Chapter 2

Literature Review

2.1 Overview

This chapter presents a detailed literature review on oxy-coal combustion, focusing on fundamental aspects of pulverized coal combustion under oxy-fuel combustion atmosphere. The difference between conventional air-fired combustion with the oxy-coal combustion has been discussed. Both wet and dry recycle oxy-coal combustion have been thoroughly reviewed and compared in this chapter. In the last section of the chapter, we have reviewed the work focusing on oxy-coal combustion-based carbon capture and storage (CCS) techniques in large scale power plants and thermodynamic analysis of the coal combustion process.

2.2 Oxy-Coal Combustion Characteristics

A mixture of around 95% pure oxygen and recycled flue gas (RFG) replaces air as oxidizer under oxy-fuel combustion (Smart et al., 2010; Maffei et al., 2013). Recycled flue gas (RFG) works as diluent to limit the AFT. The different thermophysical, chemical and optical properties of CO_2 than N_2 considerably alters the combustion mechanism in oxy-fuel atmosphere, especially the heat transfer and reaction rate. In this section a detailed review on the oxy-coal combustion characteristics mainly focussing on flame characteristics, heat transfer and numerical modelling strategies have been presented.

2.2.1 Flame Characterisation, Ignition and Burnout

Hees et al. (2016) compared the flames produced under oxy-coal combustion and conventional air-fired combustion. They reported that the flames produced under oxy-coal combustion atmosphere are less radiant than the flames produced under air combustion at the equal oxygen concentration. Hjärtstam et al. (2009) presented a comparison of the oxy-fired flames produced under three different combustion cases obtained by changing the recycle ratio of the flue gas with the reference air flame in terms of temperature, ignition behaviour and species concentration. They reported a reduction in flame temperature for oxy-fuel combustion conditions compared to reference air-fired combustion due to the greater heat capacity of CO_2 than N_2. They further added that to achieve a flame temperature identical to the reference air combustion, the oxygen concentration in the oxy-fuel combustion condition was increased to 25%. Toporov et al. (2008) conducted an experimental study of pulverized coal combustion in a pilot-scale vertical combustor in both air-fired and oxy-fired combustion atmosphere. They reported that the oxy-fuel combustion atmosphere having 21% O_2 has produced an unstable flame and low burnout. They overcame the flame instability of oxy-coal combustion by redesigning the burner. They strengthened the internal recirculation zone (IRZ) of the redesigned burner by increasing the secondary stream swirl. Jovanović et al. (2013) proposed a novel approach for the oxy-fired combustion/ignition modelling of pulverized coal. The developed model considered the possible combustion/ignition mechanisms of the particle and utilized the LES approach for turbulence modelling. They reported that the flame properties, including the ignition position, flame shape, flame stability and luminosity, were accurately predicted by the proposed model. They compared the prediction of the proposed model with the standard k-ε model to address the shortcomings of the standard k-ε model. Riaza et al. (2012) studied the ignition temperature, burnout and NO emission characteristics of coal and olive waste (10 and 20 wt.%) blends under various oxy-fuel combustion atmosphere obtained by varying the O_2 concentration from 21-35%. They found increased ignition temperature and reduced burnout under oxy-fuel combustion case having 21% O_2 compared to conventional air-fired combustion case. They achieved lower ignition temperature and higher burnout compared to air-fired combustion by increasing O_2 concentration to 30-35%. Smart et al. (2010) also reported improved burnout in oxy-fuel combustion conditions by adding biomass to coal. Bhuiyan and Naser (2015) investigated the ignition and burnout characteristics during oxy-fuel combustion of coal and biomass in a 550 MW tangentially fired boiler. They reported improvement in burnout value during co-firing of coal and biomass under oxy-fuel combustion conditions. Álvarez et al. (2011) numerically investigated oxy-coal combustion cases having 21%-35% O_2 in CO_2 in an entrained flow reactor (EFR) employing three different types of coal. They compared temperature distribution, burnout and species concentrations of oxy-fuel combustion cases with the air-fired combustion. They reported lower burnout under oxy-fuel combustion case having 21% O_2 concentration. However, burnout was improved by increasing O_2 concentration. Álvarez et al. (2013) performed numerical and experimental investigation of oxy-coal combustion. They predicted the temperature distribution, char burnout, burning rate and NO emissions during coal combustion in both air and O_2/CO_2 atmospheres. They found that the predicted values for coal burnout and oxygen concentration were more accurately predicted by FG-DVC coal devolatilization kinetics than the default devolatilization kinetics. Zhou et al. (2016) Studied the chemical and thermophysical effect of CO_2 on the combustion mechanism of a coal char of 91 µm under O_2/CO_2 combustion environment. They replaced certain amount of CO_2 with Ar (molar heat capacity of $Ar<N_2<CO_2$) to create a combustion atmosphere in which char particle temperature was comparable to conventional air combustion. Liu et al. (2017) numerically investigated the influence of swirl strength, partial pressure of O_2, blockage ratio and flue gas recycle ratio on the structure, type, shape and stability of flames. They reported that the flame stability was enhanced due to formation of internal recirculation zone. They further added that the formation of the central dark primary core destroyed the oxy-fuel flames. They found the influence of recycle ratio and swirl strength more pronounced than the other two factors. Chae et al. (2018) investigated the flame characteristics of 30 MW tangentially fired oxy-coal swirl burner. They reported that the primary oxidizer's oxygen concentration considerably influenced the flame characteristics. They observed delayed ignition close to the fuel nozzle due to the increase in flame length at reducing oxygen concentration of primary oxidizer. They further added that the favourable combustion conditions were produced at equal oxygen concentration in both primary and secondary oxidizer. Jovanović et al. (2019) studied the effect of the burner O_2 excess ratio in terms of its performance and its flexibility to work efficiently in both conventional air and oxy-fuel combustion

conditions. They assessed the effect of excess O_2 concentration on flame and emission characteristics of various oxy-coal combustion cases both experimentally and computationally. They reported that both the reactive flow field and flame type were considerably affected by the burner excess O_2. They found shorter and stable flames attached to the burner by increasing excess O_2 from fuel-rich condition to fuel lean condition. Zabrodiec et al. (2019) performed the experimental investigation of the effect of changing oxygen concentration of oxidizer on the resulting reactive flow field, species concentration and flame structure. They reported an increase in the velocity along the main vortex of flame and a decrease in velocity in recirculation regions of the flame with increasing oxygen concentration of the oxidizer. Hees et al. (2019) performed an experimental study to assess the effect of oxygen concentration on the oxy-coal swirl flames. They reported that an increase in oxygen concentration leads to more intense combustion adjacent to the burner with a somewhat similar flame structure.

2.2.2 Heat Transfer Under Oxy-Coal Combustion

Changing the combustion atmosphere from conventional air to oxy-fuel alters the heat transfer mechanisms of pulverized coal combustion. The modifications in heat transfer mechanisms of the oxy-fuel combustion atmosphere are associated with the increasing concentrations of CO_2, H_2O and particulate matter (Toporov, 2014). Many authors have studied the modifications in heat transfer mechanism under oxy-fuel combustion atmosphere mainly focussing on radiative heat transfer in lab, pilot demonstration-scale furnaces.

Smart et al. (2010) performed the measurement of convective and radiative heat flux while firing biomass with coal under different combustion atmosphere obtained by varying recycle ratio (RR). They found an adverse influence of biomass addition to the coal on radiative heat flux. They observed the opposite trend between convective and radiative heat fluxes. Lv et al. (2018) numerically investigated the co-firing characteristics of 600 MW furnace firing coal and biomass. They emphasized on burnout and heat transfer under various combustion atmosphere and for various proportions of biomass. They found reduced average heat flux in oxy-fuel combustion atmosphere compared to conventional air combustion. Guo et al. (2017) studied the combustion and emission characteristics of 35 MW boiler firing sub-bituminous coal under oxy-coal combustion conditions. They investigated the temperature, species concentration distribution, heat transfer and exhaust emission under both dry and wet oxy-coal and conventional air combustion atmospheres. They found almost similar temperature and heat flux distribution under dry and wet recycle oxy-coal combustion atmosphere at 28% O_2 concentration. They observed a strong influence of flue gas recycle ratio on heat flux under oxy-coal combustion atmosphere. They reported an increase in heat transfer to superheater and membrane wall in oxy-coal combustion atmosphere compared to conventional air combustion. They further added that the rise in recycle ratio from 0.71-0.73, heat transfer to superheater increases by 6%, whereas heat transfer to membrane wall reduces by 4%. Rebola and Azevedo (2015) performed a numerical investigation on the combustion characteristics of pulverized coal under conventional air and oxy-fuel combustion atmospheres. They reported that the oxy-fuel combustion atmosphere has a heat flux profile similar to conventional air at a recycle ratio of 0.72. They further added that the 3^0C increase in wall temperature increased incident heat flux by 10% and reduced absorbed heat flux by 7%. They concluded that the influence of wall temperature on incident wall heat flux was more predominant than the recycle ratio (RR). Crnomarkovic et al. (2014) utilized the Hottel's zonal model to study the influence of total extinction coefficient and scattering albedo on radiative heat transfer. They observed that the moderate values of extinction coefficient had attributed to maximum wall flux and heat transfer rate. They further added that the higher wall flux and heat transfer rates were obtained at a lower value of extinction coefficient than the higher extinction coefficient. Nakod et al. (2013) employed both gray and non-gray approach of radiation modelling under oxy-coal combustion (both dry and wet) and conventional air combustion atmospheres in a laboratory and full-scale furnaces. They observed reasonable agreement between predicted temperature distribution and measured data. They reported higher sensitivity of devolatilization models than the radiation models on temperature distribution. The shorter path lengths and lower flame temperatures minimized the deviations of temperature and radiative heat flux predicted by gray and non-gray radiation models in the laboratory-scale furnace. In the full-scale furnace, approximately 10% deviation between gray and non-gray radiation models predictions of radiative heat flux and 40-50 K difference in temperature were found due to longer path lengths and higher flame temperatures. Corrêa da Silva and Krautz (2015) employed the staged feed gas burner in a 0.4 MW test facility to study the heat transfer characteristics. They reported a considerable influence of stoichiometric ratio, feed gas temperature, oxygen and water vapor concentrations on the adiabatic flame temperature. The adiabatic flame temperature identical to air combustion was obtained in oxy-fuel combustion atmosphere at 31% O_2 content in oxidizer. They obtained reduced temperature in oxy-fired combustion atmosphere due to higher concentrations of CO_2 and water vapor. Li et al. (2017a, 2017b) investigated heat transfer, and combustion characteristics of 600 MW tangential fired furnace in both dry and wet recycle oxy-coal combustion atmosphere. They reported that the O_2 content of 28.3% in dry recycle and 27% in wet recycle oxy-coal combustion had produced heat transfer rate similar to conventional air combustion. Kez et al. (2019) investigated the effects of several approximations of particle and gas radiative properties and spectral resolutions on the effectiveness of the modelling of radiation heat transfer in oxy-coal combustion atmosphere. They employed narrow band correlated-k (NBCK) model to compute the wall heat flux and radiation source term. They found 50% contributions of gas radiation on the total radiation source term. They observed that the selection of complex refractive index played a significant role in the accuracy of simulation results. Yang et al. (2018) employed a full-spectrum correlated k (FSCK) model and Mie theory-based data to investigate the radiative heat transfer characteristics of both small and large scale furnace. They also presented a comparison between the predictions of the refined radiative property-based model and conventional WSGG model. They reported that the refined radiative property-based model predicted lower particle radiation source term and higher gas radiation source term compared to WSGGM. They observed the predominant influence of FSCK model in prediction of gaseous radiation in large scale furnace.

2.2.3 RANS and LES Modelling of Swirl Oxy-Coal Furnaces

CFD modelling has developed as a potentially effective and inexpensive method for designing and improving pulverized coal-fired furnaces. The comprehensive modelling approach employing the appropriate models/submodels are able to effectively handle complex physical and chemical mechanisms of pulverized coal combustion. Computational simulations save resources and time and also shorten maintenance in the full-scale boiler. Therefore, computational investigations are playing and supposed to play a crucial role in the design and development of combustion systems in the near future.

Generally, the pulverized coal combustion process is modelled employing the well-known Eulerian-Lagrangian approach. The gaseous phase submodels consider the reactive fluid flow, chemical reactions and heat and mass transfer. The particle phase submodels consider the particle force balance, particle energy balance, devolatilization and char combustion mechanisms (Tabet and Gökalp, 2015).

The CFD simulations employ RANS, and LES approaches for the modelling of the gaseous phase. The dependent variables are decomposed into time-space averaged components and fluctuations. The resulting Reynolds fluxes are modelled by solving the transport equations of turbulent kinetic energy and turbulent dissipation rate. Whereas LES directly resolves larger eddies and models the impact of the smaller eddies (Chen et al., 2012).

The structural methodology of the modelling of pulverized coal combustion is displayed in Fig. 2.1. Table 2.1 summarizes recent computational studies along with employed modelling strategies.

Reynolds averaged Navier Stokes (RANS), and large eddy simulation (LES) of oxy-coal swirl flame was performed by Warzecha and Boguslawski (2014a, 2014b), Chen and Ghoniem, (2012), Sadiki et al. (2017), Pedel et al. (2012) Franchetti et al. (2016, 2013) and Clements et al. (2015). All the studies reported that LES was able to predict the mixing and recirculation more accurately than RANS based turbulence model. Hence the prediction accuracy was enhanced using the LES model. These studies further added that the requirement of computational power was also increased for LES modelling than the RANS. Gaikwad et al. (2017) developed a simplified 2D axisymmetric model in oxy-coal swirl flame. They compared the result of the 2D simplified model with the experimental data and LES results of other authors. They showed that the result of the simplified 2D model was good enough for preliminary analysis of oxy-coal swirl flame without losing much accuracy compared to LES modelling. Chen and Ghoniem (2012) employed RANS and LES approach to model the turbulence during oxy-fuel combustion in a pilot-scale furnace. They compared the RANS and LES predictions of velocity, temperature and oxygen mole fraction with the measured data. They reported that the prediction of LES was most accurate among the tested turbulence models and captured reactive flow field and turbulent structure accurately.

Table 2.1 Summary of Numerical work along with employed models and sub-models of combustion

Facility	Fuel	Code	Modelling approaches				Ref.
			Turbulence	Radiation	devolatilization	Char combustion	
RWTH Aachen 100 kW down fired swirl burner furnace	Lignite coal	Fluent 15.0	Standard k-ε RNG k-ε SST k-ω	DO	Single kinetic rate model	kinetics/diffusion-limited	Gaikwad et al. (2017)
35 MW large pilot boiler	sub-bituminous	Fluent 16.0	Realizable k-ε	WSGGM	CPD	kinetics/diffusion-limited	Guo et al. (2017)
Downward fired cylindrical chamber of capacity 60 kW	Lignite Coal	Fluent 17.0	Realizable k-ε	P1	Single kinetic rate model	kinetics/diffusion-limited	Sadiki et al. (2017)
600 MW pulverized-coal utility boiler	Pulverized coal	Fluent	Realizable k-ε	DO	Two competing rate model	kinetics/diffusion-limited	Ti et al. (2016)
915 MW actual large-scale boiler, 2.4 MW and 0.76 MW test furnaces	Pulverized coal	Fluent	RNG K-ε	DO	Modified TDP model	Combined model of kinetics and eddy dissipation	Hashimoto and Watanabe (2016)
15 kW test furnace	Bituminous coal	Fluent	Standard k-ε	_	Two competing rate model (Kobayashi model)	Intrinsic char burnout model	Beckmann et al. (2016)
300 MW tangentially fired pulverized coal furnace	Pulverized coal	Fluent	Standard k-ε RNG K-ε RSM	DO	Single kinetic rate model	Diffusion-limited	Khaldi et al. (2016)
0.3 MW pilot-scale furnace	Pulverized coal	Fluent	Standard k-ε	P1	CPD	_	Tu et al. (2015a)
200 MW tangentially fired utility boiler	Bituminous coal	Fluent 6.3	Standard k-ε	Improved WSGG model	CPD	kinetics/diffusion-limited	Guo et al. (2015)
Drop tube furnace	Bituminous coal	Fluent 12.0	Standard k-ε	DO	Single kinetic rate model	kinetics/diffusion-limited	Cai et al. (2015)

RWEn power's 0.5MWth combustion test facility (CTF)	Pulverized coal	Fluent	Standard k-ε	DO	CPD	_	Rebola and Azevedo (2015a)
2.5 MW pilot combustion test facility	Gottelborn coal	Fluent	Standard k-ε	DO	CPD	_	Rebola and Azevedo (2015b)
_	Pulverized coal	MFIX	Standard k-ε	P1	Kobayashi's model Ubhayakar's model	A half order reaction rate of Harmor	Cai et al. (2015)
RWTH Aachen 100 kW down fired swirl burner furnace	Lignite Coal	Fluent	Standard k-ε	DO	Single kinetic rate model	_	Warzecha and Boguslawski (2015)
CRIEPI's coaxial jet burner	Pulverized coal	_	SGS turbulent model (LES)	_	FLASHCHAIN	Global 2 step kinetic mechanism	Ahn et al. (2017)
Pusher type reheating furnace	Pulverized coal	Fluent 15.0	Realizable K-ε	WSGGM	Two competing rate model	Intrinsic kinetic rate model	Chakraborty et al. (2017)
600 MW wall-fired boiler	Pulverized coal	Fluent	Standard k-ε	P1	Two competing rate model	kinetics/diffusion-limited	Du et al. (2017)
Vertical cylindrical laboratory furnace	Coal/biomass (80:20)	Fluent 6.3	_	DO	Two competing rate model	kinetics/diffusion-limited	Bonefacic et al. (2015)

Kangwanpongpan et al. (2012) focused on accurate prediction of radiative properties during numerical investigation of oxy-coal combustion. They computed radiative heat transfer by discrete ordinate (DO) model. They coupled DO model with the weighted sum of gray gas model (WSGGM) for the estimation of the radiative properties. They reported that the limitations of turbulence model and inaccurate thermochemical closure resulted in discrepancies between experimental and numerical results of the flow field and O_2 concentration, especially close to the burner.

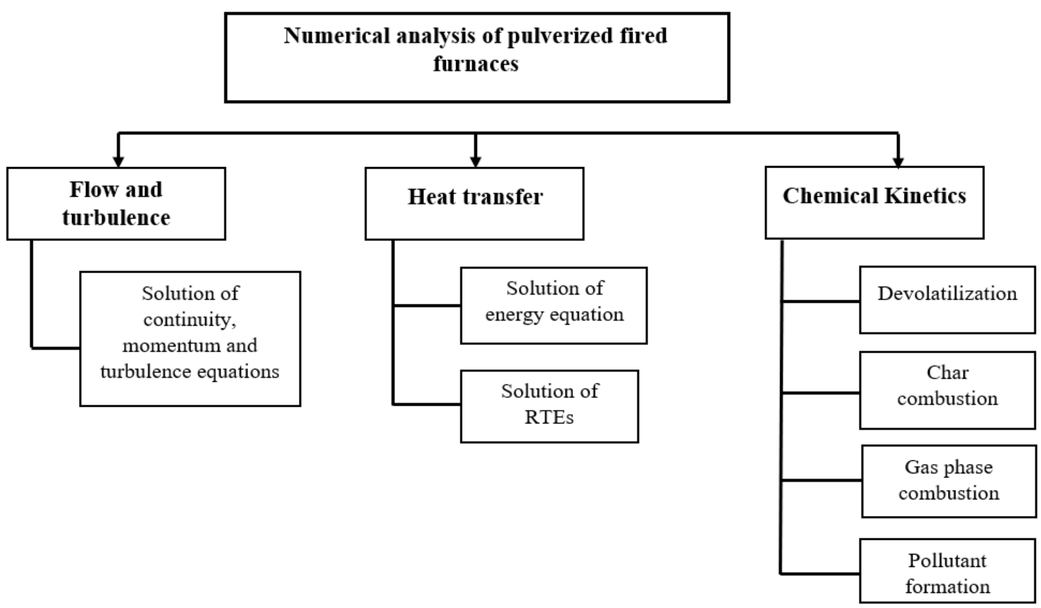

Fig. 2.1. CFD modelling of pulverized coal combustion: An overview of basic modules (Adopted from Sankar et al., 2019)

Warzecha and Boguslawski (2014) employed RANS and LES approaches of turbulent modelling to perform a computational investigation of swirl oxy-coal combustion. They observed considerable differences in temperature distribution close to the burner in the oxy-coal combustion compared to air-fired combustion. They reported that the LES had better accuracy than the RANS and LES was able to detect the outer recirculation zone. They further added that the changing of combustion environment from air to O_2/CO_2, resulted in reduced temperature and velocity distribution in the combustor. Clements et al. (2015) performed large eddy simulation (LES) and Reynolds-averaged Navier Stokes (RANS) modelling for the prediction of turbulent coal combustion under air and oxyfuel environments in a pilot scale 250 kWth furnace. They reported that LES modelling has more accurately predicted surface incident radiation than RANS modelling. However, the computational demand of LES was approximately ten times higher than RANS on the same computational grid. Elorf et al. (2016) numerically investigated the effect of swirl strength on flow and combustion behaviour of olive cake. They studied three combustion cases: air flow without swirl, axial flow with swirl, and axial and co-axial jets with the swirl. They found comparatively stabilized flames under swirling cases due to the formation of more intense internal recirculation zone (IRZ). Elorf et al. (2019) performed a 3D computational investigation of pulverized biomass flame and studied the influence of swirl strength on flow, temperature and species concentration distribution. They reported that the position of principle recirculation zone (PRZ), visible flame length and maximum gas temperature were strongly affected by varying the swirl number. Holland and Fletcher (2017) extended the comprehensive char conversion code (CCK) to develop a comprehensive char oxidation and gasification models to work under oxy-coal combustion conditions and considers the pore diffusion, film diffusion, annealing and ash encapsulation. They compared the char combustion models with the oxy-coal data and found that the CCK/oxy model had good agreement with the available oxy-coal data.

2.2.4 Emission Characteristics of Oxy-Coal Combustion

Al-Abbas et al. (2012) performed numerical modelling of 550 MW utility boiler under air and three oxy-coal combustion cases employing Victorian brown coal. They computed fuel and thermal NO formation by employing a simplified approach of chemical kinetics. They found reduction in NO_x formation by 50% under oxy-fuel atmosphere than the conventional air. They further added that the conversion rate of coal-N to NO_x has also been decreased in all oxy-fuel cases compared to the air-fired case. Chen et al. (2007) studied the CO_2, NO_x and SO_2 emission characteristics of both the conventional air-fired and oxy-fired combustion atmosphere. They reported that the flue gas had approximately 90% more CO_2 under oxy-fired combustion case compared to the air-fired combustion case. They further added that the reduction in flame temperature in the oxy-fired case resulted in lower NO_x emission in oxy-fuel combustion case than the conventional air combustion. Hjärtstam et al. (2009) also reported lower NO_x concentrations under oxy-fuel combustion atmosphere due to flue gas recycling. Hu et al. (2013) performed the experimental investigation of oxy-coal combustion and measured NO_x emission. They reported that the rise in the equivalence ratio reduces NO_x concentration, whereas rise in recycle ratio (RR) promotes NO_x formation. They observed the predominance of nitrogen release rate into the volatile matter and char on the total NO_x emission generated. Zhou et al. (2018) computed NO_x emission produced by HT-NR3 swirl burner. They employed detailed NO_x formation/destruction model to minimize NO_x formation under air staged combustion at varying stoichiometric ratio. They reported highly reduced NO_x concentration at combustor outlet employing deep air staging at burner stoichiometric ratio

0.75. Mei et al. (2015) numerically investigated the influences of fuel injection angle (α) and separation distance of primary-secondary air-nozzles (S) on MILD combustion of pulverized coal. They reported a reduction in NO_x concentration at the outlet of combustor by increasing both α and S. They further added that increase in S from 0.1 to 0.6, reduces NO_x concentration at exit by 147 ppm. Zhang et al. (2019) conducted air staged combustion of 6 different coal in an electrically heated down fired furnace. A close relationship between $CO+H_2$ concentrations in the fuel-rich region and normalized NO_x concentration was observed. They proposed a semi-empirical NO_x model and implemented in Eulerian-LES simulation. They found more accurate predictions of NO_x characteristics by the newly proposed model than the traditional model. Álvarez et al. (2013) predicted the temperature profiles, char burnout, burning rates and NO emission under both conventional air and oxy-coal atmospheres. They reported that the NO emission showed a strong dependency on the accuracy of the estimated distribution of fuel nitrogen into volatiles and char. Sung et al. (2016) assessed the effect of particle size on NO emission during pulverized coal combustion. Particle size range of 40-120 µm had a linear relationship with the NO emission. They further added that for flames with mean particle size distribution of 52 and 73 µm, the NO-reduction efficiency was approximately double than the flames with mean particle size distribution of 102 and 107 µm. Oxy-coal combustion behaviour of bituminous coal under pilot-scale furnace was studied by Guo et al. (2018). To reduce the NO_x emission under oxy-fuel atmosphere, they designed low NO_x burner. They observed a reduction in NO_x emission by 30-50% due to reduced thermal and fuel NO_x and altered NO reburning chemistry under oxy-fuel combustion than the air-fired combustion. Yang et al.

(2019) performed a numerical investigation to evaluate the effect of swirl burner arrangement and separated over fire air (SOFA) locations on NO_x emission in 660 MW boiler. They reported reduction in NO_x emission by 50% by the air staging as introduction of SOFA maintains a hypoxic regime in the lower furnace to inhibit NO_x formation. Changing the orientation of swirl burner from co-rotating to counter-rotating had decreased both the NO_x emission and unburned combustible fraction. Sung and Choi (2015) evaluated influences of combustion adjustments (air staging level, stoichiometric ratio and swirl vane angle) on NO_x emission. They reported that deep air staging lowers the stoichiometric ratio of the primary zone and results in reduced NO_x emission. They further added that the swirl vane angle had more pronounced influence on NO_x emission reduction than the stoichiometric ratio of the primary zone.

2.2.5 Effect of H_2O on Oxy-Coal Combustion

In the oxy-coal combustion, the recycled flue gas (RFG) added to the oxygen have certain amount of steam with it. The concentration of steam in the RFG is approximately 37% and 22% in wet and dry recycle oxy-coal combustion, respectively (Becher et al., 2011). The dry recycle oxy-coal combustion utilizes RFG after removal of moisture from it, whereas wet recycle oxy-coal combustion utilizes the RFG without prior removal of moisture. The oxy-steam variant of oxy-coal combustion, proposed by Carlos (2007) and Seepana and Jayanti (2010), replaces RFG with pure steam. Thus, under oxy-steam combustion, steam moderates the combustion temperature rather than CO_2. Oxy-steam combustion technology does not require recycle system. Oxy-steam combustion technology has gained recognition as next-generation oxy-coal combustion technology due to its compact systems and higher capture efficiency.

The different thermo-physical and chemical properties of H_2O than CO_2 has attributed two distinct influences of steam addition to the oxidizer. Lower volumetric heat capacity of H_2O than CO_2 may result in higher flame temperature under steam enriched combustion atmospheres. The higher emissivity of H_2O than CO_2 may also result in lower flame temperature due to enhanced radiation heat transfer under steam enriched combustion atmospheres. The temperature distribution under steam enriched combustion atmospheres is dependent on the dominance of these two influences. Mao et al. (2016) reported that the effect of heat capacity was dominant at the lower O_2 concentrations in the oxidizer (21% and 25%). Whereas, radiation effect was dominant at higher O_2 concentrations in the oxidizer (30% and 35%). Tu et al. (2015) performed a numerical investigation of the effect of steam enrichment of oxidizer on MILD oxy-coal combustion. They fixed the O_2 concentration of oxidizer at 30% and varied the steam concentration added to the oxidizer to obtain various combustion cases. The results showed higher peak temperature with improved ignition and internal recirculation rate under enriched steam combustion cases. Cai et al. (2016) reported advanced ignition under enriched steam combustion atmosphere due to distinct chemical properties of H_2O than CO_2. When higher mole fraction of steam was added into the oxidizer, ignition distance decreases drastically. Ignition distance was not much affected when the smaller mole fraction of steam was added. Lower flame temperature was reported by Riaza et al. (2011) under steam enriched combustion atmospheres (10% and 20% H_2O was added to the oxidizer) in the entrained flow reactor.

A novel approach of non-isothermal thermogravimetry was applied to study the kinetics of devolatilization and oxidation under oxy-steam combustion atmospheres by Dueso et al. (2019). They varied steam concentrations from 0-70% in the oxidizer. Hu et al. (2014) reported that the smaller steam concentrations (12-17%) of steam added to the oxidizer had insignificant influence on flame temperature. Yi et al. (2018, 2014) studied the combustion characteristics of different coal types under $O_2/CO_2/H_2O$ combustion atmosphere. They reported that the combustion atmospheres having higher concentration of H_2O were associated with delayed ignition, improved burnout and comprehensive reactivity. Li et al. (2019) studied the reaction kinetics of char-O_2, char-H_2O, and char-O_2/H_2O reactions under high temperature entrained flow reactor. They also predicted the carbon conversion rate of these reactions. They reported that the rise in steam concentration in the oxidizer leads to enhanced char-H_2O gasification reaction rate and reduced char-O_2 combustion reaction rate. Xu et al. (2016) studied the devolatilization and char combustion characteristics of oxy-steam combustion environment. They obtained reduced char yield during devolatilization in the oxy-steam combustion environment. The ignition characteristics of Victorian brown coal was investigated by Prationo and Zhang (2016) under $O_2/CO_2/H_2O$ and $O_2/N_2/H_2O$ combustion environments. They observed enhancement in char-H_2O gasification reaction with steam addition under oxy-fuel combustion atmosphere. Perrone (2015) investigated the temperature and NO_x emission characteristics of oxy-coal swirl burner. They reported lower temperature during CO_2 and H_2O recirculation than the CO_2 recirculation. Zhang et al. (2019) presented a numerical investigation of MILD oxy-coal combustion under various combustion cases obtained by varying the proportions of CO_2 and H_2O in the oxidizer at a fixed oxygen concentration of 30 vol %. They mainly emphasized on heat capacity, gasification reactivity and radiation properties. They found lower flame temperature and heat transfer with rise in steam concentration.

2.3 Oxy-Coal Combustion-Based CCS Applied to full Scale Power Plant

Carbon capture and sequestration (CCS) technologies have gained a lot of attention due to its potential to mitigate the emissions of anthropogenic CO_2 as a part of an international transition to lower carbon energy systems. The carbon capture and sequestration technologies can be categorized in three categories based on the method of CO_2 separation: (1) pre-combustion capture (i.e., CO_2 separation is performed prior to combustion process, Jansen et al., 2015; Theo et al., 2016; Valiani et al., 2017); (2) oxy-fuel combustion capture (i.e., CO_2 separation is performed during combustion under O_2 rich environment instead of air, Lasek et al., 2013; Wu et al., 2018; Yin and Yan, 2016); (3) post-combustion capture (i.e., CO_2 separation is performed after the combustion process, Cormos and Cormos, 2017; Dinca et al., 2018; Ferrara et al., 2017). In the oxy-fuel combustion process, pure oxygen is used as an oxidizer instead of air. The flue gases produced have highly concentrated CO_2 and H_2O without N_2 dilution. Pure CO_2 can be achieved after condensation of water vapor. To limit the adiabatic temperature under oxy-fuel combustion, a portion of flue gas is recycled to the boiler to maintain suitable temperature inside the furnace (Stanger et al., 2015; Toftegaard et al., 2010). Although all the carbon capture and sequestration technologies (CCS) are associated with high energy penalty, oxy-fuel combustion has been identified to have lesser carbon capture cost compared to other CCS techniques (Al-Qayim et al., 2015; Kanniche et al., 2010). Most of the equipment employed by conventional air-fired combustion can be utilized in oxy-fuel combustion. The primary equipment's of conventional air-fired combustion unit, turbines, heat exchangers and coal mills can be utilized for oxy-fired combustion (Chen et al., 2019; Koytsoumpa et al., 2018).

Air separation unit (ASU) is employed for separation of oxygen from the air. Although there are some novel oxygen production techniques such as membrane separation (Falkenstein-Smith et al., 2017; Mezghani and Hamza, 2016; Shin and Kang, 2018) and chemical looping air separation (Chen et al., 2018; Shah et al., 2012; Shi et al., 2018), yet the cryogenic air separation unit (ASU) is the most commonly used technology for oxygen production at a larger scale. There is a necessity to purify and compress CO_2 for delivery and storage. Carbon dioxide purification and compression unit (CPU) is employed for CO_2 capture and sequestration, and the use of carbon dioxide purification and compression unit (CPU) is common and inevitable to all CCS techniques. Both ASU and CPU are extensive energy consuming units. Hence, incorporation of ASU and CPU to oxy-fuel combustion cycle reduces the efficiency by 9-13% points (Liszka and Ziębik, 2010). The energy penalties of oxy-fuel CCS are needed to be decreased to make oxy-fuel power generation attractive for commercial utilization (d'Amore and Bezzo, 2017; Liszka and Ziebik, 2010).

In recent years, many studies have been performed focusing on oxy-fuel combustion-based CO_2 capture. Xiong et al. (2011a) studied the operational characteristics of the 800 MW power plant under oxy-fuel combustion conditions. They reported the 10.36% reduction in net efficiency due to incorporation of ASU and CPU under oxy-fuel combustion conditions. They found specific energy consumption for oxygen production in ASU to be 0.247 kWh (kg of O_2)$^{-1}$. Skorek-osikowska et al. (2013) presented a thermodynamic analysis of pulverized coal-fired supercritical power plant of capacity 460 MW. They estimated auxiliary power rates for technological installation of the power plant under oxy-fuel combustion conditions. They found auxiliary power rates in the range of 15.65% and 19.10% for cryogenic ASU. They significantly reduced the power consumptions of ASU and CPU by utilizing waste heat from ASU and flue gas conditioning systems. Jayanti and Kareemulla (2016) proposed oxy-fuel combustion PC supercritical power plant with CO_2 enrichment and capture. They also compared CO_2 enrichment and capture supercritical power plant (case 2) with the conventional air-fired supercritical power plant (base case) without CO_2 capture and oxy-fuel PC supercritical power plant with direct CO_2 capture (case 1). The results showed that the net efficiency of CO_2 enriched oxy-fuel CCS plant was slightly higher than the direct CO_2 capture case. The gross efficiency and gross power output of CO_2 enriched oxy-fuel CCS plant was also higher than the direct CO_2 capture case. They reported 8.74% and 8.48% reduction in net efficiency for case 1 and case 2 compared to the base case. Chen et al. (2019) performed a thermodynamic analysis of fluidized bed oxy-fired power generation system coupled with CO_2 capture. Sensitivity analysis was performed for important parameters such as furnace temperature, pressure and flue gas recirculation mode. They integrated and optimized the recovered heat from CPU, ASU and exhaust flue gases. The result showed higher amount of heat was recovered from enthalpy difference with phase change from the flue gases in acid condenser due to rise in dew point at higher pressure. This was major cause of reduction in steam turbine extraction in regenerative feed water heater and boost in steam turbine output. Cau et al. (2018a) presented a comparative techno-economic analysis of an ultra-supercritical pulverized coal fired power plant of capacity 1000 MW. They evaluated the performance of conventional air-fired, partial and full oxy-fuel power plant for comparison. They evaluated the economic performance by the expected annual cash flow. Skorek-osikowska et al. (2017) presented thermodynamic and ecological analysis of pulverized coal fired power plant integrated with CCS units. They also presented a comparison between conventional power plant working without CCS unit with three configuration of CCS power plants namely pre-combustion CCS, post-combustion CCS and oxy-fuel combustion CCS. They found that the integration of CCS units with power plant reduces net power and efficiency. The corresponding reduction in net efficiency of pre-combustion, post-combustion and oxy-fuel combustion capture power plant were 16.89%, 11.75% and 7.85% respectively compared to conventional power plant working without CCS units.

2.4 Thermodynamic Analysis of Coal Combustion

Thermodynamic analysis of the combustion processes done by flow availability to the system comprising the entire combustor.

$$\dot{A}_{in} = \dot{A}_e + \dot{I} \qquad (2.1)$$

where $\dot{A}_{in}$, $\dot{A}_e$ and $\dot{I}$ represent the incoming and outgoing flow availability rates of the system and the thermodynamic irreversibility rate within the system, respectively.

Som et al. (2005) calculated thermodynamic irreversibility, combustion and 2nd law efficiency associated with pulverized coal combustion in a tubular combustor. They computed flow availabilities at inlet and outlet of the combustor for the estimation of thermodynamic irreversibility of the pulverized coal combustion process. They found increased combustion efficiency and reduced 2nd law efficiency with an increase in inlet air pressure. They further added that the influence of air inlet pressure was more dominant for shorter combustor and smaller swirl number. They reported increased combustion efficiency when the swirl number was increased from 0 to 0.32. Reduced combustion efficiency was obtained for further increase in swirl number from 0.32 to 0.77. With an increase in air inlet temperature, the combustion efficiency was increased for the shorter combustor. For longer combustor length, reduced combustion efficiency was reported with an increase in air inlet temperature. Mondal (2008) performed comprehensive mathematical modelling of single coal particle combustion in quiescent hot gas and evaluated associated thermodynamic irreversibility of various physical processes. Chemical reactions and heat and mass transfer of gas-phase attributed to the thermodynamic irreversibility during pulverized coal combustion. In the initial ignition period, lower irreversibility rate was observed, which increased as the ignition proceeded.

A comprehensive review on thermodynamic irreversibilities and exergy loss associated with the solid, liquid and gaseous fuel combustion was presented by Som and Datta (2008). They reported that the physical transport processes and chemical reactions were the primary sources of thermodynamic irreversibility in the combustion process. They focused on the design and development of energy and exergy efficient combustion systems. Wang et al. (2018) numerically investigated the unsteady entropy generation, heat and chemical species transfer in transient oxy-combustion of single coal. The result showed that the production and transport rates of species reached the maximum level in the process of homogeneous combustion of volatiles. They reported chemical reaction as the most significant source of unsteady irreversibility. They found increased total chemical entropy generation due to oxygenation of the atmosphere. The increase of total chemical entropy generation become almost insensitive after certain oxygen mole fraction.

2.5 Research Gaps

From the available literature, we have found that numerical modelling has been used as a powerful tool to clarify the basic underpinning mechanisms of oxy-fuel combustion. However, in-depth investigation of certain important parameters that affect the combustion characteristics under oxy-fuel conditions significantly needs to be further investigated.

Based on the literature review on oxy-coal combustion, the following research gaps have been identified.

- Studies on the influence of various oxy-coal combustion atmosphere obtained by varying composition of oxidizer on char burning rate, radiative properties, temporal variation of the particle-phase variable is deficient in literature.
- Studies on the influence of inlet temperature and pressure of feed gas on flow and combustion characteristics under oxy-coal combustion atmosphere are not available.

- Studies focussing on the influence of higher concentration steam addition in oxidizer on combustion characteristics of oxy-pulverized coal combustion is missing.
- Studies showing the influence of gasification reactions are only found for drop tube furnace, where the temperature is within 1000°C. In pilot-scale furnaces, the flame temperature is more than the 1000°C, and under oxy-coal combustion atmosphere the recirculation of flue gas reduces the O_2 concentration, thereby enhances gasification reactivity. Hence, influence of gasification reaction under pilot scale furnaces needs to be investigated.
- Studies presenting the thermodynamic analysis of power plant retrofitted to oxy-fuel combustion working under Indian climatic conditions employing high ash Indian coal is deficient.

The present thesis makes an attempt to fulfil the discussed research gap in subsequent chapters. A comprehensive CFD modelling of oxy-coal combustion has been performed and validated with the available experimental data. The developed numerical models are employed to investigate the influence of swirl strength, various combustion environment, inlet temperature and pressure of feed gas on resulting reactive flow field, temperature distribution, char burning rate, radiative properties and species concentration. Influence of higher concentration steam addition in the oxidizer on the flow field, temperature and species distribution profile has also been performed employing the developed numerical model. Furthermore, the influence of char gasification reactions on temperature and species concentration profile has been investigated. The influence of above-mentioned operating parameters on NO_x emission characteristics under oxy-fuel combustion environment has also been assessed employing post-processing technique. The second part of work focusses on the numerical investigation of 660 MW supercritical power plant retrofitted to oxy-coal combustion. The thermodynamic performance of oxy-coal fired power plant with the conventional air fired power plant has been presented to find the energy penalty, CO_2 recovery rate and CO_2 purity. The sensitivity analysis of important operating parameters such as oxygen concentration, recycle ratio and oxygen purity on the performance of oxy-coal power plant has also been presented and discussed.