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Oxy–Fuel Combustion in the Lab–Scale and Large–Scale Fuel–Fired Furnaces for Thermal Power Generations

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1. Introduction

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 [1]. 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 [2]. 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 [3]. 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. 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. This chapter continues on different CO₂ 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 a comprehensive CFD modelling study on the lab-scale and large-scale furnaces under air-fired and oxy-fuel combustion conditions.

2. 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 (NO_x) and sulphur oxides (SO_x) 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 [3, 4]. 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.

2.1. Pre-combustion capture

The pre-combustion capture technique excludes CO₂ from the fuel before the burning process in the combustion chamber. This technique can be achieved by installing special equipment which captures CO₂ 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 (H₂)). The second step is to convert CO to CO₂ with steam (synthetic gas with suitable amounts of water vapour) by a process called shift-conversion ($CO + H_2O \rightarrow H_2 + CO_2$). After that, CO₂ can be separated by using a physical solvent, and finally the CO₂ becomes efficiently available for a sequestration process after it passes through a compression unit. The other remaining parts (mainly hydrogen (H₂)) will be sent to the combined cycle power plant to be used as input fuel for power production [5]. As shown in Figure 1, 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 (H₂S) removal. Although this method of CO₂ 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 CO₂ capture techniques [6].

Figure 1. Power plant with pre-combustion capture technology

2.2. Post-combustion capture

The post-combustion capture technique involves capturing CO₂, as well as reducing particulate matter, SO_x, and NO_x in the combustion flue gases (see Figure 2). 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 [7].

Figure 2. Power plant with Post-combustion capture technology

In the first separating technology, the chemical absorption of chemicals such as monoethanolamine (MEA) is used in an absorption tower to scrub CO_2 from the combustion flue gases. A high temperature level is used to separate CO_2 from the chemical solvent after delivering it to the regenerating tower. After that, a compression process is performed to capture CO_2 as seen in Figure 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 CO_2 capture [8, 9]. 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 CO_2 by separating it from the flue gases. These membranes can experience some technical problems if applied to the capture of CO_2 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 CO_2 capture power plant, and it is still under development. Finally, the third separation technology, low temperature distillation, can be used to capture CO_2 from the flue gas, but this process requires special conditions (above 75 psi pressure, and -75°F temperature) to achieve a high purity of CO_2 (about 90% CO_2) 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 CO_2 capture from power plants.

2.3. 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 CO_2 from the exhaust gases as a final process of sequestration, but it is less chemically complicated. As described earlier, the partial pressure of CO_2 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 CO_2 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 CO_2) instead of air in the combustion chamber. In this case of combustion, a high concentration of CO_2 (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 3. In Figure 3, 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.

Figure 3. Power plant with the capture of oxy-combustion technology

After removing particulates and condensing water vapour from the flue gases, the concentration of CO₂ 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 CO₂ 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 3, 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 CO₂ capture technologies due to the high reduction in NO_x and SO_x emissions besides its high CO₂ 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 CO₂ with respect to nitrogen in conventional combustion, radiative properties of gas mixtures, low oxygen molecular diffusivity in CO₂ compared to N₂ and other transport properties of the gas mixture such as viscosity, thermal diffusivity, gas phase chemistry etc. [1, 3, 10-12].

2.4. Comparison amongst different capture technologies

In short, all these three CO₂ 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 CO₂ 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 (H₂) in which CO is converted to CO₂ by the shift-conversion process. This CO₂ capture approach can be developed by either physical or chemical absorption processes to avoid any extra complexity in chemical design of power generation. However, both of these processes are very expensive and chemically complicated. Finally, capture of CO₂ 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 CO₂ and H₂O in the flue gas. After the condensation process, CO₂ concentrations will be increased to a level more suitable for the separating and compression processes. Although energy consumption for O₂ 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 O₂ production are under development in order to reduce the energy penalty for CO₂ capture power plants [13].

Recently, Kanniche *et al.* (2009) [7] comprehensively made a comparison between the leading technology systems for the IGCC, NGCC, and PC power plants with the above-mentioned CO₂ 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 CO₂ 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 CO₂ 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 CO₂ 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.

3. 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 CO₂ capture are required. Research into CO₂ 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 [14, 15], ignition behaviours [16, 17], species concentrations [18], and fuel combustion rate [19]. The heat transfer characteristics under different oxy-fuel-fired scenarios have been studied [20, 21] 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 [22–24]. 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 CO₂ in the flue gas. In addition, a significant reduction in NO_x emissions can be achieved due to eliminating N₂ from the oxy-fuel combustion processes [25]. These confirmations and support for oxy-fuel combustion technique for CO₂ 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.

3.1. Experimental and theoretical laboratory–scale projects

With increasing concerns from the Kyoto Protocol about the CO₂ 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. 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) [19] 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 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) [26]. As the gas mixture was set at 21% O_2 and 79% 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 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 O_2/N_2 and O_2/CO_2 mixtures, Zhang and co-researchers (2010) [17] and (2010) [27] 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 O_2/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 O_2/CO_2 mixture and led, as a result, to the high oxygen consumption on the char surface. Zhang *et al.* recommended increasing the O_2 concentration in the O_2/CO_2 mixture to 27% and 73% for 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.

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 [28, 29].

Recently, Venuturumilli and Chen (2009) [30] 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 (CH_4 , H , H_2 , H_2O , CO , CO_2 , O_2 , and 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. In addition to the above experimental investigations and numerical modelling, the open literature includes a number of relevant findings [31–33] 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 further research on the application of this technology prior to industrial full-scale boiler development.

3.2. Industrial large–scale demonstration developments

Developments in the lab-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 1 [34]. The implementation of these industrial-scale oxy-fuel combustion projects will greatly reduce the technology costs, especially in the ASU and CO₂ compression equipment, and make it more appropriate for commercial applications in 2022, as reported in the sequence project developments by Wall *et al.* (2009) [1].

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) [35] 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 O₂ 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 O₂/CO₂ 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.

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

Table 1. Developments of oxy-fuel combustion demonstration projects around the world, adopted from [34]

4. 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.

4.1. Coal ignition

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 [36]. For a one-step overall reaction and no heat loss, the ignition delay of volatile gases is given as follows:

$$\tau = \frac{c_v}{Q_c Y_{F,O} A \exp(-T_a/T_o)} \frac{T_o^2}{T_a} \quad (1)$$

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. 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_2O are higher than that of N_2 . As reported in many oxy-fuel experimental investigations [16, 37, 38], 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. 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_2O in the flue gas of oxy-fuel combustion, have been considered as 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 [39, 17]. 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.* (2010) [17] 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.

4.2.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 CO₂ 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) [22] 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-O₂ jet was located inside the primary stream, while in burner B, the annulus high-O₂ 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_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.

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) [40] 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 H₂) formed in the flame envelope because of the enhanced thermal dissociation. The normalized enthalpy loss variable (ξ) used to calculate the effect of convective and radiative cooling terms on the turbulent flame, and it is defined as follows:

$$\xi = h - h_{min} / h_{ad} - h_{min} \quad (2)$$

Where, h_{ad} is the conditional adiabatic enthalpy, and h_{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 - ϵ turbulence model used in the calculations and to the measurements uncertainties. In order to mathematically demonstrate the chemical effect of CO₂ 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 [41, 42]:

$$D = \frac{\tau_r}{\tau_{ch}} \quad (3)$$

Where τ_r represents the residence timescale of reactants in the combustion zone, also known as the mixing timescale, and τ_{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. $\tau_{ch} = \alpha / S_L^2$). 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:

$$D \propto \frac{\tau_r}{\alpha} \exp(-E_A / R T_f) \quad (4)$$

According to Eqs. 3 and 4, 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_2/CO_2 mixtures compared to those in O_2/N_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.

4.3. 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.

In order to reduce the char burnout time and increase the combustion rate of char particles in O_2/CO_2 mixtures, oxygen-enriched atmosphere must be used in the gas mixture [23]. 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_2 below 900K, but a low reaction order in the oxygen partial pressure is exhibited when the global reaction rate is above 1200K [43]. 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:

$$r_{gas} = k_s(T_p) P_{O_{2,s}}^n \quad (5)$$

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: $k_s(T_p) = A \exp(-E / R T_p)$.

The elevated CO_2 and H_2O 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_2O) 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) [44] 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.

4.4. 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, and recirculation of flue gas have been investigated. In this subsection, a brief summary of research under the effects of these different parameters is presented.

4.4.1. 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 safely and provide more efficient operations. However, the RFG enriched with 28 vol. % O₂ is safer than of 21% O₂ in the secondary stream of a pilot-scale burner in oxy-fuel combustion tests for high-volatile subbituminous coal [22].

The oxy-fuel combustion scenarios offer the opportunity to supply different amounts and concentrations of RFG enriched with O₂ 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 [14, 17, 45–47]. 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 O₂ 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) [33] 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.

4.4.2. 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) [47] 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 O₂/CO₂ mixture could be increased using smaller PC particles.

Huang and co-researchers (2008) [46] investigated the effect of the coal particle size on the combustion characteristics of TieFa (Tf) bituminous coal in different mixtures of O₂/CO₂ 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 O₂ 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 O₂ 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 [48]:

$$S = \frac{\left(\frac{dW}{dt}\right)_{max}^c \left(\frac{dW}{dt}\right)_{mean}^c}{T_i^2 T_b} \quad (6)$$

Where $\left(\frac{dW}{dt}\right)_{max}^c$ and $\left(\frac{dW}{dt}\right)_{mean}^c$ 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 [46].

4.4.3. 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 [49]:

$$Recycle\ ratio = \left(\frac{Recycled\ gas\ mass\ flow\ rate}{Recycled\ gas\ mass\ flow\ rate + Product\ gas\ mass\ flow\ rate} \right) * 100 \quad (7)$$

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 [35]. As previously illustrated in Fig. 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 [50].

Sturgeon *et al.* (2009) [33] 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 [10, 12, 16]. 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.

5. CFD modelling investigations on the lab–scale and large–scale furnaces under air–fired and oxy–fuel combustion conditions

In this section, an overview of the research program [10, 11, 51, 52] will be briefly discussed. This research program can be classified to have two main objectives:

- 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, and velocity. 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 [10, 51].
- 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 O₂/CO₂ 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 [52].

5.1. The pulverized dry lignite combustion in the lab–scale furnace

This subsection describes a comprehensive computational fluid dynamics (CFD) modelling study undertaken [10, 51] 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. O₂ concentration (OF25), 27 % vol. O₂ concentration (OF27), and 29 % vol. O₂ 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 [53] from a lab-scale 100 kW firing lignite unit (Chalmer’s furnace) were selected for the validation of these simulations.

5.1.1. A review of experimental setup of Andersson [53]

Chalmers 100 kW test facility has been designed to burn both gaseous and pulverized fuels. The furnace is a cylindrical refractory lined drop tube unit with dimensions: 80 (cm) inner diameter and 240 (cm) inner height. Three different oxy-fuel combustion cases are used as follows: OF25 (25% vol O₂ and 72% vol CO₂), OF27 (27% vol O₂ and 71% vol CO₂), and OF29 (29% vol O₂ and 69% vol CO₂). 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*10⁻⁵ (m³ per sec). While the carrier gas in oxy-fuel combustion cases is recycled flue gas (RGF) with a volumetric flow rate of 66.6*10⁻⁵ (m³ per sec.) that has the same oxygen concentration (30% vol dry) and recycled flue gas (68% vol dry) for all oxy-fuel combustion cases.

Inlet Flow Field Parameters		Combustion Cases			
		Air	OF25	OF27	OF29
Primary Register	Volume Flow Rate (m ³ /h)	34.87	28.94	26.85	25.11
	Mean Velocity (m/s)	7.966	6.612	6.134	5.737
	Angular Velocity (rad/s)	433.293	359.615	333.645	312.052
Secondary Register	Volume Flow Rate (m ³ /h)	81.37	67.54	62.65	58.59
	Mean Velocity (m/s)	4.995	4.146	3.845	3.596
	Angular Velocity (rad/s)	41.14	34.152	31.673	29.608

Table 2. The inlet flow field parameters of all combustion cases for primary and secondary registers of the burner

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 (λ) 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 inlet flow field parameters at the primary and secondary registers of the burner, for all the combustion cases, are summarized in Table 2. The combustor is initially fired by using gas (propane) as a pilot-fuel to start up the combusting process before switching to coal.

5.1.2. CFD results and discussion

Figure 4 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 4. 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 [53]. 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 Figure 5, 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. 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 2. 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. 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.

The oxygen concentrations (mass fraction, kg/kg) on a vertical plane through the middle of the furnace are shown in Figure 6. 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 Figure 4. 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 [53].

Figure 6. 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.

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 7a 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 7b 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 O_2 concentration of the oxy-fuel combustion cases as reported in the previous findings [17, 19, 24, 54]. 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 O_2 content, especially with high CO_2 concentration in the flue gas.

Figure 7. 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, 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

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 8 is clearly showed the increase in CO₂ 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 mechanisms in terms of homogeneous and heterogeneous coal reactions. As seen, the maximum mass fraction value of CO₂ 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 CO₂ concentration, and therefore they should be taken into consideration in design any oxy-fuel combustion boiler. All these CFD results were comprehensively validated against the available experimental data [10, 51].

Figure 8. 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 given in mm.

5.2. The brown coal combustion in a 550 MW tangentially-fired boiler

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 [55- 57]. 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 section 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 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 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_x emissions, and radiative heat transfer obtained for all combustion cases were compared.

5.2.1. Boiler description and operating conditions

The tangentially-fired Victorian brown coal 550 MW_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 Figure 9. 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 Figure 9 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 m³ 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. Table 3 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).

Burner duct	PC flow (as receive.)		Gas flow	
	Mass flow rate (kg/s)	Distribution ratio (%)	Mass flow rate (kg/s)	Distribution ratio (%)
UIB	0.93	5.7	18.71	22.1
IIB	0.54	3.3	18.22	21.5
LIB	1.57	9.4	18.19	21.5
UMB	4.82	29.7	10.3	12.2
IMB	2.78	17.2	9.34	11.1
LMB	5.62	34.7	9.8	11.6
Total	16.26		84.56	

Table 3. The mass flow rates and the distribution ratios for PC and mill gas at each inlet port of the burner ducts

5.2.2. Cases studies set up

For this numerical study, four different combustion scenarios were selected in order to estimate the performances of the 550 MW_e 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 [58]. 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 [53], 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 were 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 [10, 11, 51].

5.2.3. CFD results and discussion

In Figure 10, 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.

Figure 9. The geometric description of the CFD model for the boiler, unit 1 at Loy Yang A power station

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.

Figure 10. 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

It is clearly seen that a reduction in the levels of the gas temperature occurred when the N_2 is replaced by the CO_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_2 compared to N_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_2 concentration in the feed oxidizer gases. Furthermore, in this study, the oxygen concentration was not only the dominant factor controlling the flame temperature inside the furnace, but also the resident time of coal combustion. However, the inlet flow fields of feed oxidizer gases (O_2/CO_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. The reduction in the volumetric flow rates in O_2/CO_2 cases has given a sufficient time to burn more coal particles in the combustion zone. However, according to the Chalmers' approach [53], 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 11 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 CO₂ 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 CO₂ is achieved for all oxy-fuel combustion scenarios compared to the air-fired case. This increase of the CO₂ concentrations was also observed in the combined studies of the experimental investigations of Andersson (2007) [53] and numerical modelling of Al-Abbas *et al.* (2011) and 2012 [10, 51] which was conducted on the lab-scale 100 kW firing lignite furnace. The concentrations of CO₂ 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 CO₂ in the oxy-fuel cases can potentially increase the protection of the furnace wall against the hot flue gases. 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 4), and secondly the wall heat flux in difference furnace wall locations.

Figure 11. Distributions of carbon dioxide concentration (kg/kg) along the height of the furnace at the mid cut for all cases investigated

Combustion Media	Temp. (K)	CO ₂ (wt %)	Net Rad. Heat Flux (MW)	Carbon in Fly-Ash (%)	NO _x (ppm, dry)
Air-Fired (conventional)	635.35	18.84	778.76	2.05	218.58
Oxy-Fuel (OF25)	623.81	85.76	534.3	9.74	96.31
Oxy-Fuel (OF27)	628.27	85.01	596.37	7.04	103.2
Oxy-Fuel (OF29)	631.4	84.18	685.7	5.49	120.0

Table 4. Main predicted CFD results of all combustion cases examined at the final exit plane, and the net radiative heat flux on the furnace wall

6. Conclusion

The oxy-fuel combustion mode can potentially provide significant opportunities for near-zero emissions from the existing and newly-built PC power plants in comparison with the other CO₂ capture technologies such as pre-combustion and post-combustion. In this chapter 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 oxy-fuel combustion conditions.

The first 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 (CO₂, H₂O, and O₂), velocity, and particles consumed in the furnace. The second 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. The Chalmers' approach in a 100 kW facility unit (Andersson 2007) was selected to the present large-scale furnace in three O₂/CO₂ mixture conditions, referred to as OF25, OF27, and OF29, in terms of aerodynamic conditions and thermodynamic properties.

The findings confirmed that the combustion characteristics and heat transfer processes of oxy-fuel-fired cases can essentially be matched with the conventional combustion characteristics if the appropriate amounts of oxygen and RFG are to be optimised. Compared to the OF25 and OF27 combustion scenarios in the large-scale furnace, the OF29 case showed similar gas temperature levels and radiative heat transfer to that of the air-fired case. This was due to increased residence time of coal particles and O₂ concentrations in the gas mixture. It was also noticed that the higher CO₂ 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 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.

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