion conditions.

- The numerical simulation of the mean chemical reaction rates of fuel has been considered to be a main problem in the determination of chemical kinetic processes. This is due to reaction rate being nonlinear functions of the local temperature values and species concentrations. Detailed chemical kinetic mechanisms with the appropriate kinetic parameters of the chemical balance equations are better to use in the simulation of the fuel reaction process.

- The modified turbulent controlled combustion model, the Eddy Breakup (EBU) model, was used to calculate the mean reaction rates for these combustion simulations. More sophisticated models are available to achieve that purpose, such as Turbulent Flame Speed Closure Combustion Model (TFSCM), Eddy Dissipation (ED) model, Probability Density Function (PDF).

- Due to the complexity of the interacting processes such as turbulence, heterogenous reactions, and heat transfer, a simplified approach of the chemical kinetics used in the model for NOₓ formation. This approach might lead to losing in the essential information due to the reduction path. Therefore, other advanced approached such as detailed chemistry and advanced engineering correlations need to be taken into account.
and consideration in the calculations of the overall NO\textsubscript{x} formation. In addition, more research is required to fully understand the complex reaction processes involved in the conversion of fuel-N to NO\textsubscript{x} formation/destruction mechanisms.

- On the furnace wall surface, the effect of upstream burner geometry was partially taken into consideration in this numerical modelling due to time constraints. An incorporating of a full upstream mill ducting on the large-scale tangentially fired furnace can provide accurate gas and particle phase boundary conditions at the burner exit plane and has a great importance in establishing the efficient mixing within the furnace.

- The current developed turbulent low rank coal combustion model can be extended to include the prediction of further research in regards to the scrubbing process of CO\textsubscript{2} from the power plant and new design optimisation of the boiler.
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