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Concept of ECO Scrubbing Technology: A CFD case study in small scale furnace

B.Sc. Engineering (Mechanical) Thesis

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It is hereby declared that this thesis or any part of it has not been submitted elsewhere for the award of any degree or professional qualification.

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ABSTRACT:

The substantial rise in CO₂ percentage in the atmosphere owing to the increasing demand in electrical power is alarming and needs to be addressed. Coal continues to be a key fuel in global energy systems, accounting for nearly 40% of electricity generation. To resolve this situation, worldwide researchers are constantly investigating effective alternatives in a hope to establish a cost-effective eco-friendly power generation system. As such, eco-scrubbing technology is a trending retrofit option in existing plants. In the work presented in this paper, we performed a CFD modelled simulation on a unit of 30kW thermal load capacity. The objective of this study is to observe different combustion characteristics on four different cases: one air-firing reference case and three other oxy-fuel (25%, 30% and 35% O₂) cases. We investigated about the different significant combustion characteristics such as temperature distribution over the furnace, O₂ and CO₂ mass fraction throughout the furnace and velocity distributions through the furnace and presented comparable results later on. The results indicated that an increase of oxygen concentration in the oxy-firing cases caused slight rise in the flame temperature with occurrence of burnout in advance under oxy-fuel conditions in comparison to air-fired conditions.

1. INTRODUCTION

The fast-track globalization and economic growth have led to an escalation in the requirements of electrical power worldwide. In an attempt to mitigate greenhouse gas emissions that is released from conventional fossil and non-fossil (renewable) sources became contender for clean source of energy. However, the demand for coal in the power and industry sectors continues to grow in India, Indonesia and Southeast Asia. (IEA1)_This has resulted into the construction of several coal-fired power plants to meet the rising electricity demand. The reason behind this lies in the fact in coal being a more affordable and abundant resource than other fossil fuels. In addition, a closely related factor in the coal firing technology is the emission of carbon dioxide which is a significant contributor to global warming, and therefore needs to be addressed.

Oxygen/recycled flue gas combustion is one of the most up-and-coming processes for CO_2 recovery from pulverized coal-fired power plants. In this method, pulverized coal is burned in a CO_2 -based atmosphere rather than in air, which is a N_2 -based oxidant. CO_2 has higher specific heat than that of N_2 and is a common radiative gas. Hence, the system's combustion characteristics will differ greatly from those of a conventional combustion system. Recycled NOx and SO2 are also present in the oxidant, and the concentration of O2 can be changed by varying the quantity of recycled flue gas used. As a result, research was conducted to contemplate the properties of pulverized-coal combustion in the system thoroughly.

1.1 Carbon Capture & Storage (CCS):

The operation of power plants is given special attention since they are major mediums of CO_2 gas emissions. Many feasible developments for carbon capture and storage (CCS) from power plants are currently being researched. [1]–[8]. CCS may be used to supplement ongoing efforts to improve fuel quality as well as the transition to lower-carbon sources, such as fossil fuels in addition to biomass.

The reduction of CO_2 gas emissions involves two successive operations, as indicated by the word CCS:

- 1. Segregate and capture CO₂ gas from power plant flue gas emissions
- 2. Carbon dioxide (CO₂) storage that also comprises of its transport to site for storage

In order to use the existing source of fuel resources, research has been going on how to integrate the concept of capturing CO_2 sustainably, namely processes like pre-, post-, and oxy-fuel combustion sequestration. Oxy-fuel combustion technology has been widely regarded as one

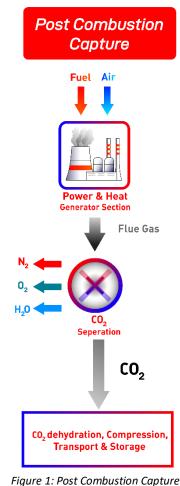
of the most viable options among the higher-than-mentioned technologies for managing and reducing a wide range of evaporated emissions from powdery coal (PC) power plants, such as dioxide, NOX, and SOX..[1], [8]–[10]

The established carbon capture technologies are classified into three categories[1], [3],[11]–[15], which are briefly represented below. (Figures 1, 2, and 3 depict the most common operations in post-, pre-, and oxy-fuel combustion technologies.)

1.1.1 Post-combustion capture:

An additional process stage is used in post-combustion capture to remove the majority of CO_2 from combustion emissions only before they are ventilated to the atmosphere. The foremost commercially advanced ways use wet clean-up with binary compound paraffin solutions. At low temperatures, the paraffin solvent holds CO_2 away from the waste gas (order 50 1C). The solvent is then heated (to about 120 1C) before being cooled and recycled, allowing it to be reused again. Under the regeneration process, CO_2 that is removed from the solvent is dried, compressed, and transported to a secure storage facility.[16]

In typical coal-fired power plants, carbon dioxide is isolated from the flue gas. Chemical absorption of mono-ethanolamine (MEA) is frequently used for its separation. [12],[16],[17]–[20]. However, standard power plant sizes are huge in contrast to the described scale of operation [16] [16], and result in the downside of plant performance, ranging from 10 to 14 percent points, occur at the current stage of production. [1], [2], [16],[21]–[27]. Sequestration unit being located down flow of the furnace and exhaust gas improvement process, retrofitting existing plants is considered relatively simple. There are no significant improvements to the original plant. [2], [28]. On the other hand, certain criteria must be met in order to exclude Sulphur dioxide and Nitrogen dioxide from the exhaust gas before CO_2 sequestration. These



igure 1: Post Combustion Capture technology of CCS

compounds has irreversible reaction mechanism with the absorbent and they gradually decline. The chilled ammonia method is conjointly included in this category.[16]

1.1.2. Pre-combustion capture:

Pre-combustion capture is often referred to as IGCC-CCS, which stands for Integrated Gasification Combined Cycle power plants with CO₂ capture. Exhaust gas containing CO, CO₂, and H₂ is formed by a chemical change in coal. The CO is reworked into CO₂ by the water-gas shift reaction, and the remaining hydrogen-containing gas is extracted before being combusted in a gas turbine.

A few technological and economic calculations [3], [15], [29] show that IGCC has improved method political economy and attributes of plant potency. And yet, high investment costs are related to plant construction IGCC plants, on the other hand, are typically much more advanced than suspension fired boilers. [30], [31] and retrofit isn't a practical approach for further use [15], [16], [30], [32], [33]. As a result, there are hardly any electricity manufacturing IGCC units with not one of them containing CCS. [13], [34], [35] Only some IGCC plants are present and therefore the incontestable accessibility

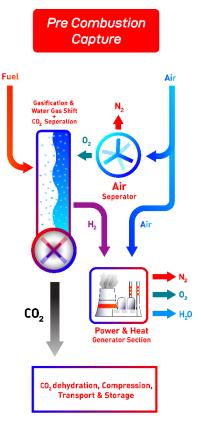


Figure 2: Pre Combustion Capture technology of CCS

is considerably less than existing demand, standard fine-grained coal-fired power plants (80-85 % vs. ~ 96 %, respectively) [1], [15], [31], [34], [36]. This is often a consequence of the restricted in operation combined with the IGCC plants' extremely merged architecture.

1.1.3. Oxy-fuel combustion:

Flue gas re-circulation is important for the regulation of flame temperature as configuration of the plant. At the last stage of combustion process the remainders of the flue gas is mostly H₂O and CO₂ [25], [27], [37]–[43]. Though carbon capture technology incorporated in a plant greatly increases the efficiency, oxy-fuel combustion requires a large amount of pure O₂, resulting in economic threat. Also large unit of refrigeration distillation for O₂/CO₂ declines the efficiency in a large point[44]. In view of the initial plant production, the anticipated efficiency decrease is 7-11%, or 15 to 30% of electricity produced (net power output).

Many considerations will affect the choice of technology. The first and foremost importance is the economy and therefore the projected growth in plant power. Equally, the maturity, planned availability, versatility in service, retrofitting or green plant engineering, local conditions, utility preferences, etc. Several technical laboratory experiments have been undertaken in the last 20 years, and the processing of coal and fossil fuels in an Oxy-fuel condition is well understood. Along with the development, on the other side, all studies also conclude that adequate indications exist of the extent of, for example, toxins, secondary products such as ash, improvements in flue gas, distribution of temperatures, and so forth.

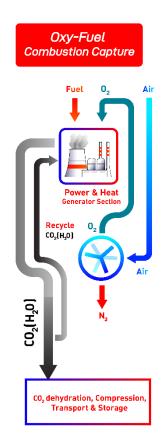


Figure 3 Oxy Fuel Combustion capture Process

1.2 Combustion model of Oxy-Fuel and Air-firing condition:

Traditional coal-fired boilers, such as those currently in operation in the energy sector, burn coal with air, which dilutes the Carbon dioxide in the flue gas by around 79% by volume. During oxy-fuel combustion, a variation with chemical elements (greater than 95% potency) and filtered exhaust gases is used to burn the fuel. With a degree of Carbon dioxide prepared for absorption, a gas composed entirely of CO_2 and water is constructed. The filtered exhaust gases is used to regulate burning rate to make up for the lost Nitrogen, ensuring that there is little gas to keep the heat in the furnace. Capture and preservation of CO_2 Post-combustion capture, pre-combustion capture, and oxy-fuel combustion are all theoretically feasible alternatives that can decrease the facility generation method's potency by 7–10%. Unit chemical element production and CO_2 compression are the major contributors to the new potency penalty. Oxy-fuel condition has been shown to vary from air-fuel condition in many respects of the combustion, including decreased temperature distribution, time lag of flame

initiation, and decrease emissions of NO_X and SO_X , according to pilot-functioning scale and experimental scale tests.

Below is a list of the contrast of variations in characteristics of Oxy-fuel fired and Air-fuel fired combustions:

• Adiabatic Flame Temperature (AFT) can be achieved increasing the O₂ composition in the combustion process, injecting through furnace for usually half an hour, than that of air (21 percent), necessitating the recycling of around an hour of flue gas.

• Because the high concentrations of carbon emissions and binary compounds in chamber gases result in higher gas emissivity, equal radiative heat transfer for a boiler retrofitted to oxy-fuel can be achieved when the O_2 proportion of the gases flowing through the burner is a fraction of the half-hour needed for a similar AFT.

• The extent of gasses streaming into the chamber is minimized by depending on the quantitative relation between flue gas recirculation and, as a result, the syngas emissions from power stations decreased to around 80%.

• Prior to air-fuel ignition, 20 percent extra air is typically used. To obtain a comparable O_2 fraction in the flue gas as air-firing, oxy-fuel needs a percent excess O_2 (defined as the O_2 supplied in excess of that needed for stoichiometric combustion of the coal supply).

• Since species (including corrosive sulphur gases) are not discarded due to recycling, concentrations of these species (including corrosive sulphur gases) are greater than in air-firing.

• Since oxy-fuel combustion with sequestration must power multiple significant unit operations, such as flue gas compression, that would not be necessary in a traditional plant without sequestration, oxy-fuel combustion/sequestration is less efficient per unit of energy generated.

Fundamentals relating to oxy-fuel combustion and therefore the relative variations when put next to standard combustion in air is mentioned below:

1.2.1. Flame & Gas Phase Temperature:

One of the most important considerations while remodelling traditional air-fired boilers to oxyfuel burning is maintaining comparable thermal and heat absorption patterns in the radiative and advection areas of the furnace. The heat and mass transfer rates within the boiler change when Carbon dioxide is specifically substituted for N2 in the oxidizing agent leading to variations in thermo-chemical properties between the two gases. The results of fuel source and working conditions, including O_2 overload, are included in the range. Lower-rank fuels have comparable temperature profiles with lower oxygen entry thresholds, while higher degree fuels need an oxygen inlet concentration at the top range of the recommended range. N₂ is not a radiating gas, although CO_2 and H_2O are. As result, heat transfer is higher at the same flame temperature when combusted with oxygen-fuel than when combusted with air.

1.2.2. Ignition & Burnout:

The oxidizer transitions from air-fuel to oxy-fuel combustion affect the devolatilization and burning of char particles. The rate of devolatilization is calculated largely because of the slight thermal conductivity difference between Nitrogen and Carbon dioxide. According to the literature, the char burnout enhances as the oxy-fuel combustion flame temperature approaches that of air combustion. The main cause of this shift is said to be the enhanced oxygen partial pressure in the vicinity of the burning particles. The increase in volume fraction time of boiler residence resulting in a lower exhaust-gas volume would increase the fatigue potential of oxy fuel relative to air fire.

1.2.3. Ash & Deposit Formation:

The dust content measured in oxy-fuel combustion is 1.5 times higher than in air combustion due to the decreased gas volume, with no noticeable change in dust particle size distribution. Burnout temperature fluctuations tend to modify the properties of particulate, that induces ash build-up, but they tend to not influence the chemical composition of ash. This means that the volume of bottom ash generated by oxy-fuel combustion would be higher than that produced by air combustion.[45]

The configuration of temperature and gas surrounding carbon particles influences coal mineral transformations during combustion. Changes can be made at low combustion temperatures (under 30 percent Oxygen in CO_2) in the distribution of the sub-micrometer-shaped fly ash to small droplets. The risk of slagging and fouling is also examined in oxy-fuel combustion. The data showed that improved combustion conditions would only lead to minor deviations from air fuel combustion.

1.3. ECO-Scrubbing Technology:

The significant and rapid reduction of greenhouse emission emissions is recognized as necessary to mitigate the potential climate effects from heating. For existing coal-fired combustion plants development efforts are concentrating on two main options for CO_2 capture, oxy-fuel combustion and post combustion capture systems. the target of the scientific research was to develop an integrated system (ECO-Scrub) employing both enhanced oxygen levels and post-combustion capture together to get the facility production and CO_2 separation efficiency required to form carbon capture practical in retrofit applications.

The ECO-Scrub technology will have significant potential industry interest because it will allow recently constructed power station with high efficiency units a possible carbon capture retrofit option. Oxy-fuel combustion offers great benefits with reference to CO_2 capture but are going to be very difficult and dear to retrofit due to the need to scale back ingress/egress of air/flue gas to below 5%. Normal design of conventional plant is 15% as built and this deteriorates with age. Whereas post-combustion CO_2 capture using an amine type scrubber or similar incurs high costs and efficiency penalties related to the CO_2 capture plant. It's been shown that there are advantages to the efficiency and price of the capture system if the quantity of flue gas are often reduced and therefore the concentration of CO_2 increased. The novel hybrid ECO-Scrub approach takes positive elements from enriched oxygen combustion which will greatly improve the performance of a CO_2 scrubbing system.

The findings on char-CO₂ reaction rates at conditions relevant to the ECO-Scrub process[46]– [48] were inconclusive and parameters requiring further investigation were identified.

1.3.1. ECO Scrub:

The study of fitting CO_2 capture to power plants is a lively research topic and therefore the concepts, the prices and therefore the performance of capture and capture-ready plants are under constant development. the bulk of those research programs are developing post-combustion CO_2 capture technologies for brand spanking new boilers or plant that needs an entire retrofit of steam cycle equipment and an abundance of knowledge has been generated.[49], [50]

The ECO-Scrub concept could also be a scheme for implementing carbon capture in modern power plants employing a completely unique combination of techniques employed in CO_2 capture, like oxygen enrichment and post-combustion, solvent scrubbing, alongside measures to increase efficiency, reduce steam consumption and generate power requirements without significantly reducing net boiler electricity generating capacity. The ECO-Scrub system is believed to possess both technical and economic potential at the outset.

The proposed approach for the ECO-Scrub system is to use limited oxygen addition to scale back the quantity of flue gas for processing, increase the efficiency of post-combustion scrubbing thanks to higher CO_2 levels and reduce the dimensions and price of post-combustion capture. There's also the potential to limit the reduction in boiler generating capacity by using oxygen to burn extra fuel, thus keeping the prevailing turbine and generation set and completing limited modifications to heat transfer surfaces to get a number of the extra stream required for a reduced-size capture plant.

There are variety of possible configurations for the ECO-Scrub process which establish the method and operational characteristics, as determined by issues like whether to recycle the flue gas, where should O_2 be injected and whether or to not preheat the O_2 . The characteristics of the proposed scheme differ from air combustion and have implications for plant control, combustion performance and warmth transfer patterns. Key parameters (such as flows, oxidant composition, FGR) which affect the ECO-Scrub process, specifically the flame stability, fuel burnout, NO_X emissions and warmth transfer. ECO Scrub's basic concept is to reduce downward gas scrubbing power consumption by maximizing Carbon dioxide composition in exhaust gases. The coal emerges from a cryogenic air separation device which combusts with O_2 rich air and supplementary oxygen. The higher CO_2 component pressure and reduced volumetric flue gas flow here, compared to the traditional post-combustion Carbon capture have resulted in lower heat demand for solvent regeneration, lower cooling need and a decrease in pump and blower power requirements.

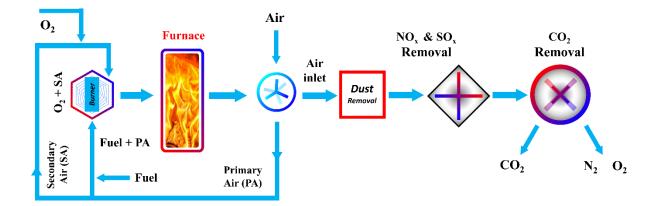


Figure 4 ECO Scrub Process diagram

This schematic diagram shows the detailed process and working of a plant implementing the eco-scrub system. Pulverized coal is combusted during a mixture of oxygen, air and recirculated flue gas. The oxygen isn't pre-heated and is injected downstream of the pulverizing mills with the secondary air, thus mitigating the danger of mill fires/explosions. If FGR is employed the flue gas is taken downstream of the gas cleaning plant (thereby avoiding the build-up of gaseous impurities) and injected into the wind box/burners.

In the initial designs, Flue Gas Recirculation wasn't considered thereby avoiding replacement of air heaters to scale back air in leakage. However, without FGR indicate problems with plant performance and therefore the possibility of high NO_X levels in high oxygen environments. Therefore, FGR is employed to moderate the flame temperature, control NO_X and make-up the quantity of missing N_2 to make sure that there's enough gas to hold the warmth through the boiler.

The higher flame temperatures related to oxygen enhanced combustion have the potential to impact on fouling and slagging. To moderate flame temperature, control NO_X and make-up the volume of missing N_2 , The FGR rate and oxygen enrichment level need to be optimized so that there is enough gas to carry the heat through the boiler. The impact of enriched oxygen combustion on the flame temperature has important implications for NO_X formation and corrosion of hearth and super heater tube bank.

Pulverized coal is combusted during a mixture of oxygen, air and recirculated flue gas. The oxygen isn't pre-heated and is injected downstream of the pulverizing mills with the secondary air, thus mitigating the danger of mill fires/explosions. If FGR is employed the flue gas is taken downstream of the gas cleaning plant (thereby avoiding the build-up of gaseous impurities) and injected into the wind box/burners.

Changes to the combustion atmosphere can impact on both the coal particle reactions and on ash deposition onto heat transfer surfaces. During enriched-air combustion, the upper particle temperatures can affect the ash deposition mechanisms and propensity, impact on submicron ash formation and therefore the presence of high concentrations of CO_2 within the flue gas may cause the formation of carbonates within the boiler deposits [51]. Substitution of N_2 by CO_2 was shown to possess a negligible effect on both the deposit weight and composition. However, increasing the O_2 concentration led to increased fly ash deposits with a more molten appearance. Ash deposition rates, deposition propensity and energy growth rates were lower under air combustion compared to oxy-fuel. However, the combustion conditions (ranging from air to oxy-fuel) don't appear to affect the mineral phases formed within the ash residues, no apparent melt was observed and therefore the carbon-in-ash values for all deposits were too small to possess any effect on deposition.

The flame temperature profiles for the combustion conditions were almost identical. The residual ash (filter ash) showed a corresponding decrease within the amount collected with increasing O_2 concentration. The trend of increased ash deposition for increased O_2 levels could be explained supported the deposition mechanisms: inertial impaction, thermophoresis, condensation and reaction[52]. Differences in observed deposition/fouling propensity are thanks to differences within the flow fields, the gas densities and therefore the physical properties of the gaseous mixtures under the various combustion conditions. The fouling factors (based on heat transfer measurements of the ash deposit) were higher for oxy-fuel conditions and lower for blends (olive/lignite) than for lignite.

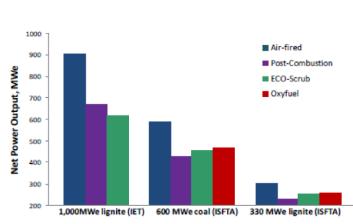
Under ECO-Scrub conditions oxygen addition within the burner region may have to be limited or flue gas recirculation want to prevent excessive tube temperatures and unacceptable tube corrosion. The upper CO_2 content within the ECO-Scrub flue gas means the warmth flux to the super-heaters are going to be higher and high-temperature corrosion is therefore likely to occur sooner in an ECO-Scrub combustion boiler than in an air fired boiler. Additionally, the upper levels of H₂O and SO₂ within the ECO-Scrub flue gas also will increase the danger of corrosion.

Co-firing with biomass is additionally likely to impact on the ECO-Scrub process, especially the flame characteristics, fuel burnout, NO_X emissions, ash deposition and warmth transfer thanks to the upper volatile content and ranging N and alkali contents of biomass fuels.

For an ECO-Scrub retrofit the most modification to the boiler is going to be the addition of a flue gas recirculating system so as to take care of flame temperatures within design tolerances of the boiler, to optimize boiler operation and control NO_X emissions membrane separation technology appears to possess considerable potential for CO_2 removal in an ECO-Scrub power station. The utilization of emerging membrane technologies (e.g., conditioned zeolitepolyimide membranes) should make this system very competitive with conventional amine absorption processes in terms of investment costs and energy efficiency.

The fundamental CO_2 capture technologies that present the foremost interesting options for the ECO-Scrub process are post-combustion CO_2 capture and full oxy-fuel combustion. The CO_2 capture retrofit was shown to possess a big impact on the steam cycle, where the main a part of the steam exiting the IP turbine is extracted and expanded to the re-boiler pressure to provide the warmth for regeneration of the solvent. Additionally, the electrical energy consumption from CO_2 compressors causes a further reduction at net electrical power. Internet power output is reduced by up to twenty percent, thanks to the drastically reduced mass flow within the LP section of the turbine, some modifications on the turbine could also be required. For the oxy-fuel retrofit, the most efficiency penalty was attributed to the energy demand from the ASU.

For both ECO-Scrub variants, because the oxygen concentration is increased the mass flow of the flue gas decreases and flue gas is recirculated so as to moderate the flame temperature and maintain flue gas temperatures at acceptable levels. Additionally, the ASU electric consumption increases thanks to the increased demand for O_2 . The HP and IP steam production increases with increasing O_2 enrichment thanks to the upper heat transfer coefficient of the flue gas as a result of the upper CO₂ and H₂O partial pressures which results in a rise in gross



electric production. In theory, an increased fouling risk is predicted for the ECO-Scrub process thanks to the upper temperatures within the burner zone.

The figures below demonstrate a visual comparison between the net power output and the net efficiency under different combustion conditions.

Figure 5 Visual representation of Net power output by different energy source

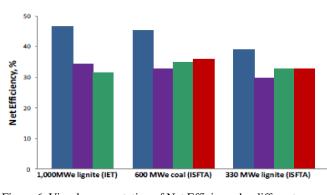


Figure 6 Visual representation of Net Efficiency by different energy source

A key issue for improving the efficiency of an ECO-Scrub retrofit may be a higher degree of integration of the CO_2 capture unit within the power station process. the utilization of low steam for solvent regeneration features a significant impact on the facility output and electrical efficiency, therefore, great attention should be paid to the warmth coupling and process

integration between power and capture island. The temperature level of any heat source or sink features a major influence on its potential use. Main heat sources are the flue gas cooler, the de-absorber head condenser, the compressor intercoolers and additionally within the sub sections of O₂/CO₂ firing mode the compressors of the ASU. Possible heat sinks are the feed water preheating train and therefore the pre-drying of lignite. Innovative concepts are needed to integrate low-temperature heat quantities and thus reduce the efficiency penalty to the general process.[53] For an ECO-Scrub retrofit there's potential to use the increased flue heating system for extra LP feed water pre-heating. The water mass flow within the intermediate system would wish to be increased thanks to maximum allowable temperature level of the plastic device within the intermediate heat transfer system of the flue heating system recovery system. The utilization a two-stage heat recovery system for feed water preheating has potential for efficiency within the ECO-Scrub mode

1.3.2. Technical benefits of the ECO-Scrub process compared with oxy-fuel combustion include:

• Use of lower purity oxygen: Both the facility demand and capital/operating costs of a low-purity cryogenic ASU, suitable for application in an ECO-Scrub retrofit, are significantly less than a high purity (99.6% or higher) oxygen plant required for oxy-fuel.

• Reduced size of ASU: ASU power consumption increases significantly with increasing O₂ enrichment and may be a major factor of the general plant energy losses and plant cost of capital. The reduced size of the ASU for the ECO-Scrub retrofit will end in lower energy

demand and lower build and operating costs. Other advantages include a smaller footprint and avoidance of oxygen storage for plant

• Lower impact on operability and plant re-engineering requirements: The inherent advantage of ECO Scrub technology is that it's potentially suitable for retrofit without drastically affecting process operations and can require less extensive plant re-engineering start-up,

• Lower impact on flame stability: Flame propagation speed and is lower and flame ignition could also be delayed in O_2/CO_2 environments; the impact being higher for oxy-fuel combustion thanks to the upper O_2/CO_2 levels. The utilization of FGR appears to be a key parameter for ensuring flame stability for both ECO-Scrub and oxy-fuel retrofits.

• Lower corrosion propensity: Oxy-fuel combustion is predicted to cause a more corrosive environment than ECO-Scrub firing, thanks to the elevated partial pressures of combustion products (such as H₂O, SO₂, HCl) resulting from the lower gas volumes and recycled flue gas.

1.3.3. Technical benefits of the ECO-Scrub process compared with conventional postcombustion capture (without oxygen enhancement) include:

• Improved heat transfer capability: The ECO-Scrub flame has an enhanced capability to transfer radiant heat without exceeding the planning limits for the utmost allowable heat flux.

• Lower NO_X emissions: a discount in NO_X emissions is predicted under ECO-Scrub firing conditions thanks to the consequences of FGR, reduced levels of thermal NO_X formation and increased rate of fuel NO_X destruction reactions

• Improved NO_X control: the appliance of O_2 enriched air staging was shown to possess significant potential for NO_X control and should be particularly suitable as a retrofit to existing boiler operating under deeper staging conditions.

• Improved burnout: The carbon-in-ash levels decrease with increasing oxygen enrichment and furnace exit oxygen levels thanks to the upper reactivity of the fuels in an O_2 rich environment and therefore the increased residence times within the heat zone of the boiler. Injection of the FGR flow through the secondary port also led to reduced CIA levels thanks to the improved fuel/ O_2 mixing which generates higher peak temperatures and hence improved burnout.

For part load operation of an ECO-Scrub plant (and other CO_2 capture options), efficient turndown of CO_2 compressors with electric drives should be possible for around 70 to 100% of design throughput for current designs.[54]

Based on the results of the economic analysis, it's concluded that the appliance of any CO_2 capture technology incurs a high-cost penalty while being advantageous in terms of reduction in GHG emissions. [55]The capital, operating and maintenance costs also because the electricity generation rise significantly for all retrofit cases compared to the traditional reference case without CO_2 capture. However, the modelling studies indicated competitive advantages of ECO-Scrub technology compared to other conventional CO_2 capture technologies, like improved net efficiency, low energy penalty for capturing the CO_2 , low NO_X emissions and minor modifications at Boiler Island. Thus, ECO-Scrub implementation might be promising in terms of both efficiency and emitted pollutants.

2. LITERATURE REVIEW

In recent years, greenhouse gas (GHG) emissions have increased dramatically in the atmosphere from fossil fuel combustion. It contributes to global climate change in a negative way. CO_2 and NO_x are thought to be the major contributor gases to GHG emissions from energy production units. People's knowledge of these environmental concerns, especially in third world countries, actually obliged the concerned authority to establish strict policies and legislation banning the use of common age-old electricity generation systems. New climate protocols, such as the Kyoto Protocol [56] [57], have already been in action to protect the climate from further damage and sustain the future demand of continuous energy supply.

Since CO_2 is the most common greenhouse gas in terms of volume emitted, climate change caused by Carbon pollutants is undeniably one of the most severe global consequences of climate change. Capturing and preserving Carbon dioxide released from burning of fossil fuels has the ability to reduce Carbon emission dramatically, enabling fossil fuels to be used as a gateway to more renewable energy systems. The emphasis is on power plant technology and procedures since power plants are considered to be the main source of CO₂ pollution. Several CO₂ sequestration and storing technics are available for power plants, for different combustion system such as pre-, post-, oxy-fuel capture [58][30][59]. Primary aim of these CCS systems is to eliminate CO₂ emissions. The properties and principles of each Carbon capture approach are described in recent literatures [1][3][60][25][61][16][22]. Of all CCS systems available, the use of oxy-fuel combustion [1][62][63][64][65]. O₂/CO₂ (oxy-fuel) combustion is evolving as a possible CCS technique due to its comparatively favorable economics [66][67] and the fact that it is more or less based on validated technology. O₂/CO₂ (oxy-fuel) combustion is evolving as a possible CCC technique due to its comparatively favorable economics and the fact that it is more or less based on validated technology. In O₂/CO₂ combustion, N₂ is stripped from the air, and the fuel is burnt in a composition of Oxygen and recycled exhaust gases. The resultant high CO₂ content in the flue gas will then be used for Carbon dioxide retrieval. Another advantage of the O₂/CO₂ combustion over conventional air-firing is the capacity for reduced NO_X exhausts. [68][69][70]

To clarify the effects of such a technology's summary, further analysis is needed. In the last two decades, a number of large and small-scale industrial demonstrations have taken place, with positive outcomes for coal burning in an oxy-fuel system. Aside from these innovations, a number of newer ones, such as separation based on membrane , chemical looping combustion (CLC), C-Cl processes [71], and so on, have the ability to cut carbon sequestration from emissions of power plants substantially [61][72][73][74]. However, these advances have not been carried out on a large enough scale to be considered for industrialization.

As a result, scientists have been intrigued by the use of green fuels in commercial power plants with CCS systems in recent years. Coal and biomass firing reduces Carbon dioxide pollutants from fossil-fuel power-plants in a more straightforward manner. A blend of CO_2 neutral fuels and CCS and recycling can be used to eliminate CO_2 from the atmosphere.

Solid fuel (Coal) combustion is considered a dynamic process in contrast to liquid and gaseous fuels combustion, since it entails many complex procedure and chemical steps. Related volatile matter (VM) and moisture content (MC) are released during the thermal extraction process, and char persists as a solid fuel in this synthesis process. As a result, during the gas-phase process, radical species such as total hydrocarbons (THC), Hydrogen cyanide, Ammonia, Nitrogen, Carbon mono Oxide, Hydrogen, and others will form in the reaction region. Using the mechanism of multistep chemical reactions on the species described above, as well as residual char, we can accurately predict various significant species and thermodynamic equilibrium temperatures.[75] Emissions are also present in everyday combustion. The equivalence ratio, residence time, temperature, and air supply all influence the evolution of animals.

In most situations, the coal combustion process in the firing device occurs after the coal straw particles have been devolatilized. This combustion mechanism has been shown to restrict many reaction parameters, including overall burnout period, incomplete oxidized carbon level, and emission from burning coal particles. [76]–[81]. Through better identifying the implications of these parameters on combustion dynamics and furnace thermal distribution under different operating cases, engineers will refine the applications of both existing and new coal power plants. The thermal performance in the thermal furnace design, such as the radiation zone (water–wall furnace) and heat exchange zone (superheater, reheater, and economizer), are crucial. [82]. The ash deposition and slag forming produced by burning pulverized char particles are important factors to consider when designing a thermal furnace, especially on heat transfer surfaces like the radiation zone and convection zone. [82] For this consequence, it's crucial to know how these factors reciprocates once the rates of volatile char (Pulverized Coal) and furnace inlet oxidant flow are adjusted in relation to current process

conditions. That being said, there is still a lack of information about the effect of these corelated factors on fuel characteristics and power station potency.

High concentration (up to 95%) of carbon dioxide flue gas is emitted due to char combustion in the recirculating exhaust gas and added O_2 (for better oxidization) condition .Flue gas containing higher than 90% CO₂ in concentration might be used as deep sea carbon dioxide storage and better oil extraction.[83]. Even if many modern coal-fired power plants have flue gas recycling equipment, only a small portion of the exhaust gas is recirculated, mostly for furnace temperature regulation, resulting in a marginal rise in CO₂ concentration in the flue gases. To generate highly concentrated Carbon dioxide, a large amount of the flue gases must be recycled. Coal burning in blends of O_2 and CO_2 is predicted to vary from conventional coalair combustion in terms of coal particle firing, combustion characteristics, thermal performance, and exhausted pollutants. This is primarily attributed to Carbon dioxide's higher specific heat than Nitrogen and its ability of gasification of charcoal. [84]–[93].

In order to continue using coal as a convenient and efficient source of energy in the long term, many improved combustion methods have recently been developed. Pre-, post- and O_2/CO_2 combustion techniques are the most effective technologies for reducing Carbon dioxide, NO_x, and SO_x exhaust and fuel consumption. [30], [94]

Carbon sequestration, which includes carbon dioxide capture and storage, can reduce coal dependency in power plants, leading to alternative fuel selection. However, flue gas from common air fired combustion has lower concentration (14-15 %) level to make capture carbon process economically feasible. Carbon sequestration is the capture and safe storage of carbon (CCS) that would either be released into the atmosphere or remain there. The aim of carbon capture and storage is to allow the use of fossil fuels thus lowering CO₂ emissions into the atmosphere, thereby reducing global warming. Fossil fuels are currently the primary source of global primary energy demand and will undoubtedly remain so for the rest of the century, accounting for over 85% of all primary energy [95]. There are three broad categories of CO₂ sequestration technologies for coal-fired power plants that are currently commercial or in production.[96][97]

When the oxy-fuel combustion campaign began in the last decade, however, a lot of research was done in terms of experimental [98]–[102] and theoretical studies [103]–[106], using various scales of furnaces. According to recent research, there have been several developments

in the oxy-fuel combustion process, which have been applied in a range of operating conditions and combustion environments to minimize the need for traditional combustion system retrofits.

The basic principle of oxy-fuel combustion is to raise the partial pressure of CO_2 in exhaust gases to make chemical sequestration and compression faster and more cost-effective. Different composition of exact Oxygen and flue gas (consists mostly of Nitrogen) ratio is used to minimize the flame temperature, instead of using air-fuel combustion condition [107]. In this case, presence of higher range of concentrated CO_2 in flue gas is identified. However, carbon capturing process is economically cheaper and feasible, using challenging oxy-fuel combustion. Comparatively in oxy-fuel combustion some changes like flame temperature level, concentration of species, radiative heat transfer etc. may be observed. There are different reasons for those changes. CO_2 having the high heat potential comparatively, different radiative and gas properties like kinetic viscosity, thermal diffusivity etc. are to name a few.

The findings of using the coal combustion technique of oxy-fuel have shown that generating exhaust gas enriched of CO₂, which can be obtained and sequestered with enriched combustion of O₂ is a viable alternative. The data demonstrate that it is theoretically feasible to retrofit this technology to pulverized coal-fired units. An O₂ content of approximately 35 percent in gas feed stream, the remainder of which is carbon-rich recirculating exhaust gas, was found to be close to flame (temperature and heat flux) characteristics in air combustion for the coals assessed for CETC-O. This technology has, in addition to enriching Carbon dioxide syngas, other benefits, such as probable emission reductions of NO_X [108], [109] and lower volume of net gas combustion at higher volumes of feed with O₂. The above contributes to better thermal efficiency and less sensitive heat losing in flue gas. It is also able to reduce oxygen-fuel costs by reducing the scale of flue gas cleaning equipment [110]. While the goal of oxy-fuel condition is ultimately to combusts fossil fuels into purest Oxygen gas, the O₂/CO₂ variant offers an immediate adoption route as it reduces the need for extreme temperatures components and questions about coal-combustion chemical mechanism with very high O₂-pure combustion temperatures. [111]

Detailed research on the reaction properties of O_2/CO_2 furnaces is important since the partial pressure of CO_2 and O_2 has risen considerably and due to a major decrease. Since the oxy-fuel campaign started a decade ago, many theoretical and analytical studies have been carried out on different forms of charcoal in experimental and existing furnaces. These experiments may provide knowledge that is valuable to preserve burning characteristics similar to traditional

combustion. Consequently, an economical basis can be developed for upgrading existing power plant equipment or constructing a new power plant system under the various conditions of combustion of oxy-fuel. Latest research [107], [112], [113] has demonstrated that oxygen-fuel burning equipment can still be used. It is undoubtedly sufficiently suited for use in large-scale coal-fired power plants. Thus, further research and investigation into this approach to should be carried out in laboratory-scale and pilot-scale furnaces and then we can take on the large-scale applications.

Using the ANSYS CFX 12.0 code, Tian et al. [114] created a CFD model to study the combustion of coal in a 375 MW utility boiler that operates on tangentially-fired. Here, the reaction of CO with O₂ was used to boost the projections made for the model. The reason behind this is the constraints in the CFD code in the field of multi-step reaction of hydrocarbons. That being the case, the validated model in comparison to computed data from Yallourn plant helped to investigate the flame form, temperature profile and the heat flux incident on the wall. Various combustion air distribution scenarios and out-of-service firing groups were numerically investigated. The predictions revealed that considerable amount of variation was present in lots of aspects of the furnace's combustion, which is entirely dependent on which burner groups are switched off during full load services.

Wang [84] used experiments on a furnace (600 mm*2134 mm) of horizontal, non-swirl combustion chamber in addition to 1-D modeling to investigate the pulverized coal combustion using waste CO₂ and O₂. They concluded that a CO₂/O₂ atmosphere with CO₂-to-O₂ molar ratios ranging from 2.23 to 3.65 could perhaps achieve fine-coal combustion. Their research did not include NO_x emissions [84]. Payne et al. [85] reported their findings on coal combustion in oxygen-recycled flue gas mixtures shortly after Wang [84] published their article. They conducted their experiments on a test furnace of small scale (1m*6 m, 3 MWt) and evaluated the effect on efficiency using a 2-D boiler output model. The results implicated that the combustion of coal without the presence of air could be sufficiently accomplished under utility boiler conditions. In Japan, researchers looked into the properties of pulverized coal combustion of a with O_2/CO_2 were found to be lower than that with air [86], [88], [89]. The spread of a flame in the presence of pulverized coal clouds was calculated in a microgravity furnace [115] and found to be much slower in an O_2/CO_2 atmosphere than in an O_2/N_2 atmosphere, even though it could be improved by making the O₂ concentration higher in CO₂.[87]

Tan [116] found a little bit rise in the heat flux values within the furnace with the O_2 concentration 35% and CO_2 65% as compared to O_2/CO_2 combustion study to the air-firing (reference) one, except for the values with O_2 concentration 28% to be marginally down.

The efficiency of oxy-combustion simulation is largely related to the concerned models while summarizing a range of CFD investigations in large-scale cases. In a 550 MWe tangentially fired utility boiler, Al-Abbas [106] investigated oxy-fuel combustion. Homogeneous reaction mechanisms and WSGG model could achieve comparable gas temperature and radiative heat transfer. Habermehl [117] concluded that with oxygen concentrations of 27 percent and 30 percent by volume for wet and dry flue gas recycle, respectively, based on a mathematical analysis on a 1200 MWth opposed firing boiler. At oxygen concentrations of 24 percent and 29 percent a close adiabatic flame temperature could be achieved. Black et al. [118] indicated that the 25% and 30% range is optimal O₂ concentration. It also ensured the match of temperature and heat transfer of air-fired combustion although this research relied on the traditional WSGG model, likely to be inaccurate in terms of radiation predictions.

Recently, several researchers have focused their efforts on gaseous reaction kinetics and radiative properties models to improve oxy-combustion. Yin et al.[119] simulated a laboratory scale 0.8 MW oxy-fuel furnace to build an updated WSGG model with new methods of combustion. In the findings of oxy-fuel combustion, over-prediction of temperature and under-prediction of CO stage was seen. Nikolopoulos [82] used the ECO-Scrub technology numerically applying on a large boiler. In oxy-fuel combustion, the complete and radiative heat fluxes increased, according to the simulation results that might have resulted due to the presence of special cases in it.

Good flame distribution and uniform heat flux incident on the furnace walls: these two factors contributed to the popularity of tangentially-fired boilers using pulverized form of coal. However, they do have a few issues. To begin with, substantial quantity of combustible matter is present in the fly ash. Also, there are instabilities occurring under off-load variations in addition to imbalanced heat with fluctuations in gas temperature deviation in the super-heaters, re-heaters, and more.[120] The CFD technique allows researchers to investigate the combustion phenomena and impurity formation within the furnace in greater depth. Few researchers have attempted to use CFD to model three-dimensional large-scale tangentially fired power plants. [121], [122]

Studies have found that flame stability and temperature are significantly altered.[123], [124] It is important to assess the efficiency and heat transfer while designing a boiler for oxy-fuel combustion. It also needs to be noted that the heat transfer and heat exchange must be comparable to the ones in an air-fired boiler for the retrofit scenario. Even without significant changes temperature levels close to air-fired flame can be achieved. [125]

According to the Intergovernmental Panel on Climate Change (IPCC), a single measure alone would not be sufficient to stabilize atmospheric CO_2 concentrations, and a combination of measures with the like of decreasing demand, better efficiency, CO_2 segregation will be needed [95]. These technologies are predicted to take a major role in reducing carbon emissions from conventional fuel power plants around the world. Carbon sequestration is the method of trapping and storing carbon that would otherwise be released into or remain in the atmosphere. This is referred to as carbon capture and storage (CCS) (CCS). However, CO_2 capture technology has yet to be demonstrated, and the demand for fossil fuel power plants continues to rise at full tilt to meet global energy demands. In this context, policymakers have questioned the idea of a "CO₂ capture ready farm." While a precise definition has yet to be developed, a capture-ready plant must have devised schemes in place to harbour future changes, such as adding more facilities, taking into account any potential power loss, and also the transportation and storage capacities of CO_2 .

For CO₂ capture from power plants, there are three major technology options [96], [126]:

- Post-combustion capture.
- Pre-combustion capture.

• Exclusion of nitrogen from the combustion phase (also known as oxy-fuel combustion or O_2/CO_2 recycle combustion, but also including processes like chemical looping).

The ECO-Scrub principle is contingent to a synthesis of two fundamental CO_2 capture technologies: partial oxy-fuel mode in the furnace and solvent scrubbing after combustion. [94] Coal is combusted in an oxygen-rich environment to the point that no or only minor boiler and power island modifications are necessary. Flue gas recycling for temperature and heat flux changes is minimized in this manner. Since the partial pressure of CO_2 in flue gases has increased, a traditional amine scrubbing system is used to extract CO_2 , but with lower solvent loading requirements. Furthermore, post-combustion of traditional amines can be accomplished in smaller facilities, lowering capital and operating costs.

The key goals of the ECO-Scrub project, discussed in another paper are [94]:

- Calculating the energy penalty for CO₂ capture using an ASU and a scrubber at the same time.
- Examining the significant improvements that must be made to the boiler and steam turbine island in order to retrofit an existing power plant.
- To compare the results of an operational electricity generation power plant with a retrofitted one that includes post-combustion CO₂ capture.

The ECO-Scrub retrofitting alternative has been evaluated thermodynamically and economically elsewhere [94]. Thermodynamic modeling calculations were conducted for a 330MWel lignite-fired power plant and a 600MWel hard coal plant. Comparatively, the ECO-Scrub technology has a higher gross and net electrical efficiency. Although the cost of the proposed technology is lower but performance is not satisfactory.

Lusatian dried lignite and Polish hard coal were examined in a 0.5 MWth test facility by Kass [127] who supplied pure oxygen (99.95 vol%) mixed with hot flue gas to reach almost same O_2 concentration level as atmospheric air. There is an impact of excess air and O_2 distribution both on the maximization of CO_2 and minimization of other gas pollutants. And it was one of the significant goals of the mentioned work. Approximately 3.24% of O_2 mole fraction is needed to achieve high CO_2 concentration (92.15%). There are also some negative consequences of this increase. There was also staged combustion (O_2 in primary air is less than secondary air) found to lessen unwanted pollutant release.

A 2D CFD modelling was performed by Vascellari and Cau [128] on a 2.4MW combustor which operates under two conditions: one is 21% O2 and 79% CO₂ and the other case is 30% O₂ and 70% CO₂. For the first condition, although velocity profile remains almost similar but a slight drop is noticed in temperature. Due to heavy recirculation field and the char reaction burnout remains almost unchanged. But temperature contour becomes more similar to the air-fired case if we can keep the mass constant and burnout also decreases if we do so.

Influence of recycled flue gas on O₂ concentration going through the furnace was investigated by Hjarstman on a 100kW unit [129]. Three cases were examined (25, 27 & 29% O₂) of which

25% case provided almost similar results compared to reference case. And higher peak temperature was provided by reduced recycled flow along with slower gas speed and quicker burnout. For OF 27 and 29 conditions CO level goes higher but in the exiting flue gas, concentration is lower. Whereas Tan et al. [116] performed investigation on a 0.3 MWth unit and found almost identical temperature profile and heat transfer result.

CFD simulations were performed by Erfurth et al. for a 1200 MWth PF boiler with swirl burners.[130]. Several oxy-fuel scenarios were explored, with variations in O_2 mol fraction and whether wet or dry flue gas recycle was used. The Exponential Big Band Model's greyband variant was used to model the radiation (EWBM). When O_2 was 21 vol%, in-furnace temperatures fell. In order to preserve the same adiabatic flame temperature, the O_2 concentration was increased to 27 percent (wet) or 30 percent (dry). During oxy-fuel combustion, wall heat fluxes increase. For 30% case, temperature and enthalpy are different from reference air-fired case. In the convective part of the boiler retrofitting is possible and no distinct changes are required in spite of outlet gas composition being different. Gasification reactions contribute to the burnout phenomena in high concentration cases of CO_2 and H_2O , although the temperature at the exit of the furnace remained under that that of reference case.

Investigations on pulverized coal combustion was performed by Liu [125] in a 20kW unit. He examined the air-firing and oxy-fuel cases. In OF cases, Mass fraction of O_2 was a bit differentiable from reference case and of course there were noticeable distinction in temperature profile (decrease) and also char burnout phenomena.

In brief, approximately 30% mole fraction of O_2 achieve considerably similar temperatures and combustion conditions to air-fired case. Comparatively, as usual lower temperature is found in the furnace. If the temperature field is assumed to be fixed, while gasification reactions contribute more, burnout remains high. Proper radiation modeling is critical since higher CO_2 and H_2O levels result in higher emissivities and increased wall heat fluxes.

Although eco-scrubbing sounds so exciting and promising in terms of environmental aspects, there aren't much published work worldwide on this topic. In our project we aim to look at different impacts of eco-scrubbing application through CFD simulations and finally present a case study on the results we find after performing proper investigations on aforementioned technology.

3. PHYSICAL SETUP

Numerical analysis on the combustion characteristics is conducted with biomass(straw) along with coal in a 30 kWth solid fuel swirl stabilized furnace which categorized in the scale of

semi- technical once through type. 315 mm inner diameter corresponding with a length of 1.9 m had been defined as combustor prime dimensions. the [131] [The configuration data for the setup is seen in Table 2.1 on page 18]. Refractory lining with thickness of 80 mm is coated in the inner and outer insulation shell, which also provides cooling through hole between two layers, drawing ambient air from atmosphere. The combustor chamber consists of 8 measuring ports indicated as 1 from 8, with 1 being the topmost. These ports are used as deposit probe injection, thermocouple, sampling of gas lines etc. Partial flue gas flow is used to extract fly ash from reactor to ash sampling device. Depending on the setup's precise operating conditions, the sampling rate ranges from 60 to 150 L/min. The ash from the machine is separated into three fractions: "bottom," "cyclone," "filter". Unless otherwise mentioned, the three fractions are responsible for the findings of the concentration of fly ash.[8]

Fuel particles (solid pulverized coal) are fed onto a vibrating table (Scan-Vibro) by a loss-in-weight operated twin-screw feeder (K-Tron K-ML-KT20-H-110L), which

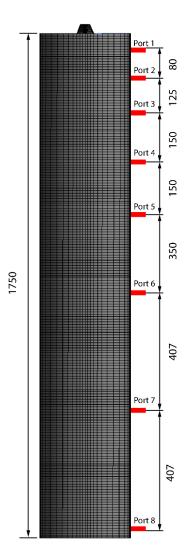


Figure 7: Schematic diagram of the computational domain of the 30 kW swirl stabilized furnace.

serves as both a conveyor and a leveling system. Vibrating table consume the crashing of fuel particles which are guided through primary burner. A portion of primary oxidant is mixed from vibrating table to balance the O_2 feeder in the latter part. Furthermore, to balance the oxygen level primary oxidant is flown through the central burner directly with the residual flow of O_2 . During the start-up of an experiment, the break between the two main oxidant flows is modified to ensure the maximum solid fuel feeding stability. The configuration of the combustion

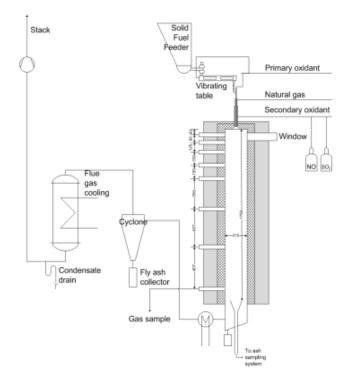


Figure 8: Schematic of the 30 kW swirl burner setup.

Table 1: Design data configuration	on
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Parameter	Value
Reactor inner diameter	315 mm
Reactor height, total	1.9 m
Port 1, distance from burner	43 mm
Port 2, distance from burner	123 mm
Port 3, distance from burner	248 mm
Port 4, distance from burner	398 mm
Port 5, distance from burner	548 mm
Port 6, distance from burner	898 mm
Port 7, distance from burner	1305 mm
Port 8, distance from burner	1712 mm
Flue gas sampling position	Port 8
Flue gas sampling rate	3 L/ min
Deposit sampling position	Port 7

chamber is depicted in the figure above of the burner. It has three tubes: two for main and secondary oxidants, as well as a single natural gas inlet for reactor heat-up and transfer to the flames of solid fuel. Secondary oxidant is injected in two streamsaxial and tangential flows. Axial and tangential flow ratio known as swirl number dictates the swirl wave generation, generated at the bottom part. Figure 2.4 on provides a detailed schematic of the burner.

At the reference conditions, 20% primary oxidant flow is fed as for the overall flow of natural air flow and oxy-fuel cases. Stoichiometry and combustion characteristics are modified contributing the shift in linear velocity of main oxidant exhaust from burner. However, swirl number is unchanged for both air and oxy-fuel conditions combustion for differentiating from each other. Rotameter readings indicates the change in flow of O₂ which can be regulated with

manual valves. In oxy-fuel case,

proper mixing of O₂ defines the control over the rate of mass-flow.

As the reactor is one way through type and absence of ducts makes the recirculation of flue gas null. Oxidant mixing chamber produces the optimum ratio of O_2/CO_2 molar mixture from O_2 , CO_2 tank which also controls the primary and secondary O_2 flows maintaining same compositions. Only secondary and partial tangential oxidant flow is mixed with NO₂, SO₂ in

order to balance and recirculate flue gas prior to oxy fuel combustion. In normal case (air fuel combustion), solely pressurized air is supplied as oxidant.

Flue gas is continuously injected through the 8th port, keeping the ratio of fuel mixture balanced. Until joining on-line gas analyzers, the gas sample is filtered and dried. There are two analyzers available (Rosemount NGA 2000), one for measuring O₂, CO, and CO₂, and the other for measuring NO and SO₂. NO₂ has not been tested because it is thought that at the low oxygen excess concentrations and temperatures used, only trace levels escape the reactor. It would, however, almost certainly be lost before it reaches the flue gas sampling position.[132]

3.1. Mesh

First input the geometry into ANSYS default mesh and then run basic mesh which creates unstructured tetrahedral mesh. For creating hexahedral structure mesh, we follow the procedure described below.

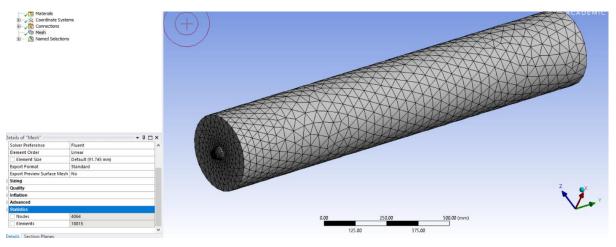


Figure 9: Unstructured Mesh without sizing

Choosing Multizone method with mapped mesh size as hexa/prism. The output we get is as followed,

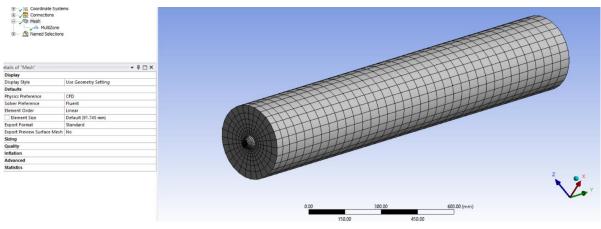


Figure 10 Structured mesh without sizing

Now, taking edge sizing in outer edge of the burner with number of divisions 10

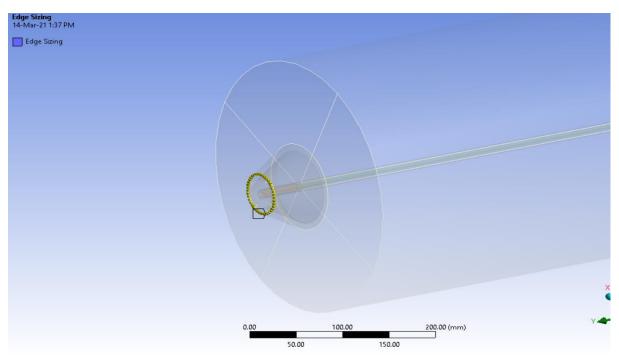


Figure 11: Sizing of the top of burner

Similarly, other edges were taken under divisional sizing which are

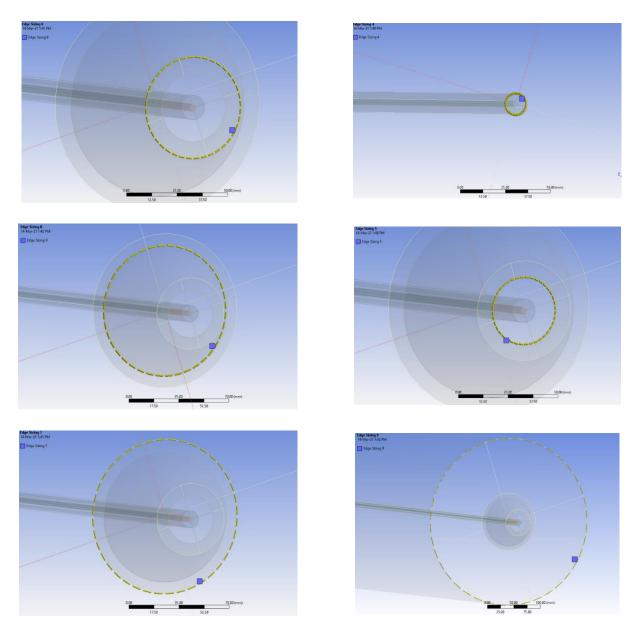


Figure 12: Sizing of Different edge of burner

After All of these sizing we reached in the optimum size of the mesh with **maximum skewness 0.5**

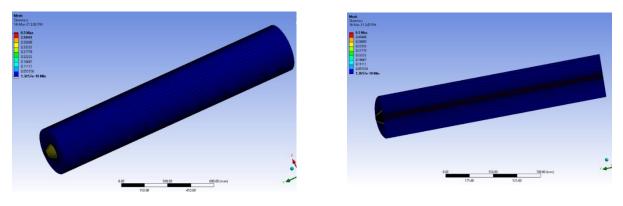


Figure 13: Skewness of mesh (max 0.5)

The orthogonal quality range is 0.86-1. The report is

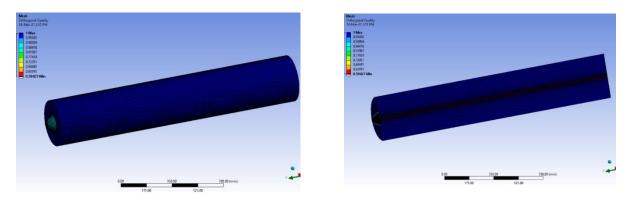


Figure 14: Orthogonal quality of mesh (range: 0.86-1)

The final mesh with cell number **263434**

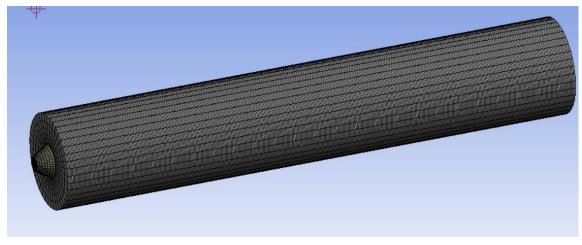


Figure 15: Final Mesh

3.2. Grid independency:

Total three grid sizes having number of cells of 132796 (12 mm element size), 263434(8.6 mm element size) and 389147 (7.46 mm element size) are considered. It can be concluded that the grid size having number of cells 263434 is optimum for further investigation with minimum computational time.

Grid No	Element Size	Element Number
1	12 mm	132796
2	8.6 mm	263434
3	7.46 mm	389147

Table 2 Mesh element size & number

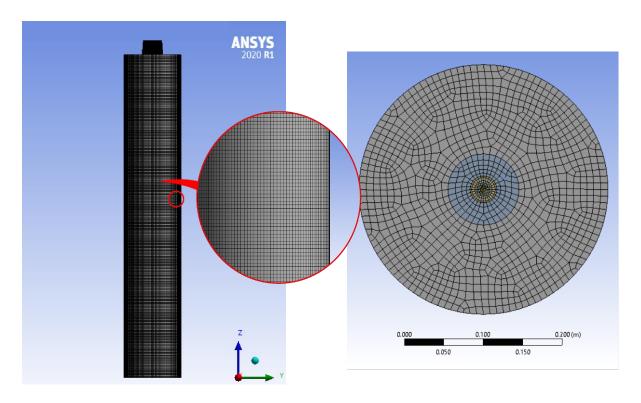


Figure 16: Mesh of Furnace

4. MATHEMATICAL MODELLING

A commercial Computational fluid dynamics (CFD) code, ANSYS 2021 R1 Academic Version, was used to model coal and biomass combustion, along with customized subroutines. The combustion of coal and straw particles is modeled in this study using different methods with the inclusion of both gas and particle conditions. Under the Eulerian approximation/formulation, Navier–Stokes's conservation equations define the gas phase. The source term in the Eulerian transport equation's general form used in Reference [133] couples heat transfer, particle trajectories, and turbulence.

4.1 Eulerian Transport Equation:

The general form of Eulerian transport equation used in [134] couples the heat transfer, particle trajectories and turbulence through the source terms. The general form of Eulerian transport equation used is:

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

The Eulerian PDF transport equations are derived by substituting into the closed composition PDF transport equation. Using the Direct Quadrature Method of Moments (DQMOM) approach, the unknown terms, ρ_n and $\langle \Phi_k \rangle_n$ are determined by forcing lower moments of this transported PDF to match the RANS lower moment transport equations and is as follows:

Probability (magnitude of the nth delta function):

$$\frac{\partial \rho \rho_n}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i \rho_n) = \nabla (\rho \ \Gamma \nabla \rho_n)$$

Probability weighted conditional mean of composition:

$$\frac{\partial \rho s_{k,n}}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i s_{k,n}) = \nabla (\rho \Gamma \nabla s_{k,n}) + \rho (M_{k,n} + S_{k,n} + C_{k,n})$$

Where ρ_n is the probability of the nth mode, and $S_{k,n} = \rho_n < \Phi_k >_{n+1}$ is the kth species probability weighted conditional mean composition of the nth mode. The terms, $M_{k,n}$, $S_{k,n}$, and $C_{k,n}$ represent mixing, reaction and correction terms respectively.

4.2 Standard \mathbf{k} **–** ε **model:**

The k- ε model is a widely used turbulence model, especially for industrial applications, and it is included in most CFD codes. Despite numerous flaws found over the last decade, it is widely accepted that the k- ε model produces accurate and practical estimates of major meanflow features in the vast majority of complex situations. The standard k- ε model compiles of a series of equations that can be summarized by [135]:

The turbulence kinetic energy, k, and its rate of dissipation, ε , are obtained from the following transport equations, respectively:

$$\rho \frac{\partial k}{\partial t} + \rho U_j \frac{\partial k}{\partial x_j} = P + G - \varepsilon + \frac{\partial}{\partial x_j} \left(\mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) [136]$$
$$\rho \frac{D\varepsilon}{Dt} = \left(C_{\varepsilon 1} P + C_{\varepsilon 3} G + C_{\varepsilon 4} k \frac{\partial U_k}{\partial x_k} - C_{\varepsilon 2} \varepsilon \right) \frac{\varepsilon}{k} + \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) [137]$$

Where:

$$P = -2\mu_t S: S - \frac{2}{3} [\mu_t (trS) + k](trS) [4]$$
$$G = -\frac{\mu_t}{\rho \sigma_\rho} \nabla \rho [138]$$
$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} [139]$$

where *P* is the shear production, *G* is production due to the buoyancy force and μ_t is the the turbulent viscosity, determined by solving the transport equations for the turbulent kinetic energy and its rate of dissipation.

4.3 Discrete transfer radiation modelling (DTRM):

Discrete transfer radiation modelling (DTRM) is a common preference for the modeling cases of heat transfer, which is generally listed on the weighted-sum-of-gray-gases model (WSGGM). In the calculation of gas radiation, this model is vital as it also accounts for particular concern within the oxy-firing projects. For this purpose, choosing the absorption coefficient, surface and angular discretization are crucial for accurate radiation characteristics prediction. [140]. The premise of DTRM is that one ray can use a solid angle to assess the strength, thus referring the amount of rays with directions, chosen in (RTE) to be solved for each ray as it travels from one boundary to the next. Thus, the background of this method is that the coefficient of absorption and therefore temperature is believed to be constant within one cell (control volume).

For the change of radiant intensity, dI, along a path, ds, the equation can be written as:

$$\frac{dI}{ds} + \alpha I = \frac{\alpha \sigma T^4}{\pi}$$

Where

 α = gas absorption coefficient

I= intensity

T= gas local temperature

 $\sigma = Stefan - Boltzmann Constant(5.669 \times 10^{-8} W/m^2 K^4)$

The DTRM integrates the aforementioned equation along a series of rays emerging from boundary faces. If α is constant along the ray, then I(s) can be estimated as [141]:

$$I(s) = \frac{\sigma T^4}{\pi} (1 - e^{-as}) + I_o e^{-as} [142].$$

where I_o is the radiant intensity at the start of the incremental path. This value is determined by applying the appropriate boundary conditions. Furthermore, the ray tracing parameters: polar divisions and Azimutal divisions are set to be 2 and 8 respectively in this simulation so that a more accurate solution can be achieved in addition to reducing computational costs.

4.4 DDM (Discrete Droplet Method):

The DDM (Discrete Droplet Method) has been widely used to model the lower degree coal combustion. The coal straw (particle) is usually assumed as in the form of rectangular shape containing non interacting packets. This model can be observed and controlled in the computational map introducing particle parcels in the domain of flow region. The equations are solved to obtain for different factors such as particle's momentum, heat, and mass transfer between gas phases.

$$m_p \frac{du_{id}}{dt} = \bar{\mathbf{F}}_{idr} + \bar{\mathbf{F}}_{ig} + \bar{\mathbf{F}}_{react}$$

In the equation, all the external force magnitudes acting on particle phase equals the mass particles times inertia of particulate phase. Where $\bar{F}_{idr} = \frac{1}{2} \rho_g A_p C_D |u_{rel}| u_{rel}$, the drag coefficient is dependent on Schiller and Naumann's formulation [143] .Here C_D , drag coefficient is a function of the cross sectional area (A_P) of coal particle and Reynolds number (Re). The relative velocity is measured using gaseous and particle phase velocity .The gravitational force is $\bar{F}_{ig} = V_p (\rho_p - \rho_g) g_i$. The reaction force applied on the coal particle is m_{vp} defining the formula $\bar{F}_{react} = V_p (\frac{-m_{vp}}{dt})$ also define the devolatilization function. Trajectory of particle has an effect of the reaction force although negligible in contrast of other forces in the equation. Stochastic means assess the reaction force's course.

4.5 Eddy Breakup (EBU) model:

This combustion simulations use the Eddy Breakup (EBU) model, which is a turbulencecontrolled combustion model. EBU, first suggested by Spalding [144] and later updated by Magnussen and Hjertager is an efficient tool for modeling common combustion calculations [145] that can be used to write the mean reaction rate:

$$\bar{\rho}\bar{\mathbf{r}}_{fu} = \frac{C_{fu}}{\tau_R}\bar{\rho}.\min(\bar{\mathbf{y}}_{fu},\frac{\bar{\mathbf{y}}_{OX}}{S},\frac{C_{fu}.\bar{\mathbf{y}}_{pr}}{1+S})$$

Time scale of turbulence (τ_R), is dependent on the characteristics of local flow which defined the fuel consumption rate. τ_R is termed as turbulent kinetic energy (K) to its dissipation rate (ε) ratio. Minimization of the first two operator value strictly search for the presence of fuel or oxygen in a restricting amount. Third term is a probability function, defines the probability of the reaction. The exact values for analytical co-efficient C_{fu} and C_{pr} are computed on basis of the precise turbulence structure of the flow region. It's worth noting that raising the values of these coefficients causes the chaotic reaction rate to intensify. For the same purpose as before, C_{fu} and C_{pr} were fixed at the value of 3.0 in air-fuel fired and 0.5 in oxy-fuel fired situations, under these special conditions of this analysis.

4.6 Reactions:

In comparison to single step mechanism, multi-step modelling provides more satisfactory results as studied by Al Abbas and Naser [146] After investigating related studies, we used three step homogeneous and heterogeneous reactions as shown on the following part.

Even after quite strong predictions about species and temperature profile, there were found some inconsistencies in the simulated numerical results which were generated incorporating total of 8 species (volatile and char, O_2 , N_2 , CO_2 , CO, H_2 , and H_2O) in three step mechanism.[147] Such inconsistencies might have got influenced due to the use of single step mechanism and thus it was quite essential and predictable to bring the aforementioned species into count to get desired temperature and species profile. Moreover, one-step model's inability to capture equilibrium and CO_2/CO ratio made researchers think of multi-step modelling which also technically helped the fuel conversion rate and CO/CO_2 output rate subjected to temperature and partial pressure. [82], [148]

4.6.1 One-Step Chemical Reaction:

Irreversible one-step mechanism of solid fuel mixed with air or O₂/CO₂ was considered for all of the combustion cases. There are two major reaction mechanisms in coal combustion. The first method is homogeneous volatile matter reactions (VM). Since there wern't much remarkable differences found between methane and other gases, methane (CH₄) is considered as an instance in this reaction.[102] The heterogeneous reaction is the second phase. Following chemical reactions were considered during oxy-fuel combustion, as shown below.

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O + heat$$

The equation for char that has been oxidized (heterogeneous phase) is:

$$C_{char} + O_2 \rightarrow CO_2 + heat$$

The combustion reaction heat (Δ H) of above mentioned reactions are found to be 802310 and 393520 kJ/kmol, respectively, based on the combustion model. [146]

4.6.2 Two-Step Chemical Reaction:

Since single-step reaction mechanisms have limitations in terms of temperature and essential critical intermediate species (CO), mechanism using two-step reaction may produce CO in the mid-phase and char burn-out reactions below.

These two reactions can be used to express the devolatilization chemical mechanism:

$$CH_4 + \frac{3}{2}O_2 \rightarrow CO + 2H_2O + heat$$

 $CO + \frac{1}{2}O_2 \leftrightarrow CO_2$

The heats of reaction of are 307880 and -110190 kJ/kmol, respectively. However, these two chemical reactions can be used to express the reaction for char burned with oxygen:

$$C_{char} + \frac{1}{2}O_2 \rightarrow CO + heat$$
$$CO + \frac{1}{2}O_2 \leftrightarrow CO_2$$

There is a significant impact of reverse reaction on the equilibrium state and heat emission rate, which is subject to special interest due to it's high temperature level. Many investigated referred studies in the literature have used the aforementioned chemical reactions. [114], [149]–[151]

4.6.3 Three-Step Chemical Reaction:

As previously mentioned, the flame envelope zone is the furnace's highest zone of temperature when compared to other areas. So, during computational simulation coal particles, the dissociation reaction of the main gaseous component should be taken into account. In addition to the main dominant species, the three-step reaction mechanism will reliably produce CO and H_2 . Consequently, to correctly describe the dissociation processes in this mechanism, the hydrocarbon fuel (methane) and residual char (Cchar) are presented below [130]

These three chemical reactions can be used to express the chemical reaction for devolatilization:

$$CH_4 + O_2 \rightarrow CO + H_2 + H_2O + heat$$

 $CO + H_2O \leftrightarrow CO_2 + H_2$
 $O_2 + 2H_2 \leftrightarrow 2H_2O$

Above equations have heats of reaction of 549710, 868360, and 483660 kJ/kmol, respectively. Given the fact that due to their lower effect on the char reaction the gasification in both the air-

fired and oxy-fuel combustion instances, is addressed and taken into account to enhance the simulation's certainty and precision

These three heterogeneous chemical reactions can be used to express the method for char oxidization:

$$C_{char} + \frac{1}{2}O_2 \rightarrow CO + heat$$
$$C_{char} + CO_2 \rightarrow 2CO$$
$$C_{char} + H_2O \rightarrow CO + H_2$$

As separate subroutines, the enthalpy (ΔH) of the reactions are considered and for all combustion cases they were incorporated as source term. Al-Abbas and Naser's recent simulation analysis contains detailed numerical knowledge about the multiple reaction process.[152]

For devolatilization, Badzioch and Hawksley's [153] reaction model is considered. The kinetic rate constant and the temperature background of the fuel particles are heavily influenced by the unpredictable output rate in this model[106]. The Arrhenius equation [154] is used to account for this phenomenon.

 K_d (P_g- P_s) is used to calculate the oxygen diffusion rate, where P_g denotes the partial O₂ pressure (far from the particles boundary layer), P_s denotes external surface partial pressure of oxygen, and K_d is given by the equation below.[155]

$$K_d = \frac{2.53 * 10^{-7}}{R_p} (\frac{T_p + T_g}{2})^{0.75} \frac{P_A}{P}$$

where R_p denotes the particle radius, T_p denotes the particle temperature, T_g denotes the the far region gas temperature, and atmospheric and local pressure are defined by P_A and P respectively. K_cP_s defines the rate at which char oxidizes in every unit particle surface area. The Arrhenius expression for the kinetic rate is as follows:

$$K_c = A_c \exp(\frac{-E_c}{T_p})$$

where A_c represents the pre-exponential factor (kg /m² s (N m²)) and the activation energy (J/ kmolK) is denoted by E_c . It is suggested by studies to use A_c value as 497 (kg /m² s (N m²)) and 8540 (J /kmol K) to be used as E_c value [104]. Finally, the rate at which char is formed can

be expressed as follows: $\left(\frac{1}{K_d^{-1}+K_c^{-1}}\right)P_g 4\pi R_p^2 \frac{P_A}{P}$ and can be dominated with respect to the K_d and K_c rates comparatively lower. [106]

Char and ash are assumed to be the rest amount of coal particles after devolatilization. And it's formation is simulated with global power-law (Bri). Various rate constants selection (like preexponential factor (Av) and energy of activation (Ev)) is vital for correctly modelling of combusting fuel particles.

5. OPERATING CONDITIONS

5.1 Fuel Characterization:

As fuel, a bituminous coal, was used in this analysis. Table 1 summarizes the proximate and ultimate study of the chosen fuel. Heating values (LHV) of 27.09 MJ/kg are characteristic of the coal. Reference 151 provided the particle size distribution for coal. The coal's average particle size is 47 millimeters. The solid fuel feeding device has been set at a set point corresponding to a thermal load of 30 kW in all cases considered. Based on the experimental analysis, a constant total thermal load is determined. [156]

Coal Chara	cteristics					
Proximate	Fixed	Volatile	Moisture	Ash	N/A	N/A
Analysis	Carbon	Matter (VM)	Content	Content		
	(FC)					
	50.40	34.86	5.03	9.62		
Ultimate	Carbon	Hydrogen(H)	Nitrogen(N)	Sulphur(S)	Chlorine	Oxygen(O)
Analysis	(C)				(Cl)	
	80.70	5.41	1.69	0.726	0.016	11.46

Table 3 Coal Characteristics

Table 4 Kinetic parameters

Kinetic parameters											
Fuel type	Processes	Activation Energy,	Pre-exponential	factor,							
		E (J/kmol)	A(1/s)								
Coal	Devolatilization	1.559x10 ⁰⁸	4.68x10 ¹¹								
	Char	1.2×10^{08}	9.48x10 ⁴								
	Combustion										

5.2 Boundary Conditions:

The Primary Oxidant Flow is set to be 20% of the overall Oxidant Flow. For all of the walls, a constant wall temperature was assumed with a no-slip boundary condition (where u,v, and w = 0) and a wall emissivity of 0.85.

Fuel	Fuel	Inlet O ₂ (%)	Inlet	CO ₂	Inlet	N_2	Oxidant	Swirl
	Flow		(%)		(%)		Flow*	Number
	(kg/hr)						(Nl/min)	
		21	-		79		620	
		25	75		-		490	
Coal	3.99	30	70		-		390	1.8
		35	65		-		325	

Table 5 Boundary Conditions

6. COMPUTATIONAL SETUP & MODELLING

1. Firstly we select the transient method for the whole simulation setup and also gave the gravity value input towards the Y-direction.

General (?)	🕫 Viscous Model	×			
	Model	Model Constants			
Mesh	Inviscid	Cmu			
		0.09			
Scale Check Report Quality	 Spalart-Allmaras (1 eqn) 	C1-Epsilon			
	k-epsilon (2 eqn)	1.44			
Display Units	O k-omega (2 eqn)	C2-Epsilon			
	Transition k-kl-omega (3 eqn)	1.92			
Solver	 Transition SST (4 eqn) Reynolds Stress (7 eqn) 	TKE Prandtl Number			
Type Velocity Formulation	Scale-Adaptive Simulation (SAS)	1			
	 Detached Eddy Simulation (DES) 	TDR Prandtl Number			
Pressure-Based Absolute	 Large Eddy Simulation (LES) 	1.3			
O Density-Based O Relative	k-epsilon Model	Energy Prandtl Number			
	Standard	0.85			
		Wall Prandtl Number			
Time	 Realizable 	User-Defined Functions			
○ Steady	Near-Wall Treatment	Turbulent Viscosity			
Transient	 Standard Wall Functions 	none 🔻			
	Scalable Wall Functions	Prandtl and Schmidt Numbers			
	O Non-Equilibrium Wall Functions	TKE Prandtl Number			
	Enhanced Wall Treatment	none			
✓ Gravity	Menter-Lechner User-Defined Wall Functions	TDR Prandtl Number			
Gravitational Acceleration		none			
dravitational Acceleration	Options	Energy Prandtl Number			
X [m/s ²] 0	Buoyancy Effects Only Turbulence Production 🔻	none			
	Viscous Heating	Wall Prandtl Number			
Y [m/s ²] 9.81	Curvature Correction	none			
Z [m/s ²] 0	Production Kato-Launder	Turbulent Schmidt Number			
2 Links 1 0	Production Limiter	none 👻 👻			

Figure 17 Operating condition and Viscous modeling properties input

- 2. Next in the viscous modelling we used standard k-epsilon model and the near wall treatment was specified as standard wall functions and other parameters are used default.
- 3. In radiation modelling, we used discrete transfer eadiation modelling with 10 energy iteration per radiation iteration and maximum number of 5 radiation iteration. For species modelling we selected species transport modelling with both volumetric and particle surface reactions and specified the diffusion energy source. For turbulence interaction we are using finite-rate/Eddy-dissipation option.

Radiation Model		X Species Model	Mixture Properties
Model Off Rosseland P1 Discrete Transfer (DTPM)	Iteration Parameters Energy Iterations per Radiation Iteration Maximum Number of Radiation Iterations Residual Convergence Criteria 0.001	Off Species Transport Non-Premixed Combustion Permixed Combustion Partially Premixed Combustion Composition PDF Transport	Mixture Material Mixture Material Edit Import CHEMKIN Mechanism Number of Volumetric Species 7 Number of Solid Species 1
Discrete Transfer (DTRM) Surface to Surface (S2S) Discrete Ordinates (DO) Monte Carlo (MC) Solar Load Model		Reactions Volumetric Vall Surface Particle Surface Electrochemical Chemistry Solver	Turbulence-Chemistry Interaction Finite-Rate/NO TCI Finite-Rate/Eddy-Dissipation Eddy-Dissipation Concept Coal Calculator
Off Solar Ray Tracing Solar Irradiation Solar Calculator		None - Explicit Source Options Inlet Diffusion Influsion Energy Source Full Multcomponent Diffusion Thermal Diffusion	Select Boundary Species Select Reported Residuals Thermodynamic Database File Name S~1\v211\fluent\fluent21.1.0\\jsat\data\\thermo.db

Figure 18 Radiation Model & Species Model

4. From the above-mentioned data, we inserted the proximate and ultimate analysis value of coal as shown in the figure below. We also put the high calorific value of the coal and chose the one-step mechanism.

		Coal Stre	eam	S
		Number of	of C	oal Streams 1
			Coa	al Stream ID 1
oal Propertie	s			
Proximate An	alysis	U	tim	ate Analysis (DA
Volatile	0.3489	14 0	C (0	.807113
Fixed Carbon	0.5044	54 H	1 0	.054108
Ash	0.0962	87 0	0	.114616
Moisture	0.05034	45 1	1 0	.016902
		5	5 0	.007261
Mechanism		0	ptio	ns
 Two-Ste 		on		
✓ Include S	02			
✓ Include S Settings	02			
		Name coa	l-pa	rticle
Settings	Material I		· ·	
Settings Coal Particle N	Material I xeived HC	CV [J/kg]	2.70	09e+07
Settings Coal Particle M Coal As-Rec	Material I eived HC ecular W	CV [J/kg] /eight [kg/	2.70 /kmc	09e+07 bl] 30
Settings Coal Particle M Coal As-Rec Volatile Mole CO/CO2 Spli	Material I ceived HC ecular W it in Read	CV [J/kg] /eight [kg/	2.70 /kmc	09e+07 bl] 30 tts 1
Settings Coal Particle M Coal As-Rec Volatile Mol CO/CO2 Spli High Te	Material I ceived HC ecular W it in Read mperatu	CV [J/kg] /eight [kg/ ction 1 Pro	2.70 /kmc oduc e Yie	09e+07 bl] 30 tts 1 eld 1
Settings Coal Particle M Coal As-Rec Volatile Mole CO/CO2 Spli High Te Fra	Material I ceived HC ecular W it in Read mperatu ction of	CV [J/kg] /eight [kg/ ction 1 Pro re Volatile	2.70 /kmc oduc e Yie (DA	09e+07 bl] 30 tts 1 eld 1 F) 0.7
Settings Coal Particle M Coal As-Rec Volatile Mole CO/CO2 Spli High Te Fra	Material I ceived HC ecular W it in Read mperatu ction of I Coal Dry	CV [J/kg] /eight [kg/ ction 1 Pro re Volatile N in Char Density [k	2.70 /kmc oduc e Yie (DA	09e+07 bl] 30 tts 1 eld 1 F) 0.7

Figure 19 Coal Calculator

5. Then in discrete phase modelling we chose the interaction with continuous phase and also selected unsteady particle tracking which will track the fluid flow with respect to

its time step. Maximum number of steps were given input as 5000 with step length factor 5. We chose automated tracking scheme solution with defined tolerance in accuracy and also selected droplet heat-mass solution to use.

E Discrete Phase Model			×	Discrete Phase	Model				
Interaction	le Treatment		Interaction	Particle Treatment					
✓ Interaction with Continuous Phase	✓ Interaction w	ith Continuous Pha	se	Unsteady Particle Tracking					
Update DPM Sources Every Flow 1	teration 🗹 T	rack with Fluid Flov	v Time Step	Update DPM	Sources Every Flow	Iteration	✓ Track with Fluid Flow	Time Step	
DPM Iteration Interval 10	Inject	t Particles at		DPM Iteration Int	erval 10	*	Inject Particles at		
Contour Plots for DPM Variables		Particle Time Step		Contour Plots fo	or DPM Variables		O Particle Time Step		
Mean Values	• F	Fluid Flow Time Step	p	Mean Values			Fluid Flow Time Step		
	Particl	le Time Step Size [s	5] 0.001				Particle Time Step Size [s] 0.001	
	Clear	r Particles					Clear Particles		
Tracking Physical Models	UDF	Numerics	Parallel	Tracking	Physical Models	UDI	F Numerics	Parallel	
	g Option gh-Res Tracking			Max. Refinemen Track in Al Coupled Heat Ø Droplet Combustin Multicompi Averaging	Control nce 1e-05 ents 20 boolute Frame -Mass Solution g onent de Based Averaging	Aut High Or Lov Trade Vaporiz Mass (Heat ()			

Figure 20 Discrete Phase Model

6. Next, in the discrete phase, we created an injection of coal (combusting particle), direction towards the normal to the surface and coal will be injected through the primary oxidant inlet. The particle size was specified as 47 μm at 300k with a flowrate of 0.0011083 kg/s.

njection Name			Injec	tion Type								
njection-1			surf	face	*)						
						Re	lease Fr	om Surfaces Fil	ter Te	xt	-) = =
						in or pl	ilet_po ilet_so utlet lane-4 vall-solid					
Particle Type					Laws							
○ Massless ○ Inert ○	Droplet 💿	Combusting	O Mu	lticomponent	Custom							
Material	Diamete	r Distribution	n	Oxidizing S	pecies		Discrete	Phase Domain				
coal-particle	 uniform 	n		• o2		•	none		•			
vaporating Species	Devolati	lizing Specie	s	Product Sp	ecies							
h2o	▼ vol			• co2		•						
Point Properties Physic	al Models	Turbulent Dis	persion	Parcel	Wet Co	ombus	stion	Components		UDF		Multiple Reac
Variable	Value										Stag	ger Options
Diameter [m]	47e-06		-									Stagger Positio
Temperature [K]	300		-									ger Radius [m
Start Time [s]			_								0	
	0		•									
Stop Time [s]	20		*									
Velocity Magnitude [m/s]	0		• C	onstant						•		
Total Flow Rate [kg/s]	1.1083e-3		- C	onstant								

Figure 21 Injection Properties

7. Then comes the reaction part. Here we used two-step reaction mechanism: 1. Devolatilization (Volumetric) 2. Char combustion (Particle surface) with their distinct activation energy and pre-exponential factor as specified below. And for char combustion we imported C_{Char} from the fluent database and added to the reactions. We also specified the rate exponent and stoichiometric coefficient in the reactions. Similarly other two and three step reactions were imported in the reaction model.

Reactions								×	Reactions					
ixture coal-volatiles-	air			Total N	umber o	f Reactions	2 🌲		Mixture coal-vola	atiles-air		Total Num	ber of Reactions	2 🌲
leaction Name	ID 1		on Type	Wall Surface 〇	Particle	Surface 🔘 I	Electrochemic	al	Reaction Name reaction-2	ID F	Ceaction Type	Wall Surface 🖲 Pa	rticle Surface 🔾	Electrochemic
lumber of Reactants	2	*		Number of Pr	oducts	4 🌲			Number of Rea	ctants 2		Number of Produ	icts 1 🌲	
Species		Stoich. Coefficient	Rate Exponent	Species		Stoich. Coefficient	Rate Exponent	A	Species	Stoich. Coefficie	Rate ent Exponent	Species	Stoich. Coeffici	Rate ent Exponent
vol	•	1	0.2	co2	Ŧ	1.31937	0		C <s></s>	• 1	0	co2	• 1	0
o2	•	2.05784	1.3	h2o	*	1.96934	0)	02	• 1	1			
				n2	-	0.04427	0) 🖵	Arrhenius Rat			v Minine Deba		
rrhenius Rate				Mixing Rate							000	Mixing Rate	B 0.5	
Pre-Exponential	Facto	or 4.68e-11		A 4		B 0.5				ential Factor 94				
Activation Energy [J/	kgma	l] 1.559e+0	08							ure Exponent 0	20+00	Particle Surfac		
Temperature Ex	·									ckward Reaction	Specify	c <s></s>	,	•
Include Backward Third-Body Efficie		6	Specify						Third-Body	Efficiencies	Specify	Diffusion-Limiter	d Species	*
		2	Specify						Pressure-D	ependent React	ion Specify	Diffusion Rate C	onstant 5e-12	
Pressure-Depend	ient F	Reaction	Specify						Coverage-Dependent Reaction Specify		Effectiveness Factor 1			

Figure 22 Reactions Model

8. Then we input the boundary conditions. First, we specified the boundary conditions of primary oxidant. Flow rate of primary oxidant is given as mass-flow inlet 0.0015996 kg/s at specified temperature. Next, we inserted the values of secondary inlet in a similar way.

🚺 Mass-Flo	w Inlet						Х	Mass-Flow Ir	ilet							×
-								Zone Name								
Zone Name				inlet_so												
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Figure 23 Inlet Boundary conditions

9. Then simple solution algorithm was used for solution methodology. After that, calculation was run after standard initialization.

7. VALIDATION

This CFD study is validated by comparing the achieved temperature values in different cases in reference[131]. For validation three different oxy-fuel and one air firing case were chosen. In the figure below, it can be seen that the peak temperature ranges from air fire to oxy-fire is 1100 °C to 1300 °C.

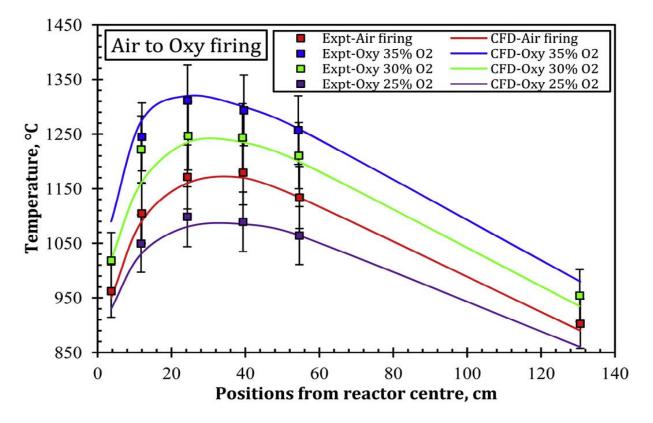
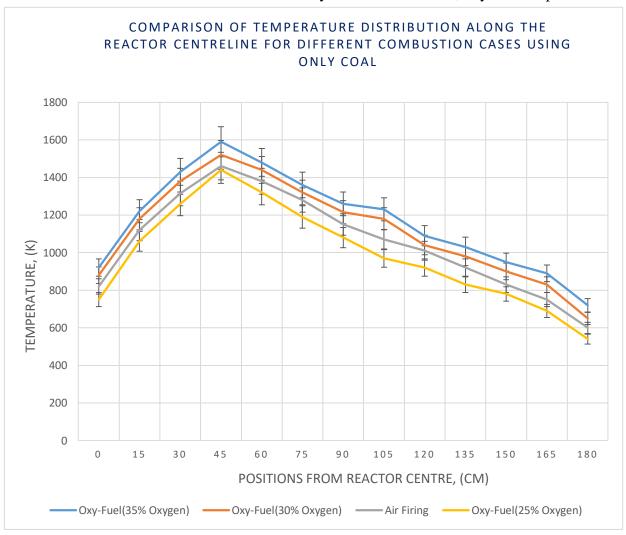


Figure 24: Temperature in four different coal combustion cases[131]

According to this paper analysis it is similar to the reference paper. In this figure below, the graph shows that temperature range from air firing to oxy-fuel firing is 1400K to 1670K (1127°C to 1397°C)



It is observed that both of these results are very close. In both cases, oxy-fuel temperature is

Figure 25 This paper temperature for four different coal combustion cases using

slightlyhigher than the air-fuel temperature. In both cases, at the end of the reactor the temperature became low. So that, it can be said that fuel is consumed entirely. Thus, proper combustion was happened in all the cases.

8. RESULTS AND DISCUSSIONS

In this research, effect of pure coal combustion in air and oxy-fuel atmospheres affects combustion characteristics such as flame temperature, burnout, and pollution are shown. One air fuel and three different oxy fuel cases are considered in this research. All the cases are modeled with 30 kW thermal input. To reduce CO_2 from the power plant, use of carbon-dioxide neutral fuels and OF combustion can be added to coal. In this section, the computational analysis results of this research will be discussed.

8.1 Differences among combustion environment for Air-fire to Oxy-fire

Performance of any power plant is highly dependent on the combustion environment. The flow analysis and species fraction analysis are showing the difference. When the combustion environment is air-fuel, the result of these analysis are different from oxy-fuel environment and it also varies in different oxy-fuel cases. This research would make a distinction between the different cases considered. Here, combustion process for different oxy-fuel and air-fuel will be discussed elaborately. While retrofitting, the temperature of flame for air-fuel and temperature of flame for oxy-fuel should match. This criterion has huge important in combustion case analysis. The oxy-fuel cases which are taken into consideration for this research is Oxy-Fuel 25% (25% O₂ & 75% CO₂), Oxy-Fuel 30% (30% O₂ & 70% CO₂) and Oxy-Fuel 35% (35% O₂ & 65% CO₂) and the results were analyzed based on flow, species, temperature profiles of combustion flames, and SO_x and NO_x emissions.

8.1.1 Case-I: Air-Fuel - Temperature, Axial flow, O2 and CO2 concentration contour

In this case, It is seen that the axial velocity is higher around 6.5 m/s and the peak temperature is around 1500K. The concentration of oxygen is 0.21 max and carbon-dioxide concentration is around 0.18. The lower concentration of CO_2 is the result of zero inlet boundary condition of carbon-dioxide. The static temperature is highest in the upper portion of the reactor and it is gradually decreasing which shows that the combustion was completed perfectly.

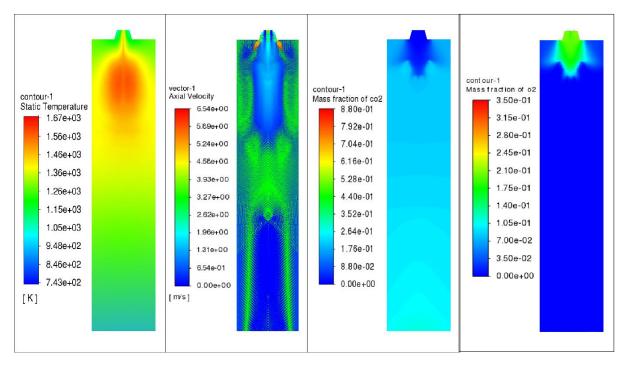
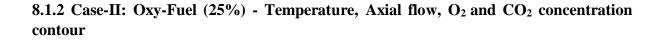


Figure 26: Air Fuel Case



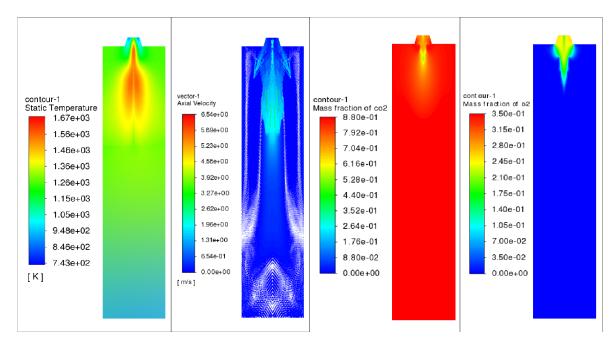
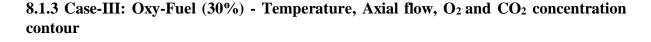


Figure 27 25% Oxy-Fuel Case

In this case, it is seen that the axial velocity is higher around 5.6 m/s and the peak temperature is around 1450K. The concentration of oxygen is 0.25 maximum and carbon-dioxide concentration is around 0.78. The higher concentration of CO_2 is the result of inlet boundary

condition of carbon-dioxide. The static temperature is highest in the upper portion of the reactor and it is gradually decreasing which shows that the combustion was completed perfectly.



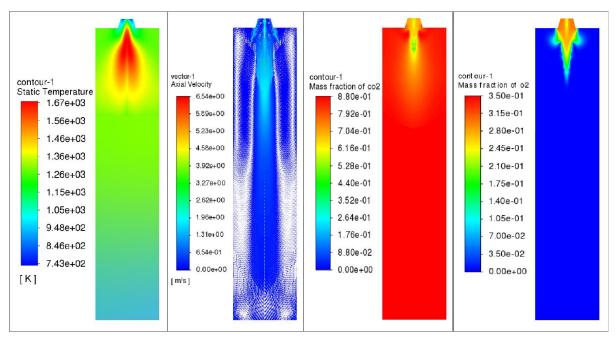


Figure 28: 30% Oxy-Fuel Case

In this case, it is seen that the axial velocity is higher around 4.8 m/s and the peak temperature is around 1590K. The concentration of oxygen is 0.30 maximum and carbon-dioxide concentration is around 0.8. The higher concentration of CO_2 is the result of inlet boundary condition of carbon-dioxide. The static temperature is highest in the upper portion of the reactor and it is gradually decreasing which shows that the combustion was completed perfectly.

8.1.4 Case-IV: Oxy-Fuel (35%) - Temperature, Axial flow, O_2 and CO_2 concentration contour

In this case, it is seen that the axial velocity is higher around 4 m/s and the peak temperature is around 1670K. The concentration of oxygen is 0.35 maximum and carbon-dioxide concentration is around 0.88. The higher concentration of CO_2 is the result of inlet boundary condition of carbon-dioxide. The static temperature is highest in the upper portion of the reactor and it is gradually decreasing which shows that the combustion was completed perfectly.

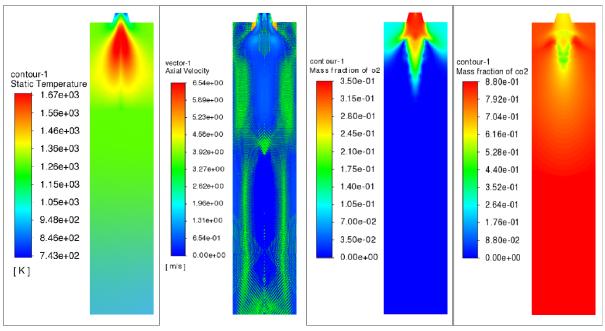


Figure 29: 35% Oxy-Fuel Case

8.2 Comparison of Static Flame Temperature (O₂ &CO₂ among Air-Fuel to three Oxy-fuel Cases

In the figure below there are temperature variation for three different combustion cases are presented according to the previous discussion. From the result it can be seen that with the increase of oxygen concentration in the combustion environment, static temperature also increases. Though in 25% oxy fuel cases has lower peak temperature than the air fuel peak temperature. The reason behind this difference is CO2. Carbon-dioxide has higher heat absorption capacity then nitrogen. In air firing case, oxidant was combination of oxygen and nitrogen while in oxy-fuel cases, the oxidant mixture was combination of oxygen and carbon-dioxide. But, when the oxygen concentration rises in OF30 and OF35 cases, static temperature also rises in significant amount.

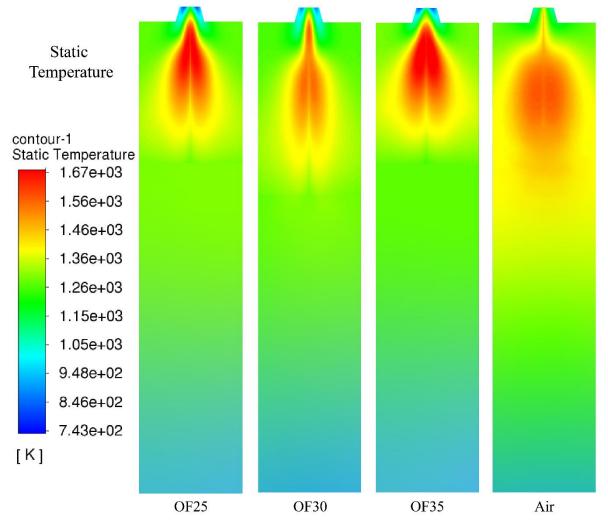


Figure 30 Static Temperature of different combustion cases

8.3 Comparison of flow among Air-Fuel to three Oxy-fuel Cases

The axial velocity (m/s) for four different cases are presented in the figure below. In both AF and OF situations, the volume flow rate of primary oxidant is 20% of the total volume flow rate of oxidant, as stated in the operating condition portion. Secondary oxidant flow is calculated on the basis of swirl number, total volume flow rate of oxidant flows, secondary flow will be the resultant of axial and tangential flow. For better mixing, a feature is introduced in the burner which is swirl stability. It has huge effect on the combustion flame structure. Swirl flow stabilize the flame efficiently and helps the oxidizer to burn the fuel completely. In this study for all the cases, swirl number was considered constant 1.8. The fuel particles (here only the coal) are directly injected into the reactor through the primary oxidant inlet. The secondary oxidant which is swirl oxidant flow was fed through secondary oxidant inlet. In the figure there are two recirculation zone are observed. They are mainly in the upper section of

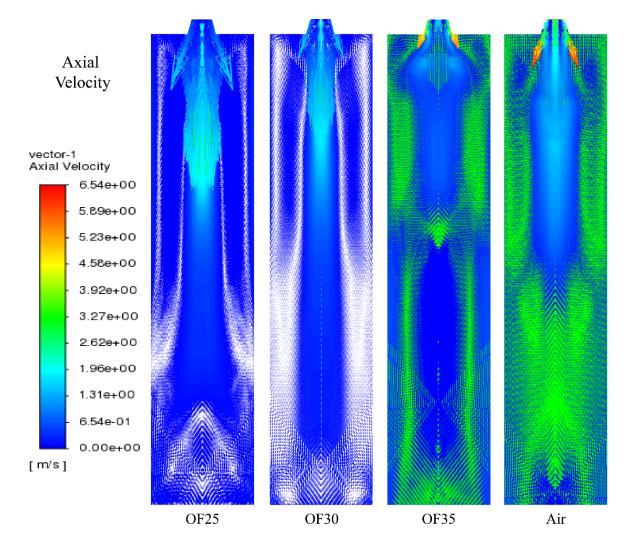


Figure 31 Axial Flow Distribution of OF25, OF30, OF35 and AF

the reactor. Swirl flow is the reason for creating this recirculation zone and internal recirculation were also observed in the burner area. From the air and oxy-fuel case, it can be said that with the increase of oxygen concentration, the velocity of the different cases decreases and resident time increases. This phenomenon helps to get better combustion reaction. Thus, stable flame temperature is achieved.

8.4 Comparison of Species Concentration (O_2 & CO_2) among Air-Fuel to three Oxy-fuel Cases

The main species of combustion is O_2 and CO_2 . The mass fraction of these two species for all the cases are presented in Figs. 6 and 7 respectively. The variation in the analysis amount of O_2 and CO_2 concentration in the process of air to oxy-fuel combustion are noticeable. As per the Eddy Break-up (EBU) model, O_2 concentration in the reaction affects the flame and

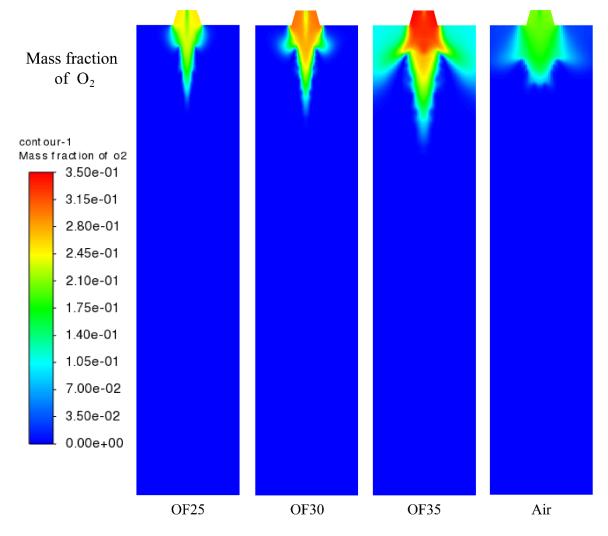


Figure 32 Mass Fraction of O2 for all cases

ignition characteristics in furnace area. Based on the combustion environment, a comparable form of O_2 distribution is expected for the air-firing case and the OF-25 case. Because of the higher oxidizer flow, the distribution is relatively broad. By comparing OF-30 and OF-35 to air and OF-25, there is a large rise in concentration. As a result, O_2 accessibility is greatly improved, and O_2 use is accelerated. This would result in a stronger combustion state in the reaction field, with a higher flame temperature. On the basis of chemical characteristics and properties Carbon-dioxide has advanced specific heat characteristics compared to N2. For this reason, CO_2 has higher heat absorption capacity. Thus, comparing air fuel and oxy fuel cases, the increasing concentration of carbon-dioxide has great impact on combustion environment. In the below figures, the mass fraction of CO_2 and O_2 for all the cases are presented.

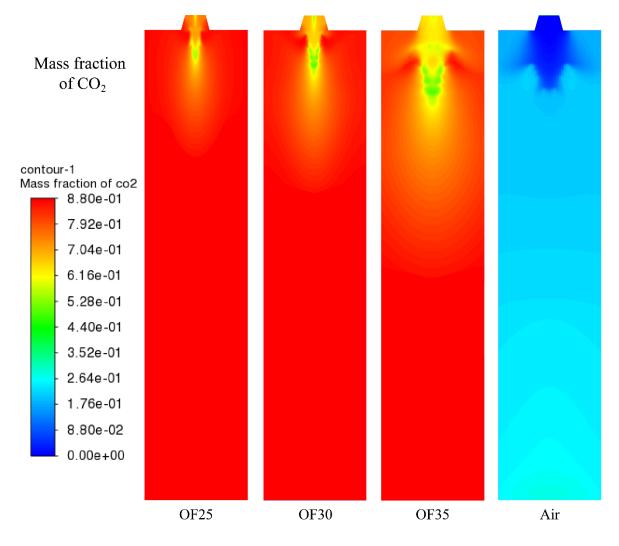


Figure 33 Mass Fraction of CO2

8.5 Residence time of all combustion cases

For combustion cases, perfect residence time has importance like every other variable. The reaction is dependent on fuel particle & oxidant residence time in the combustion area. The combustion flame temperature is related to residence time and the flow rate of the flue gas. In the table below the residence time for all the cases are shown. When the oxygen percentage rises, the residence time also increases. In coal powerplant while retrofitting, residence time affect significantly on combustion output. The result also varies according to reactor.

Oxidizer	Residence time, T(s)
Air fuel	2.60
Oxy-Fuel (25%)	3.47
Oxy-Fuel (30%)	3.70
Oxy-Fuel (35%)	4.20

Table 6 Residence Time For different cases

9. CONCLUSION & FUTURE WORKS

In this research, a computational fluid dynamics analysis was done for pure coal combustion. Total four cases were analyzed in this study. Three different oxy-fuel cases and one air-fuel case were simulated by using ANSYS Fluent 2021 Academic version R1. For changing combustion situation in four cases, oxidant variation was introduced. Here, different oxygen, carbon-dioxide and nitrogen concentration was used and to retrofit flame temperature and then, species concentration were matched. The comparison of the simulations under the different cases, it could be suggested that 30% oxygen concertation is more acceptable. The amount of emission of these cases are still under research. In future, the emission level and the solution to reduce emission will be added with this study.

The ECO-Scrub technology will be of serious prospective interest in the industry in the near future. The reason is that it will permit a probable carbon capture retrofit choice in the newly built power plants with high efficiency, thus helping to reduce adverse effect on the environment. The ASU plant energy consumption is an important component of total plant energy losses for the ECO-Scrub and oxyfuel processes, and existing cryogenic technology is continuing to show cost reductions as a result of improved compressor efficiencies, more effective process equipment, and bigger plants. Emerging air separation concepts based on high-temperature oxygen ion transport membranes are also showing promise, with the potential to increase power generation efficiency and lower capital costs. The development of oxygen transport membranes for oxygen production on a commercial level is still in the primitive stages, and further work is needed to demonstrate this technology. Using the CFD modelling, further optimization is required in reaching the final temperature as well as narrowing down the velocity range and minimizing the NOx and SOx emissions. The significance of numerical analysis of oxy-fuel conditions scenarios prior to their industrial implementation is highly emphasized by the present research.

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