Modelling of NOx and SOx emission: A CFD case study in a small-scale furnace

B.Sc. in Mechanical Engineering Thesis

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Research Certification:

The thesis title “Modelling of NOx and SOx emission: A CFD case study in a small scale furnace” submitted by Faria Noor (160011013), Rezwana Sarwar (160011017) and Musarrat Khan(160011075) has been accepted as satisfactory for the Degree of Bachelor of Science in MechanicalEngineering on March 2021.

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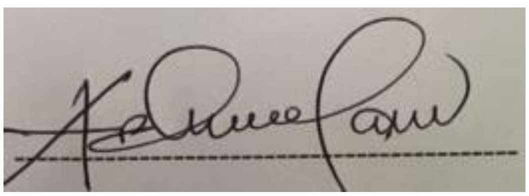

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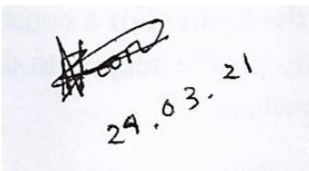
<u>Candidate's Declaration</u>

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

Signature of the Candidates



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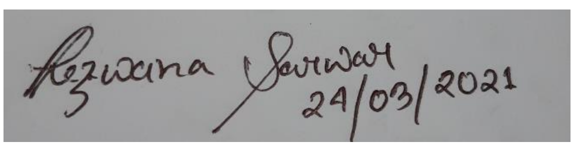

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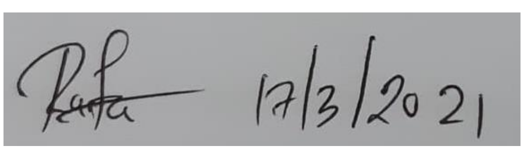

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Abstract: A CFD case study was done to learn the impact of Flue Gas Recirculation in a horizontal axis small scale furnace. Flue Gas Recirculation was performed to seehow the emissions are affected with a change in recirculation ratio. The aim was to find out the optimum Recirculation Ratio at which the emission is minimum but the efficiency of combustion is not compromised. A comparative analysis was presented in order to determine the various factors affecting NOx and SOx emission.Ansys FLUENT 2020 R2 was used to simulate the combustion environment. It was found out that by using flue gas recirculation, NOx and CO_2 emissions can be reduced significantly, and SOx emission can be reduced only slightly. The temperature contour for the recirculation scenarios were comparable to that of the air fired case. Increasing temperature also resulted in an increase in NOx emission.

Keywords: **NOx, SOx, Flue Gas Recirculation, Combustion, Ansys FLUENT**

Nomenclature

RR=Recirculation Ratio

NOx=Nitrogen Oxides

SOx= Sulfur Oxides

Ac =pre-exponential factor (s^{-1})

D=Diameter of the particle (μm)

Ec=Activation Energy (kJ mol^{-1})

IFRF= International Flame Research Foundation

AASB = Aerodynamically Air Staged Burner

DTRM = Discrete Transfer Radiation Method

CTF = Combustion Test Facility

GCV =Gross Calorific Value

RFG = Recycled Flue Gas

PFG= Product Flue Gas

GHG=Greenhouse Gas

VM =Volatile Matter

HC=Hydro Carbon

FC =Fixed Carbon

FGR= Flue Gas Recirculation

1.Introduction

Fossil fuels have been the number one offender behind the destruction of atmosphere and yet it is difficult to satisfy energy needs without it. People have moved back and forth and efforts have been made to minimize the impacts keeping the efficiency constant to some extent. CO_2 emissions from fossil fuel comprises of 75% of total emissions which contributes to severe problems like global warming. Among other pollutions, NO_X and SO_X are the most significant and harmful ones. Using coal as a fossil fuel has been detrimental to the atmosphere because these oxides critically endanger the planet and human health. Acid rain is a phenomenon created from these sulfur pollutions, which is toxic to humans and objects alike. NO_X pollutions are dominant in creating photo chemical smog, which is disastrous to the environment. Therefore, there is continuous research going on to diminish the release of these pollutants into the air from these plants.[1][2] A huge number of power plants operate using these fossil fuels. However, amount of CO_2 that is being released from these plants is significantly low these days because it comprises of about 21% oxygen and 79% nitrogen. This nitrogen oxidesare usually released in the atmosphere. [3]This is one of the major emissions of power plant alongside sulfur oxide emissions and is an extremely harmful component. Various cleaning technologies have been adapted by companies for cleaner air. Then again the combustion efficiency of these processes are not good enough always for running the plants. Most of these techniques do not solve NO_X and SO_X emissions together but is capable of doing one or the other. The wet flue gas desulfurization system removes a huge chunk of SO_X, about 80.3%. This however does not do anything for the removal of NO_X and hence is one dimensional. [4]

There have been studies to use glycerol in these fuels to heavily increase the oxygen content of fuel. This helps in reduction of NOx emissions and can be used as compensation for EGR (exhaust gases recirculation) penalties. It was observed that using 8% and 13% EGR rate, NOx, CO and soot can be cut down together. This improves CO- NOx and soot- NOx trade off approximately 2 times for each of the species. [5] In recent times, coal combustion using oxygen in place of direct air has gain popularity for a number of reasons. Since nitrogen is deducted beforehand, the exhaust is CO_2 rich and gives an effective route for removal of nitrogen related impurities. Using oxygen for coal combustion has various benefits that improves the overall efficiency of the process. For starters, the recovery and removal of CO_2 is an expensive procedure but using this process, the complexity significantly reduces, and CO_2 can be accessed easily. Since the amount of nitrogen in the fuel is minimum to begin with, it reduces the chances of nitrogen pollution significantly. Furthermore, recirculation decreases the amount and gradually diminishes the nitrogen pollution. Again since the amount of exhaust is low, it is very apparent that the efficiency of boiler will hike. The flue gas received can be recirculated thus making the entire process environment friendly.

We aimed to model the NOx and SOx emissions and observe the presence of each of these components in the net flue gas. Flue Gas Recirculation (FGR) was used as a tool to cut down NO_X emissions. FGR is a process of reducing the peak flame temperature which reduces NO_X emission by reducing the amount of oxygen in the combustion area.[6] Recirculating CO_2 as a flue gas has been our main mode of operation to cut down on these emissions in oxyfuel combustion. However, there remains the significant threat of compromising the combustion efficiency which ultimately is fatal to the workability of the entire model. Hence, it is imperative to figure out an optimum point that tackles the threat of reduction of efficiency and yet has significant impacts in reducing emissions. In order to find the optimum ratio, we went for a trial and error mechanism and created simulation for NO_X and SO_X emissions against various recirculation amount CO_2 as inputs. From those simulation results we aimed to create a picture of the entire process and to somehow predict the trend of these recirculation percentages on combustion efficiency. Comparative analysis of the impacts of NOx and SOx emissions was done separately to see and predict how differently these two respond to minor changes of the ratio and whether or not there is any change at all.

Bhuiyan et al. performed a numerical investigation on the radiative and convective performance on the combustion of pulverized Russian Coal. Testing of various combustion environment was done. Air fired was used as reference case and three recycled flue gases were used. The temperature distribution for the reference case was similar to that of RR72%. The flame temperature was found to increase with O_2concentration and decreasing RR. Highest peak radiative heat flux and flame temperature was achieved for the lowest recycle ratio of RR65%. The flame for the RFG fired case was concentrated more towards the center comparted to the air fired case. [7]Wei et al. used a numerical simulation program and CFD software AIOLOS was used to find the concentration profiles of CO, NOx and SOx during co-combustion of coal and biomass. It was found that lower temperature of combustion reduces NO formation but final concentration of SO_2 remains unaffected. To reduce emission, biomass with low nitrogen and sulfur content, high volatile matter and low heating value was recommended. [8]Li et al. performed an investigation on effects of flue gas recirculation ratio and fuel types on the NOx and SOx emissions. The effects of air pre heating on the NOx emission has also been analyzed. Flue gas recirculation was found to be an effective way to reduce the NOx and Sox emission. Furthermore, NOx emission was rapidly reduced with the increase in recycle ratio while there was a simultaneous increase in the SOx emission. Volumetric combustion was recommended as a way to reduce both NOx and SOx emissions. Higher percentages of biomass resulted in smaller amounts of NOx and SOx formations. [9]Smart et al. tested the cofiring of biomass and coal under oxy fuel combustion conditions using south African and Russian coal, both types blended with 20% by mass of Shea Meal. O_2 values were kept at 3% and recycled ratios between 65% and 75% was used, it was found that the highest radiative heat flux corresponds to the lowest recycle ratio. Co-firing showed lower radiative heat fluxes and improved burnout. [10]

Croiset et al. performed two types of experiments (combustion in once through O_2/CO_2mixtures and experiments with recycled flue gas) focusing on the implications of O_2/CO_2 recycle combustion on NOx and SOx emissions. Performing combustion in air as a base case , NOx and Sox were measured at different locations of the reactor. It was observed that the higher O_2 concentration in the feed gas increases NOx and SOx emission rates. Combustion in air showed the highest NOx emission rate because large amount of nitrogen was in the combustion medium to produce thermal NOx.Combustion in recycled flue gas has less NOx emission than once through combustion in O_2/CO_2 mixtures.The non-recycled flue gas was more enriched with NOx than the recycled one.SO_2 emission was slightly higher in the once through combustion than the recycled one. [11]Hu et al. investigated the emissions of CO_2, NOx and SO_2 from the combustion of a high-volatile coal with N_2- and CO_2-based, high O_2 concentration (20, 50, 80 and 100%) inlet gases in an electrically heated up-flow-tube furnace at elevated gas temperatures (1123–1573 K).The impact of varying fuel equivalence ratio was observed in case of NOx and SOx emissions.It was seen that there are two types of S in the coal (one is volatile and the other type is combined with fixed carbon in char).Decreasing SO_2 was observed in the fuel rich region because of the retention of sulfur in the char or unburned carbon. NOx emission indexes (mg-N/g-Coal-fed) monotonically decreased with the increase of fuel in both fuel-lean and fuel-rich combustion. Temperature had little effect on SO_2 emissions and a large effect of temperature on NOx emission. NOx emissions at peak increased by 50–70% for the N_2-based inlet gas processes and by 30–50% for the CO_2-based inlet gas processes from 1123 to 1579K.[3]Gopan et al. proposed a thermodynamic approach to better understand the fundamental impact of FGR (flue gas recycle) on the efficiency of oxy-combustion systems. It's been seen that the second-law losses associated with flue gas recycle are significant and highly non-linear with recycle ratio. It was suggested in the paper that for systems employing cold recycle, FGR should be kept below 33%.[12]Scharler et al. took a computational fluid dynamics approach to investigate the effect of flue gas recirculation in case of air staging combustion. In the paper , proper air staging and flue gas recirculation ratio were analyzed. More homogeneous temperature distribution inside the furnace was noticed with increasing recirculation ratio.[13]Oki etal. stated that recirculating CO_2 can have significant impacts on increasing the thermalefficiency of power plants during combustion which is otherwise difficult using carbon capturetechnologies. The coal will be gasified using a mixture of oxygen and recirculated CO_2. This willevidently simply the system since so separation unit is required as the CO_2 concentration isvery high in the exhaust gases. Recirculating decreases emissions and yet balances the fall ofefficiency.[14]Liu et. al discussed the impacts of recirculating flue gases to negate global warming. Study and experimentation revealed that overall conversion of fuel nitrogen to NO was about one fourth using O_2/CO_2 pulverized coal combustion. To avoid mixing effects, the experiments were conducted in a one dimensional premixed reactor for NOx. However to keep the combustion intensity intact it is necessary to recirculate 40% heat. This could be achieved with oxygen as low as 15%. Hence the emission of NOx can be decreased to about one seventh. At the same time desulfurization efficiency can be improved drastically.[15]

2. Methodology

2.1. Computational Domain:

The details of the computational domains are given in figure 1-4. It consists of a burner section followed by a ceramic lined furnace and a converging section. Figure 4 shows a closeup of the burner section. A slight gap (8mm) is kept in between the inlet of the primary and secondary air to separate the two inlets. Solidworks 2019 was used to create the geometry.

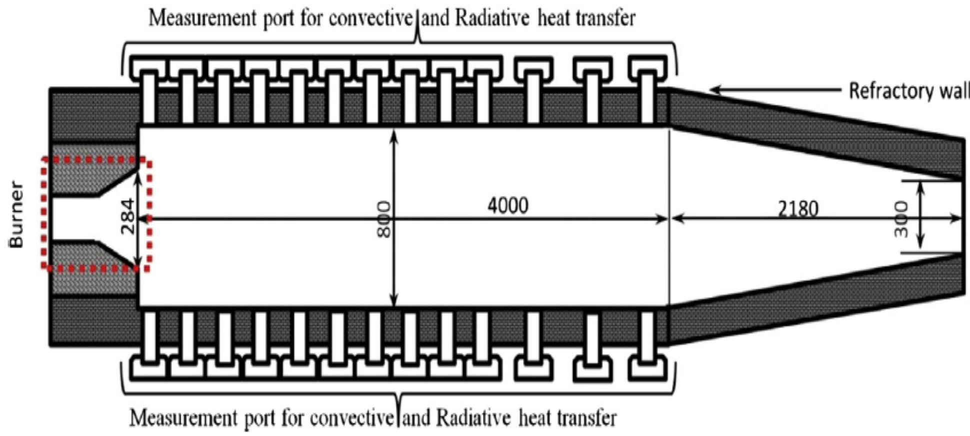


Figure1: Schematic of combustion test facility used in present study (all dimensions in mm)[7]

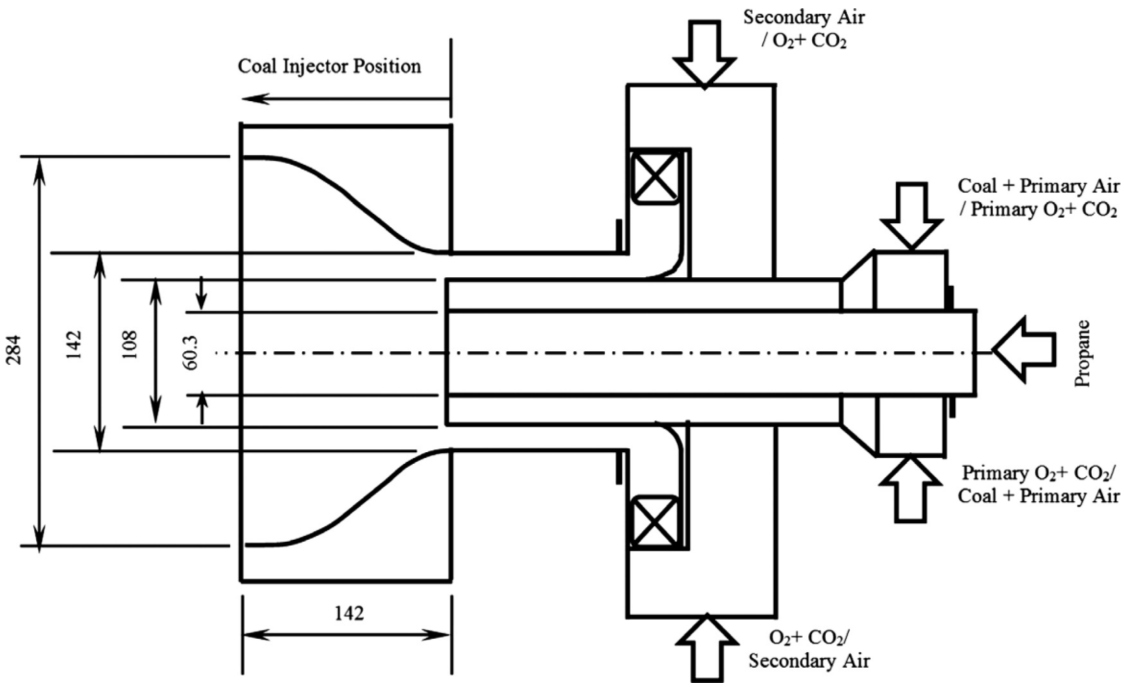


Figure 2: An IFRF Aerodynamically Air Staged Burner (AASB) specification.[7]

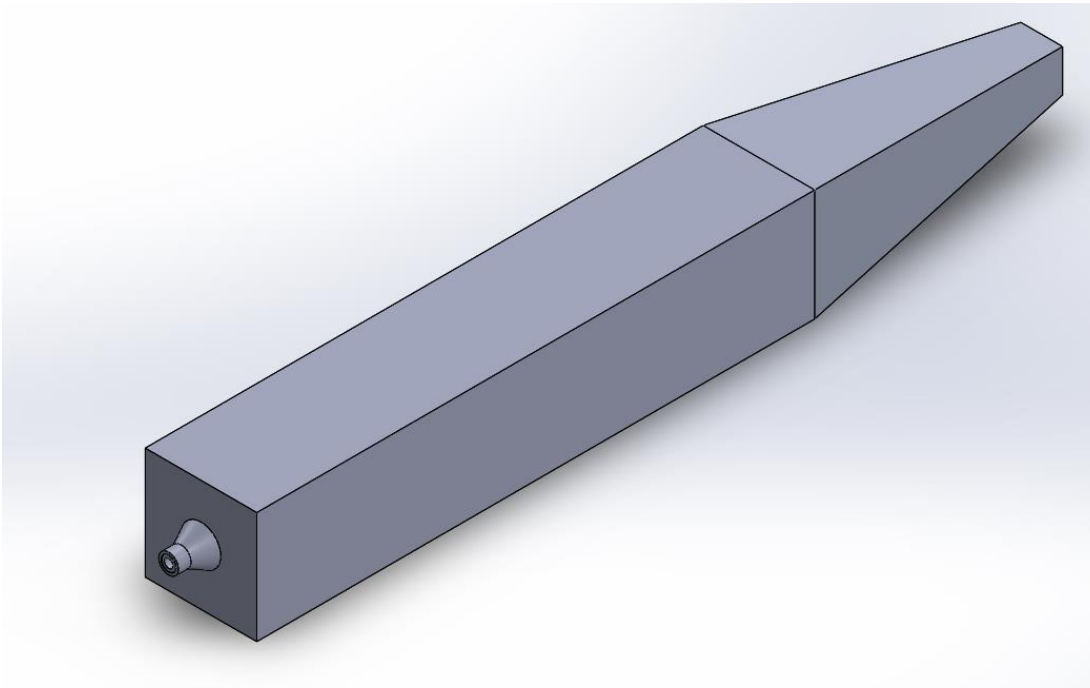


Figure 3: Isometric view of the furnace in Solidworks 2019

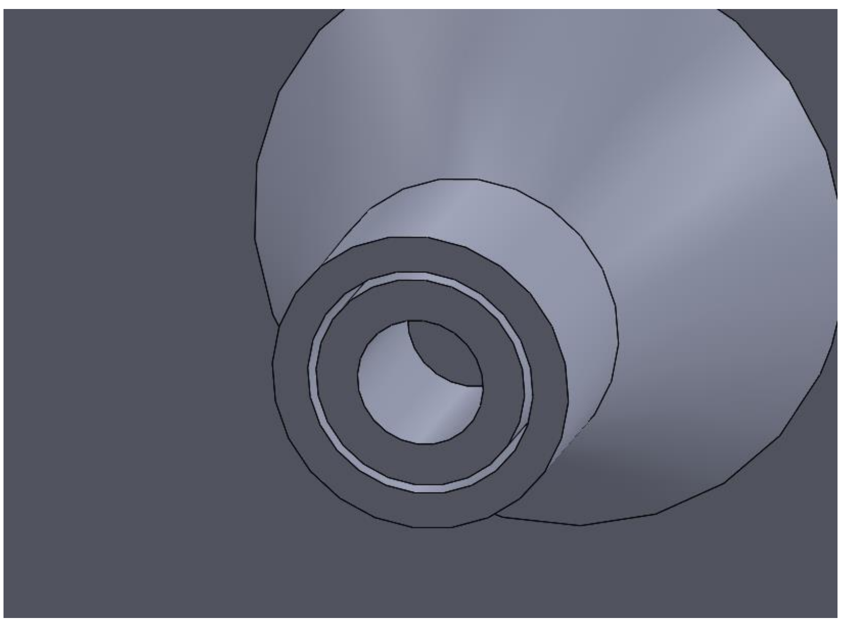


Figure 4: Closeup of the inlet of the burner section

2.2.Mesh

Table 1: Mesh details

Physics preference	CFD
Solver preference	Fluent
Nodes	3478
Elements	15946
Tetrahedral cell	15946

Table 1 shows the details of the mesh used for our simulation. The node number and element number were 3478 and 15946, respectively. Tetrahedral meshing was used, which is the default meshing feature of Ansys.

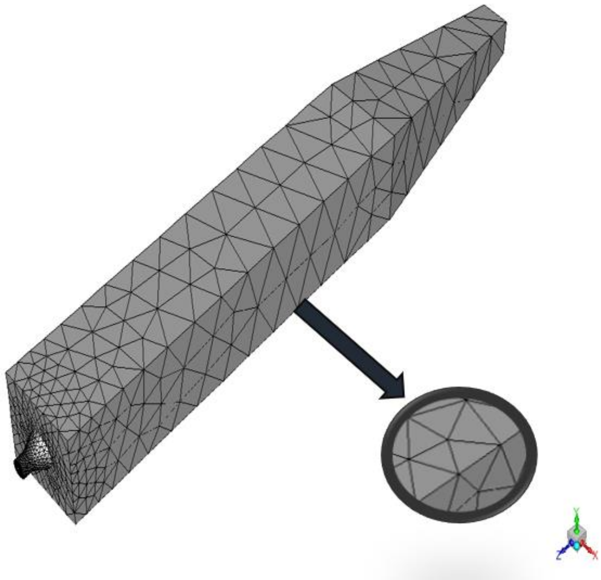


Figure 5: Meshing

Figure 5 shows the tetrahedral mesh elements.

2.3.Chemical Reactions

The chemical reactions considered in this study are given below-

Homogeneous reactions

$CH_4 + O_2 \rightarrow CO_2 + H_2 + H_2O$ + Heat

$CO + H_2O \rightarrow CO_2 + H_2$

Heterogeneous reactions

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

In order to simplify the whole simulation and reduce computation time, the reaction was considered as a single step reaction.

The steps considered for coal combustion:

1. thermal decomposition

2. burnout of the volatile matter

3. oxidation of char

Table 2: Model Formulation

SPATIAL DISCRETISATION	2ND ORDER UPWIND
Pressure formulation	SIMPLE
Gas phase model	Eulerian partial differential equations
Particulate phase model	Discrete droplet method (DDM)
Devolatilisation	Single reaction model
Char combustion	Global power-law
Turbulence	The k-e turbulent model
SOx modelling-char mass fraction	1
Radiation	Discrete transfer radiation method (DTRM)

In table 2, we see the various models used for our simulation in Ansys FLUENT. For turbulence modeling, the k-e turbulent model was used for its success with the relevant studies in the field. In terms of the SOx Modeling, all SOx was assumed to be Char. The

DTRM Radiation model was used, which assumes all radiation leaving the surface element in a certain range of solid angles to be a single ray.

Table 3: Proximate analysis of the coal

Proximate analysis, %wt	
Ash content, %ar	11.98
Moisture content, %ar	6.23
Combustibles, %ar	81.82
Volatile matter, %daf	43.43

Table 4: Ultimate analysis of the coal

Ultimate analysis %wt

Carbon, %ar	65.91
Hydrogen	2.09
Nitrogen, %ar	2.09
Sulphur, %ar	0.34
Oxygen, %ar	8.89
GCV, kJ/kg 27,098	27098

The ultimate and proximate analysis of the coal used for simulation is given in table 3-4.The total amount of combustibles is the sum of the volatile matter and carbon content. The calorific value was also given as an input in the coal calculator of Ansys FLUENT.

Table 5: Kinetics parameters for the particle combustion modelling

Kinetics parameters	Pre-exponential factor Ac	Activation energy Ec
Devolatilisation	$4.2 * 10^{14}\ s^{-1}$	230 ($kJ\ mol^{-1}$)
Char oxidation	497 ($kg\ m^{-2}\ s^{-1}\ (N\ m^{-2})^{-1}$)	155 ($kJ\ mol^{-1}$)

The kinetic parameters are shown in table 5. For our model, we input the Char oxidation parameters.

2.4. Boundary Conditions

Table 6: Inlet Boundary Conditions

Flow parameters	**Primary Flow**
Mass flow, kg/h	110
Temperature, K	343
O2 concentration, (kg/kg)	23.15
Coal supply, kg/h	68
Flow parameters	**Secondary flow**
Mass flow, kg/h	620
Temperature, K	543
O2 concentration, (kg/kg)	23.15

The inlet boundary conditions for the primary and secondary flow is given in table 6. The O_2 concentration of the species is given and the remaining species is assumed to be Nitrogen.

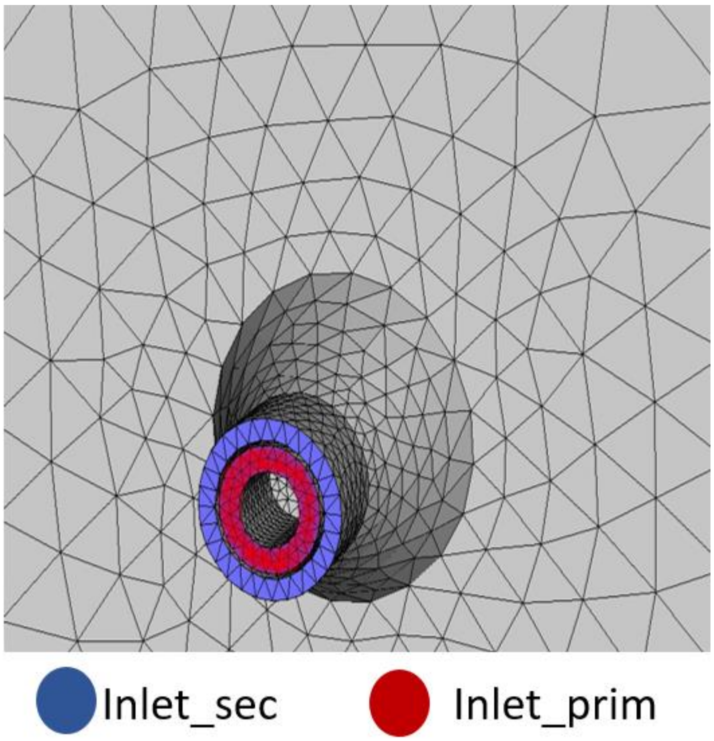


Figure 6: Primary and Secondary air inlets

Figure 6 shows the primary and secondary air inlets.

Outlet Boundary Conditions

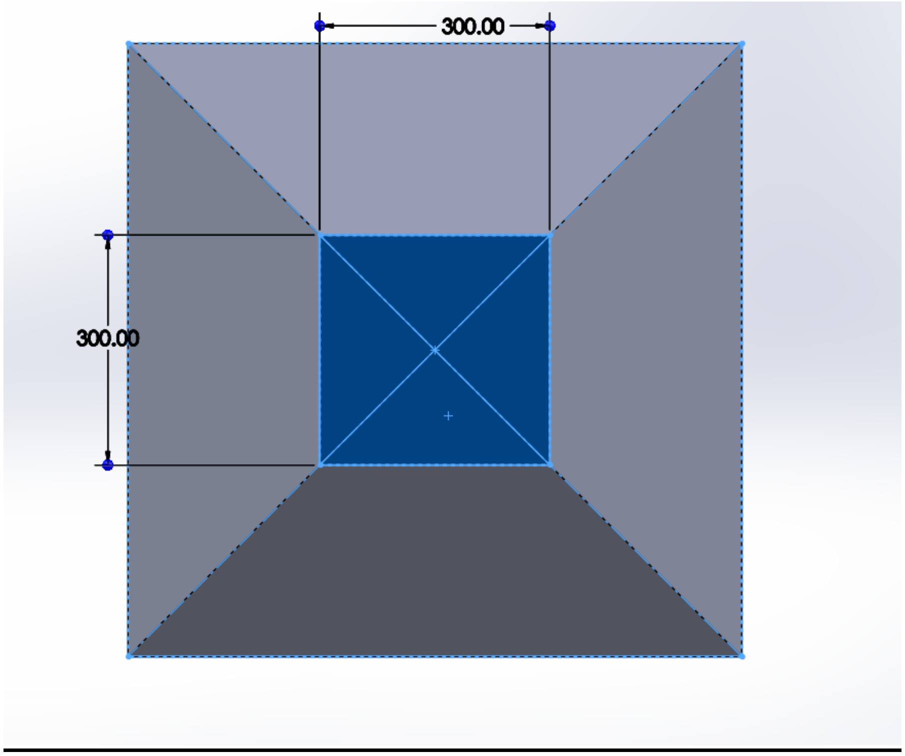


Figure 7:Outlet surface

Figure 7 shows the outlet surface of the geometry used.

A zero pressure gradient was applied at the outlet of the furnace for all variables.

2.5.Particle size distribution

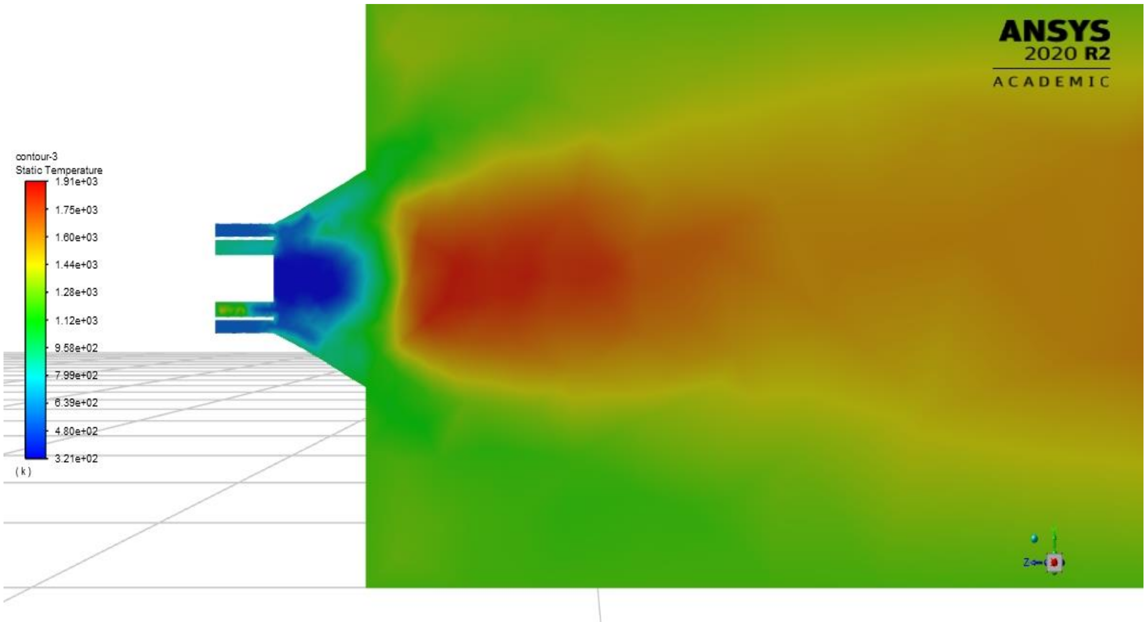
Coal particles are injected at a flow rate of 68kg/h along with the primary air.The injection time was set as 1000s.

Russian pulverized high volatile bituminous coal was used as fuel and the calorific value was considered 27,098 kJ/kg. The particle sizes were considered 75–300 μm with d_{min}=75 μm and d_{max}=300 μm. Considering the number of the particles, d_{mean}=75 μm was considered and given as input.

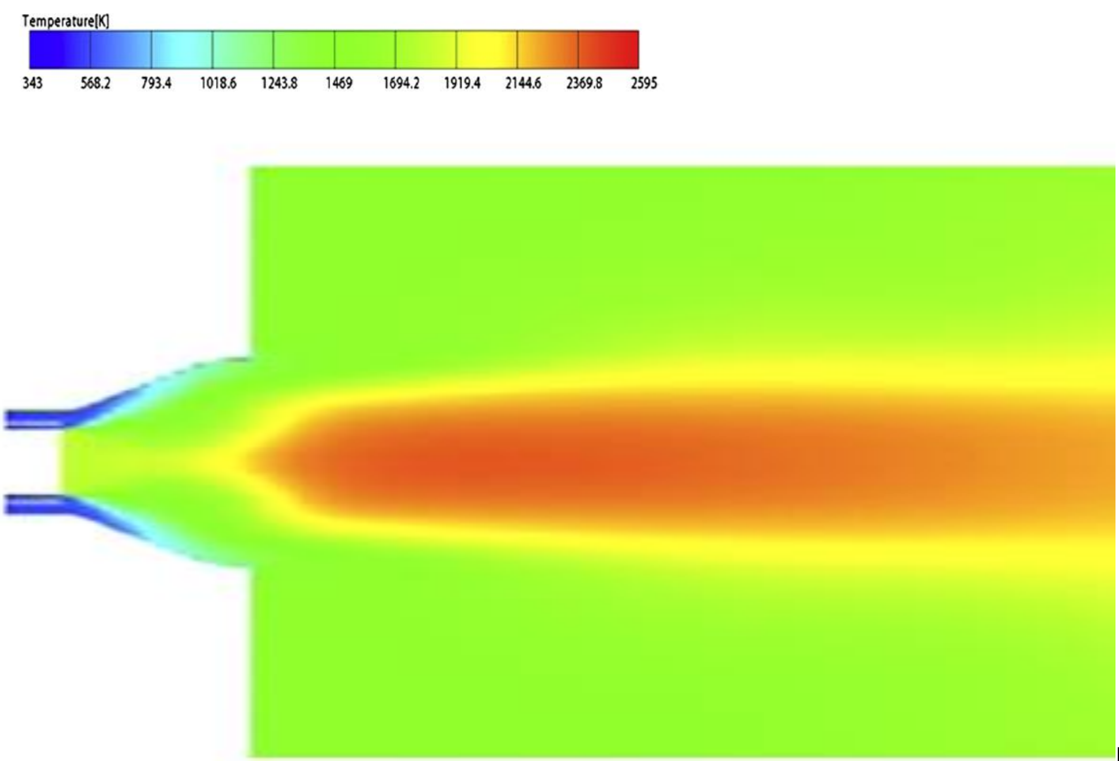
2.6. Numerical descriptions

Commercial CFD Tool Ansys FLUENT (version 2020R2) is used to solve the 3 dimensional governing equations. The SIMPLE pressure formulation is used, which uses a relationship between velocity and pressure corrections to enforce mass conservation in order to obtain the pressure far fields. The value 10^{-4} was considered absolute residuals. The time step size was given as 0.01 and the simulation was run till a quasi-steady state was achieved. The second order upwind scheme was used for almost cases. Standard initialization was done setting temperature as 800K in all the zones, which helps to achieve the steady state.

3.Model Validation:



(a)



[7]

(b)

Figure 8: Comparison between the temperature contours of the a)present study and b) Bhuiyan et al.

From the temperature contour in figure 8 we see that the highest temperature achieved in the model used by Bhuiyan et al. was around 2100K and the simulation was done in AVL Fire ver.2009.2. The highest temperature we were able to achieve using our model was around 1900K, which was reasonably close to the temperature achieved by Bhuiyan et al. We used Ansys FLUENT (version 2020 R2) for our simulation and the slight discrepancy of the temperature could be caused by a number of factors- use of a different software, meshing, simulation run time, coal composition etc.

4. Results and Discussion

4.1. Air Fired Case

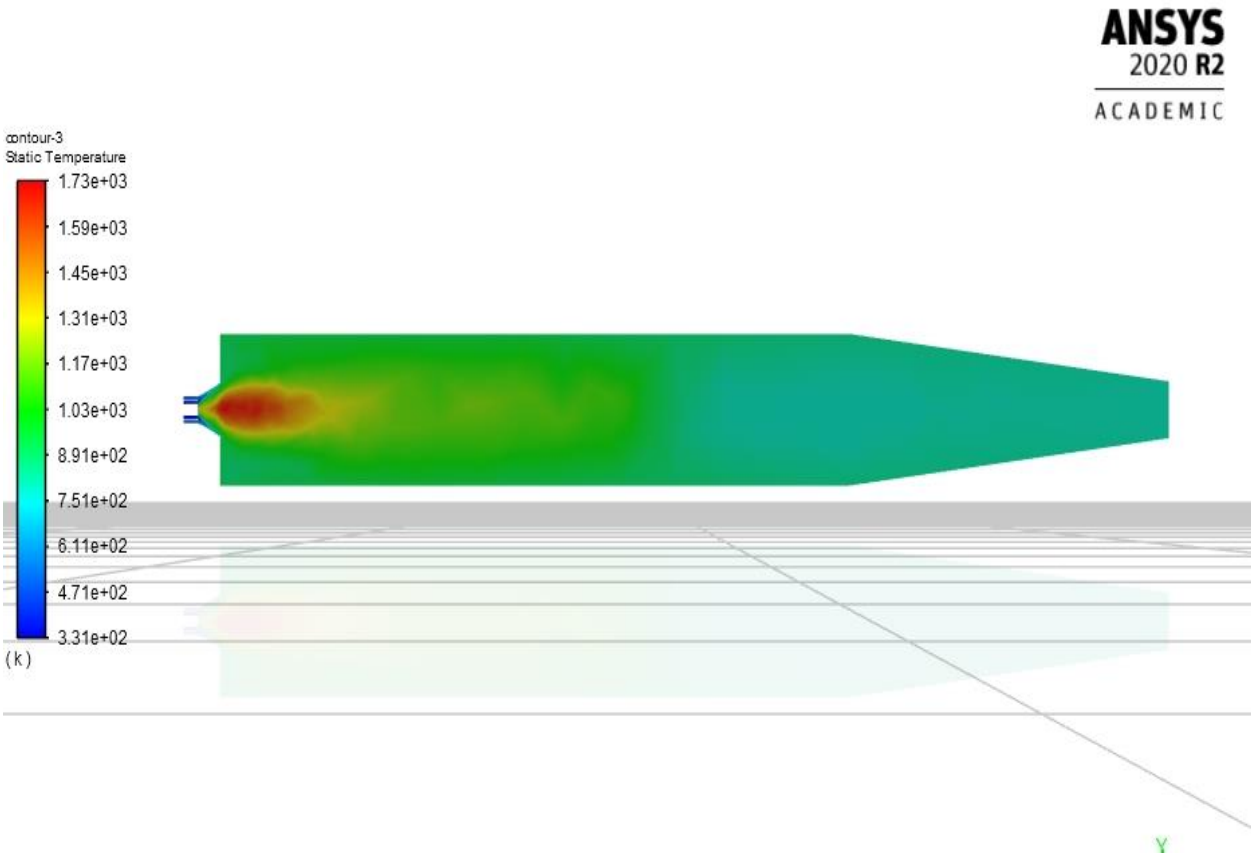


Figure 9: Static Temperature Contour (Air Fired)

In case of air fired combustion, after supplying the primary and secondary air through the inlets, a flame with very high temperature has been seen in the vicinity of the burner. This is an evidence of combustion. The temperature contour in the Figure depicts the highest temperature inside the furnace as 1730K.Moving towards the furnace outlet, the temperature decreases gradually.The lowest temperature is achieved near the furnace outlet.

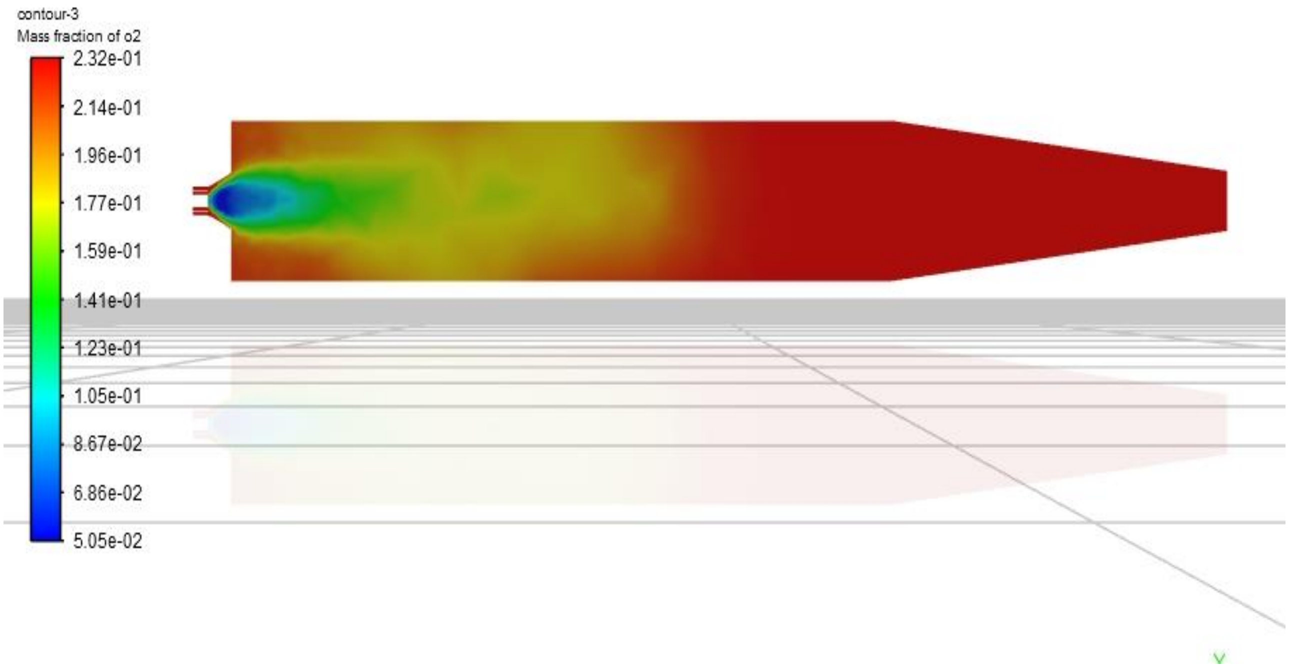


Figure 10: Species Contour Of Oxygen (Air fired)

Figure 10 shows the mass fraction of oxygen inside the furnace. When the combustion takes place, the available mass fraction of oxygen drops drastically. The lowest mass fraction of oxygen is in the flame region as the available oxygen in that location is burnt for combustion to produce the highest temperature. Moving towards the furnace outlet, an increase in the mass fraction of oxygen is noticed. The highest mass fraction of oxygen inside the furnace is around 2.32e-01.

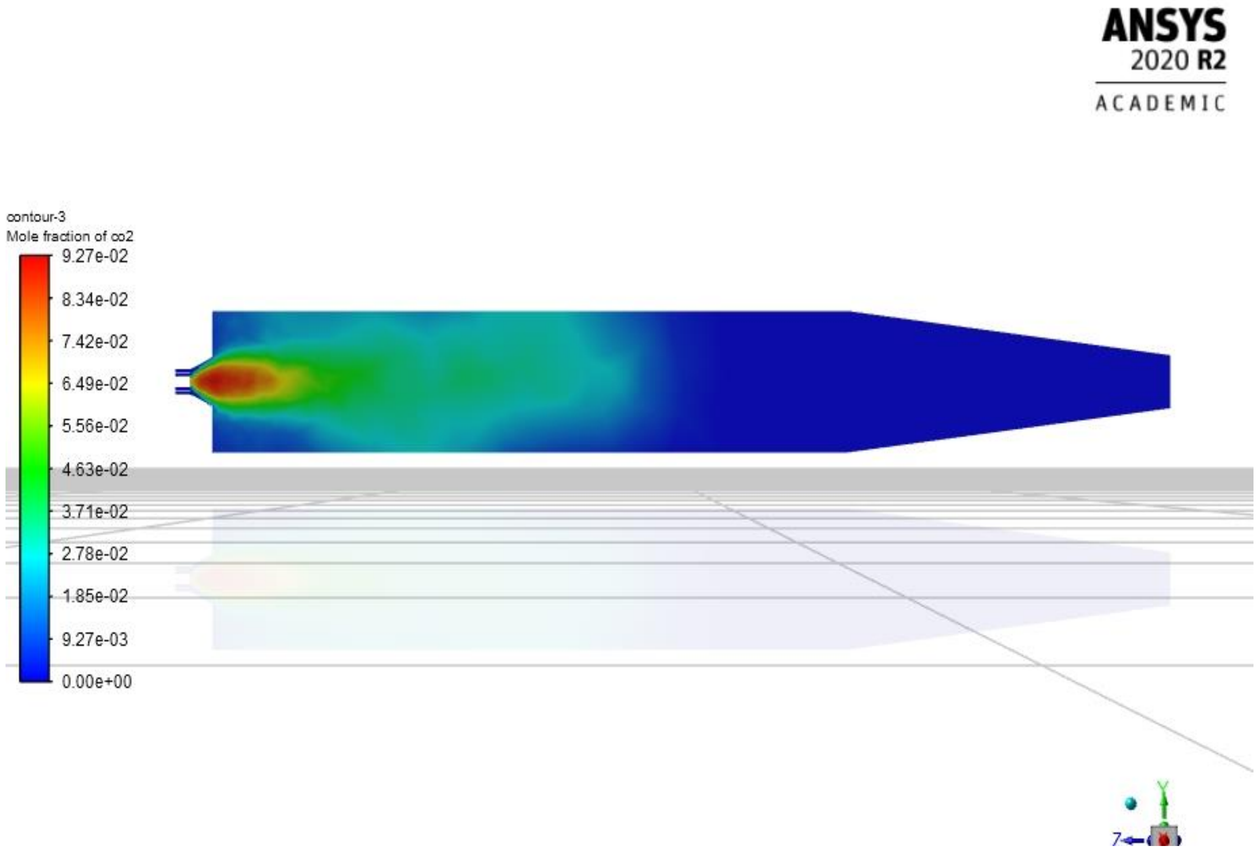


Figure 11: Species Contour of Carbon di-Oxide

The species contour of carbon di-oxide exhibits the amount of carbon di-oxide produced in the furnace due to combustion. Figure 11is showing the amount of CO_2 in mole fraction. As the combustion takes place in the flame region, the highest amount of CO_2 is produced. The highest mole fraction inside the furnace was around 9.27e-02. Right after the combustion the mole fraction of CO_2 gradually decreases towards the furnace outlet. The decreasing amount of carbon di-oxide has been seen because of unburnt oxygen available in those parts of the furnace.

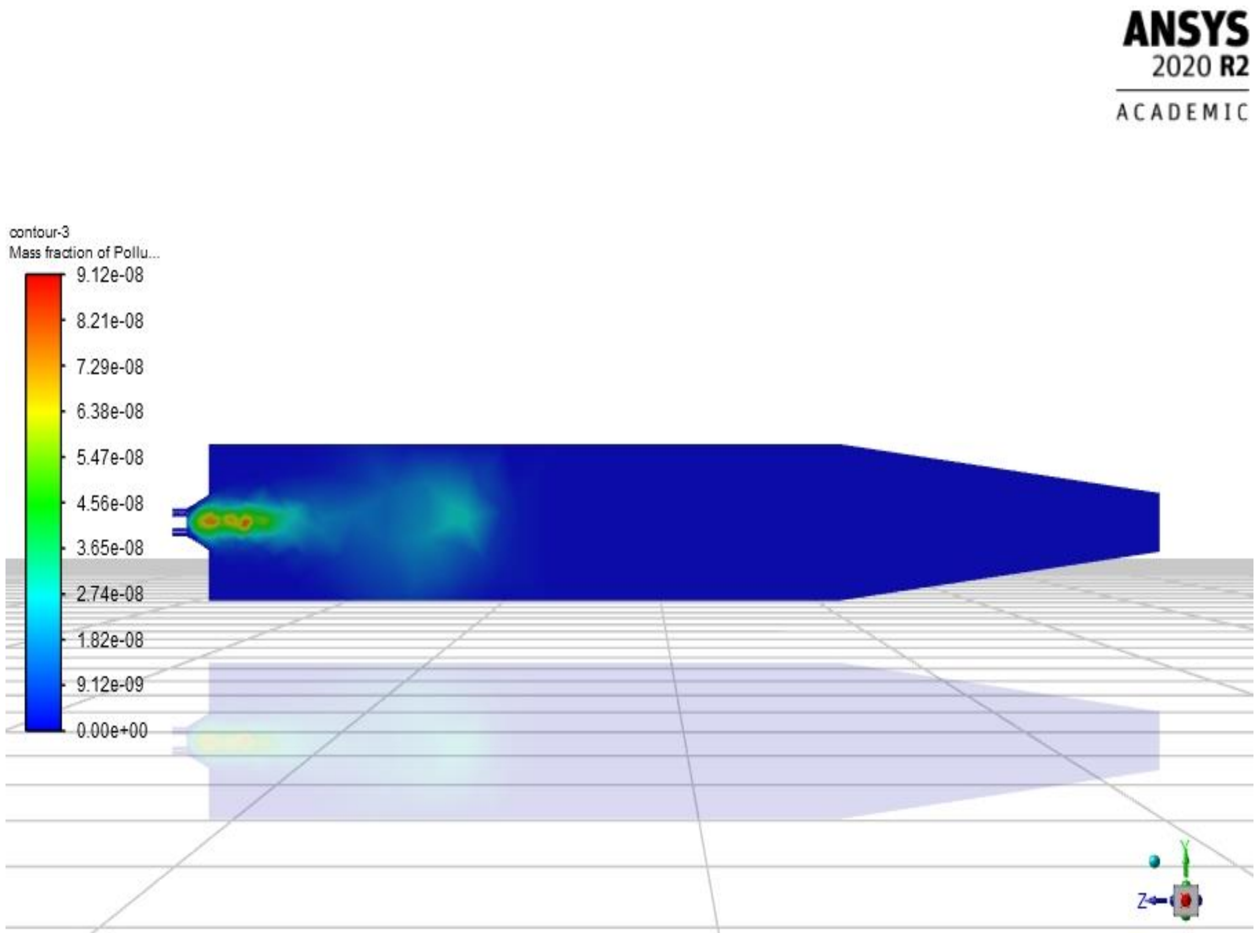


Figure 12: Mass fraction Contour of NOx (Air Fired)

Figure 12 shows the mass fraction contour of NOx produced from combustion inside the furnace. NOx is one of the major pollutants resulting from combustion. The nitrogen from the supplied air and the pulverized coal particles reacts with the oxygen when the temperature is significantly high. Thus thermal NOx is produced in the flame region. That's why,In the Contour, we can see the highest amount of NOx in the flame region where the combustion takes place. It's evident that with increasing temperature, NOx increases. In our case, the highest mass fraction of NOx produced from combustion was around 9.12e-08. Formation of NOx is also an evidence of successful combustion.

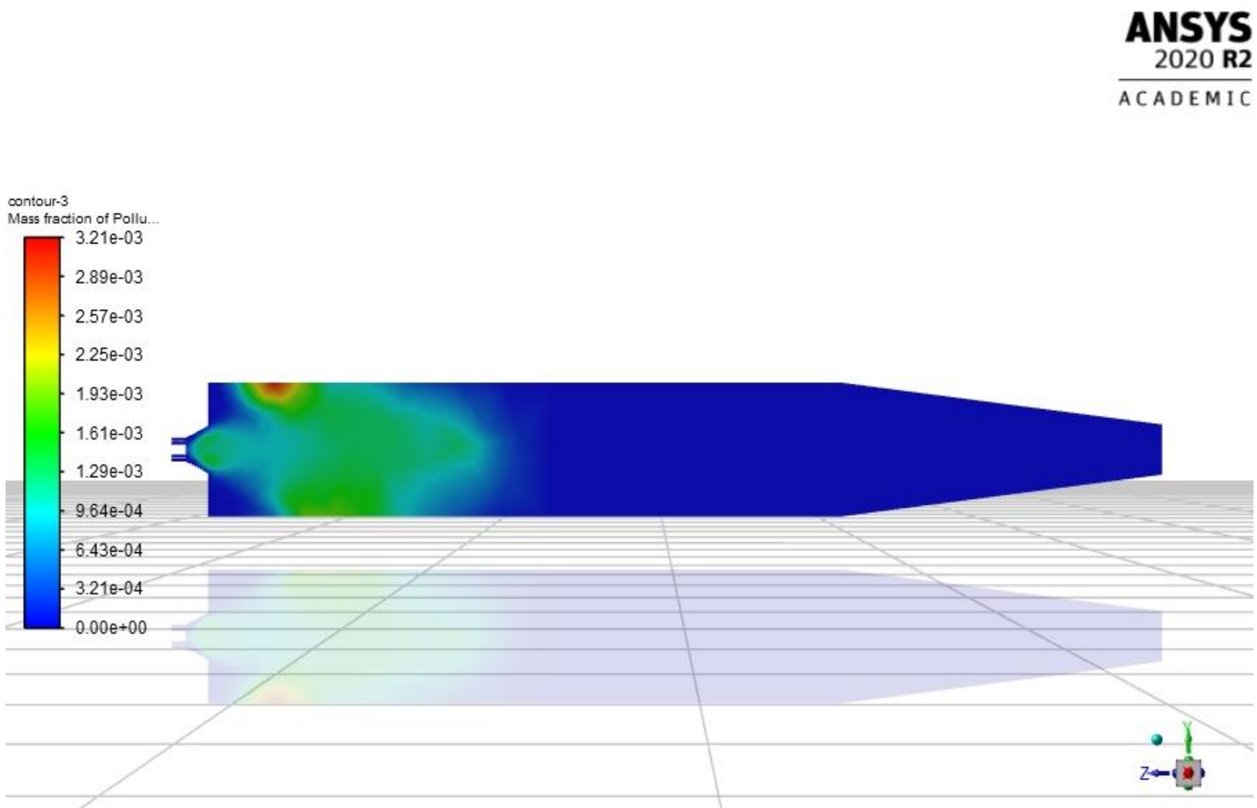


Figure 13: Mass fraction of SOx (Air fired)

Figure 13is showing the mass fraction contour of SOx in case of air fired combustion. SOx is one of the major pollutants resulting from combustion. When combustion takes place , the sulfur content of the pulverized coal reacts with the oxygen. Thus SOx is produced and it’s one of the major components of the flue gas. Figure depicts the formation of SOx inside the furnace in the flame region. This formation of SOx is an evidence of successful combustion and the highest mass fraction that has been noticed was around 3.21e-03.

4.2. 65% RR Case

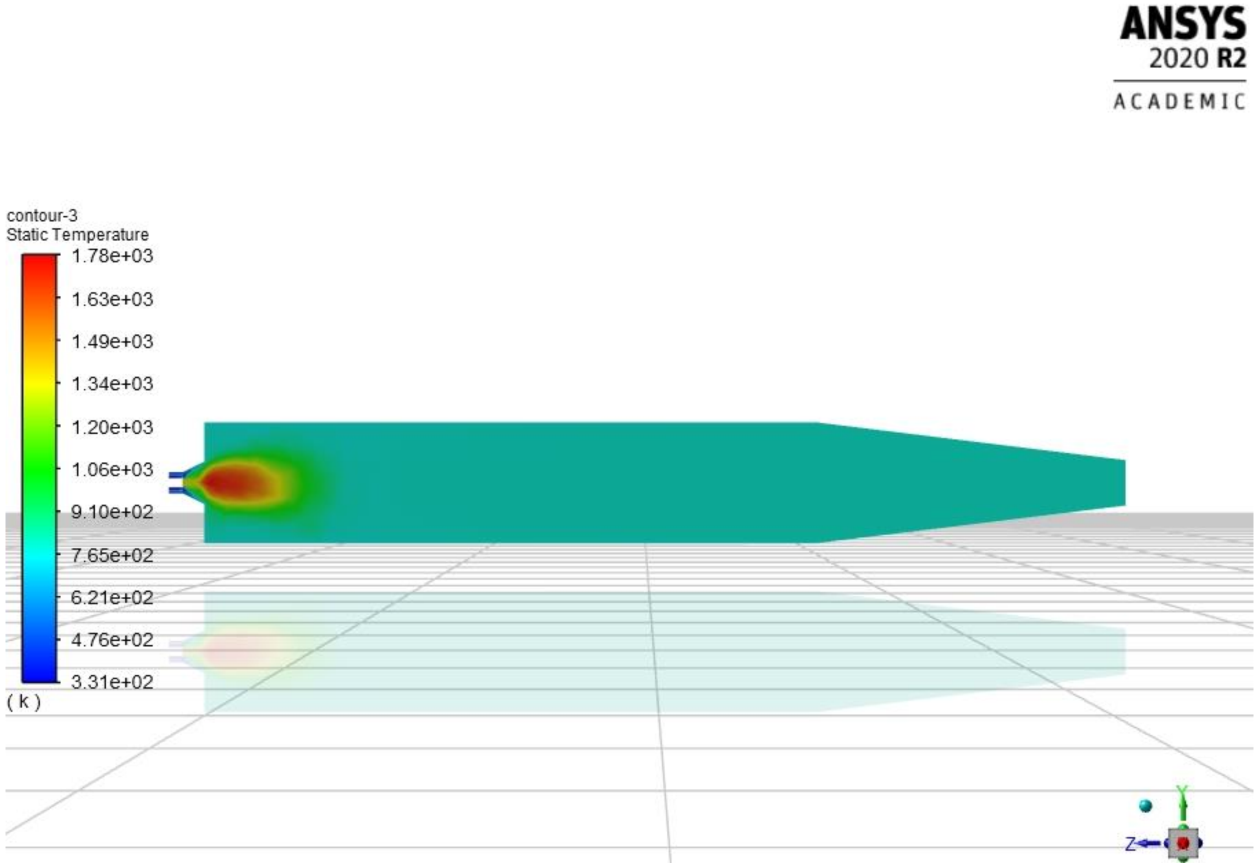


Figure 14: Temperature Contour (65% RR)

Figure 14shows the temperature contour in case of 65% recirculation ratio of the flue gas. The temperature contour for 65% recirculation ratio is comparable to the temperature contour of once through air fired combustion. There has not been any significant change in the flame shape or in combustion region and temperature.

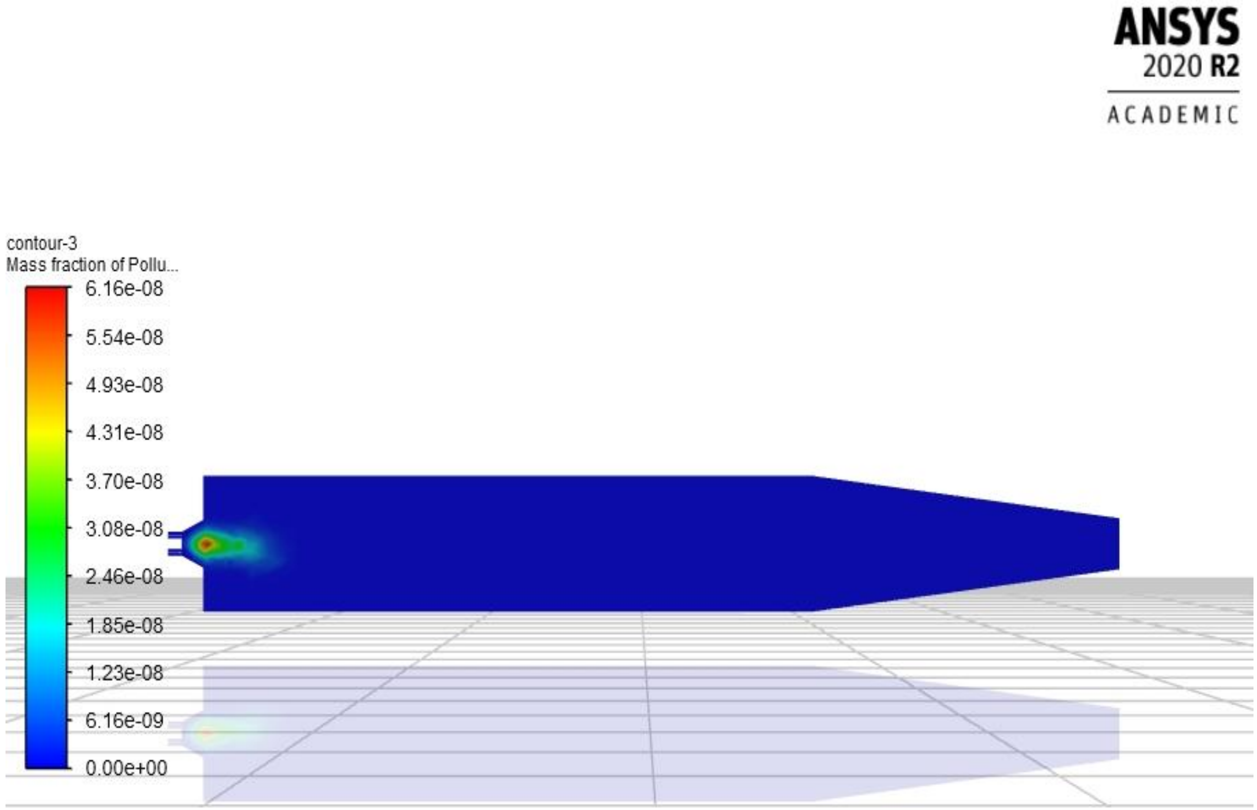


Figure 15: Mass fraction contour of NOx (65% RR)

Figure 15exhibits the mass fraction contour of NOx in case of 65% recirculation ratio of the flue gas. After recirculating the flue gas, significant changes have been noticed in case of NOx formation. The contour shows the maximum mass fraction of NOx as 6.16e-08. It’s evident that after recirculating the flue gas, the formation of NOx which is one of the major pollutants of combustion reduces significantly. The reduction of NOx formation results from lesser amount of nitrogen in the inlet as we are recirculating flue gas through the inlet which is mostly carbon di-oxide.

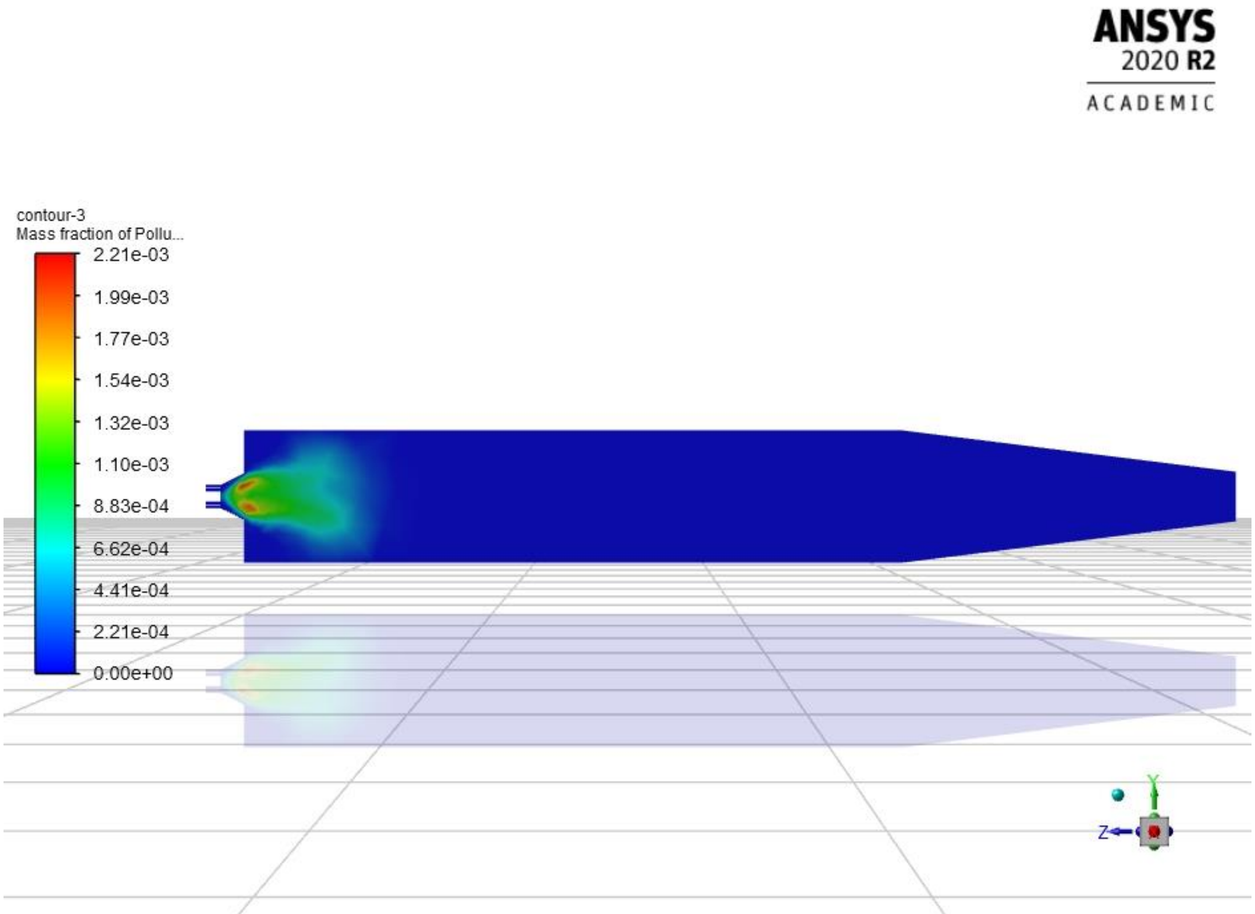


Figure 16: Mass fraction contour of SOx (65% RR)

Figure 16shows the mass fraction contour of SOx with recirculation ratio of 65%. After recirculating the flue gas, the formation of SOx in the flame region ensures that successful combustion. There has not been any drastic change in case of SOx formation. A slight decrease in SOx formation has been noticed when we recirculated the flue gas through the inlets. The highest mass fraction is in the flame region and the contour shows the maximum mass fraction value of SOx with 65% RR as 2.21e-03.

4.3. 76.85% RR Case

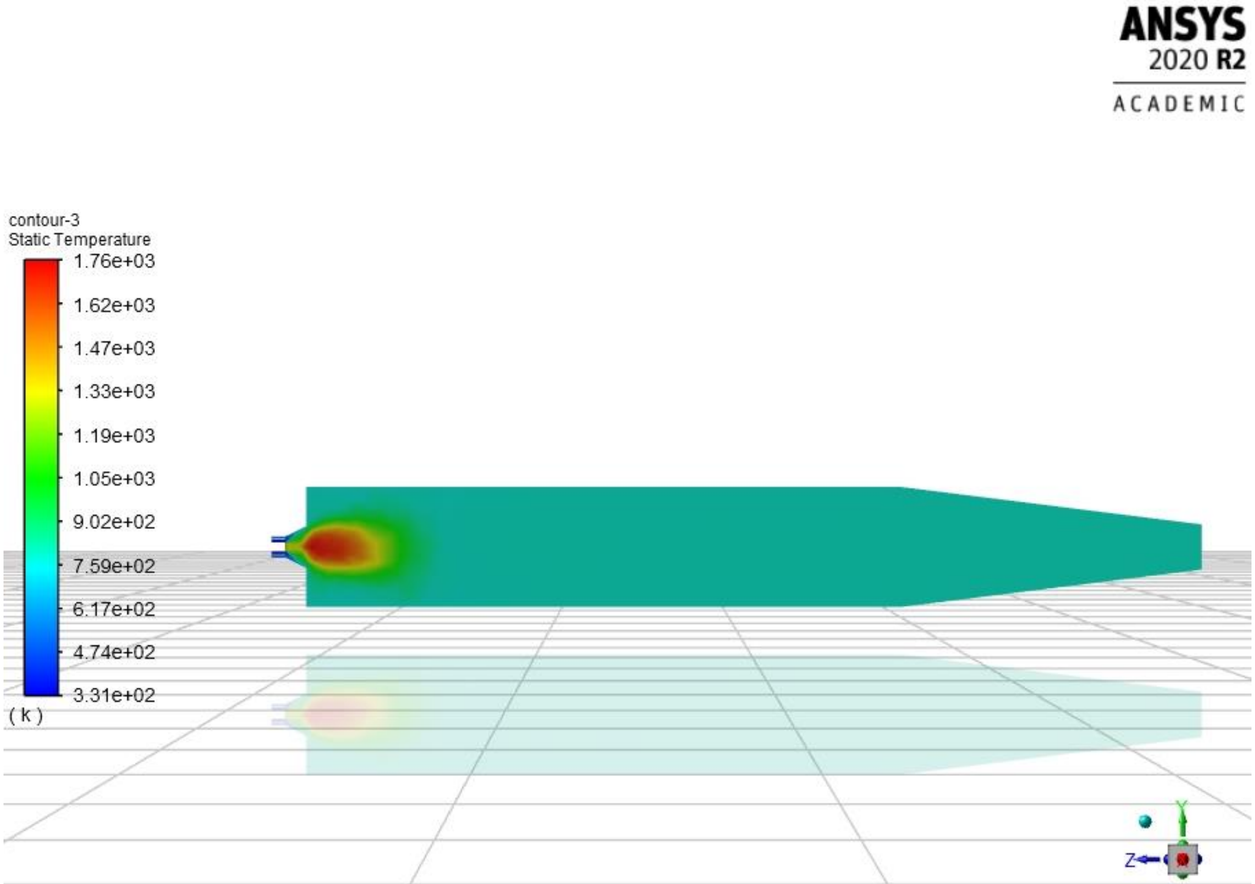


Figure 17: Temperature contour (76.85% RR)

Figure17depicts the temperature contour when recirculation ratio of the flue gas is 76.85%. It's been noticed that the temperature contour with 76.85% RR is comparable to the previous temperature contours of once through combustion and of combustion with 65% RR. There has not been any drastic change noticed in the static temperature contours. In case of flue gas recirculation the flame shape and high temperature are signs of successful combustion inside the furnace.

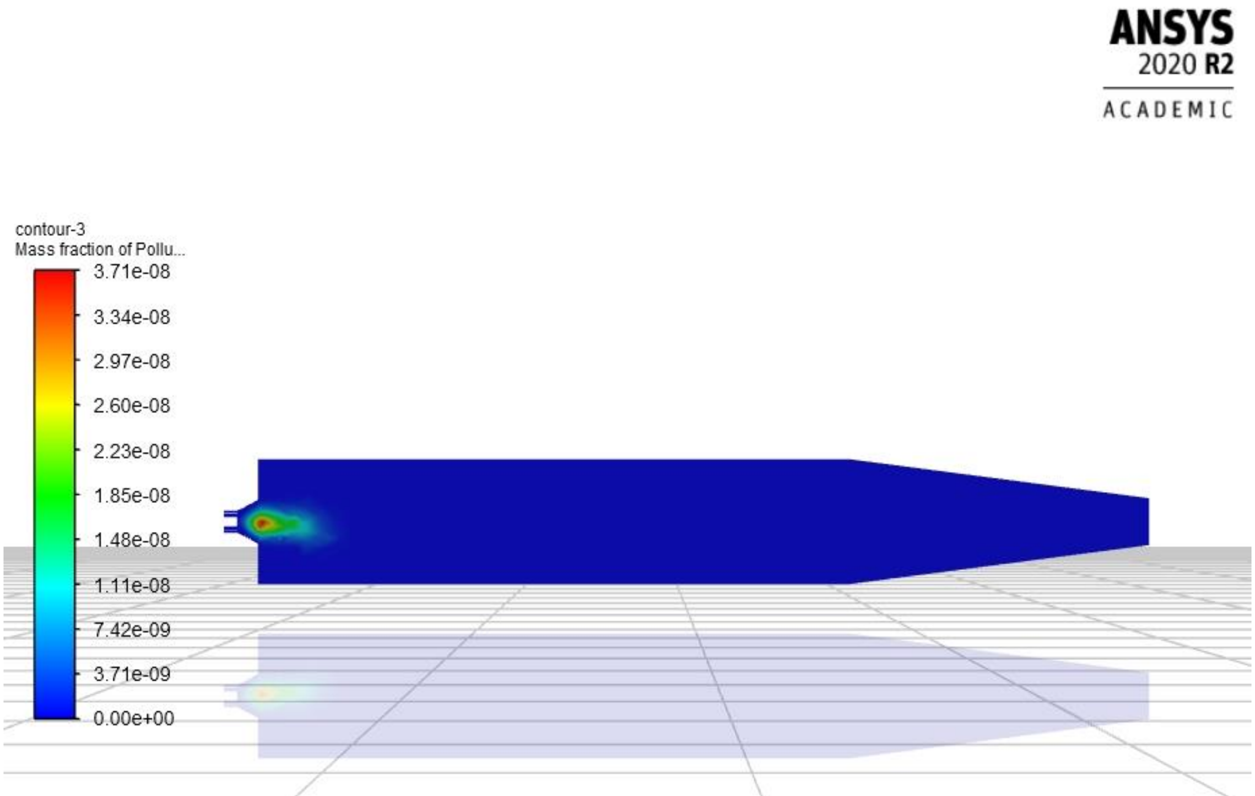


Figure 18: Mass fraction contour of NOx (76.85% RR)

Figure 18exhibits the mass fraction contour of NOx when the recirculation ratio is 76.85%. A significant effect of recirculating the flue gas on the mass fraction of NOx emission has been noticed. With the increasing recirculation ratio , the mass fraction of NOx emission decreases. In the contour, the maximum mass fraction of NOx is shown as 3.71e-08 which is lesser in amount than the previous cases. As the recirculation ratio is increased, the availability of nitrogen is decreased in the inlets. The flue gas which is mostly carbon di-oxide causes the reduction of NOx in the furnace. The contour shows the highest amount of NOx in the flame region as we know that with increasing temperature , emission of NOx increases. The highest mass fraction of NOx depicted by the contour is 3.71e-08.

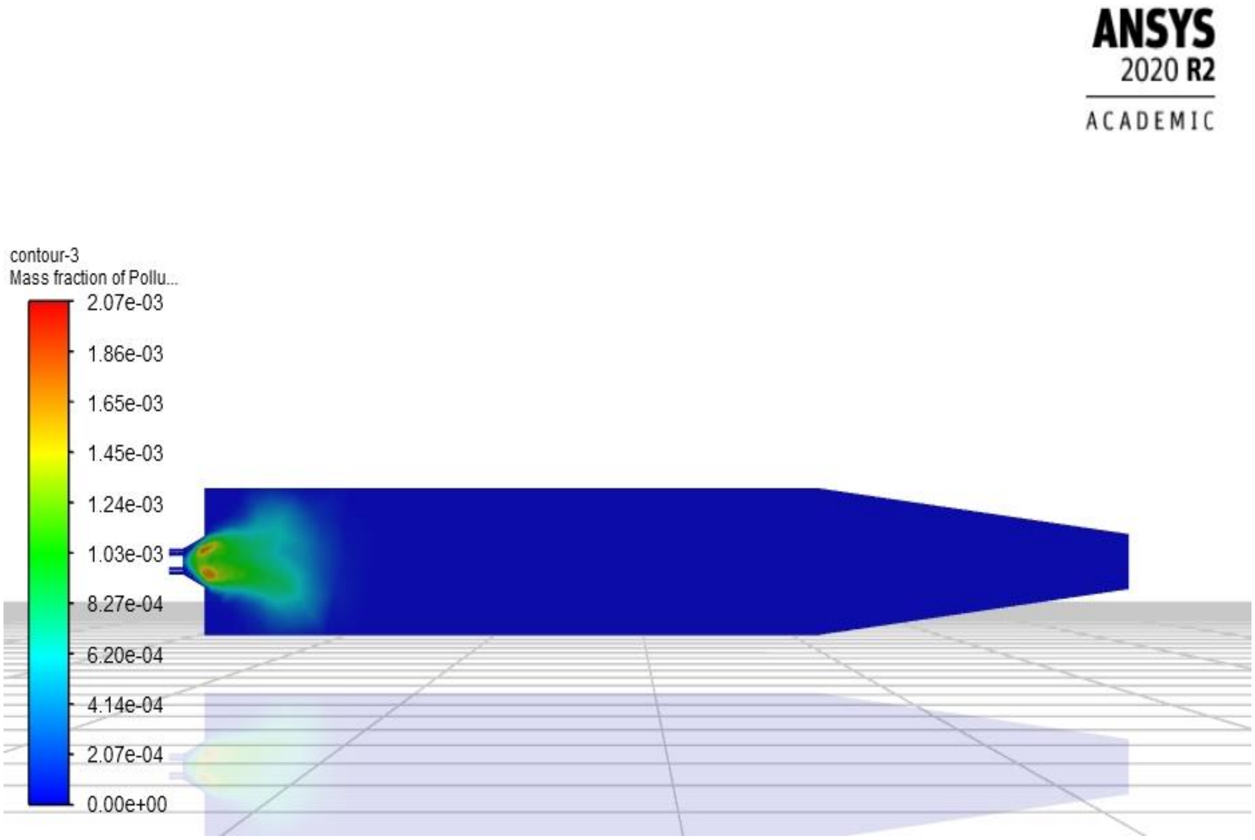
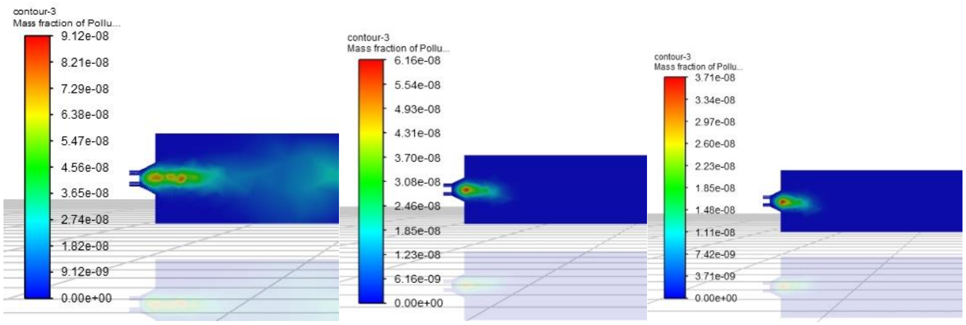


Figure 19: Mass fraction contour of SOx (76.85% RR)

Figure 19 shows the mass fraction contour of SOx when the recirculation ratio of 76.85%. SOx is one of the main pollutants of combustion which basically results from the sulfur content of the pulverized coal.Even though there is not any drastic change in the mass fraction contours of SOx ,with different recirculation ratio, very slight changes have been noticed. The recirculation of flue gas slightly decreases the SOx formation. A value of 2.07e-03 has been shown as the highest mass fraction value of SOx.

4.5. Comparison between NOx contours



Air Fired 65% RR 76.85% RR

Figure 20: Side by Side Comparison of the NOx Contour

We have worked on three different cases: once through air fired combustion, combustion with 65% RR and combustion with 76.85% RR. In case of air fired once through combustion, the mass fraction of NOx is 9.12e-08. With 65% RR it comes down to 6.16e-08 and with 76.85% RR it further decreases and comes down to 3.71e-08. From this, it is evident that recirculation flue gas reduces the NOx emission during combustion. With increasing recirculation ratio, the NOx emission decreases because of the unavailability of nitrogen in the inlets. As flue gas is mainly carbon di-oxide, the formation of NOx reduces significantly because of flue gas recirculation.

5. Conclusion:

From our research, we have come up with the following conclusions:

1. Recirculation of flue gas reduces NOx emissions significantly. When the RR is 65% , NOx emission is reduced by 32.46% and when the RR is 76.85%, the NOx emission is reduced by 59.32%.
2. Recirculation of flue gas reduces CO_2 emission as we are recirculating the flue gas without releasing it into the atmosphere.
3. Flue gas recirculation slightly reduces SOx emission.
4. Achieved combustion temperatures are comparable in all cases.

6. Recommendations:

In the future we suggest the following improvements to get more accurate results-

1. In the future, we want to use finer mesh where the temperature gradient is most significant. We want to achieve mesh independent result in order to save computational time and power without compromising the accuracy. We also want to incorporate symmetric grid.
2. We also hope to run the simulation for a longer period of time to achieve better and more accurate results.
3. We want to measure the NOx and SOx emission for different RR with an aim to finding the optimum RR to fulfill two conflicting objectives, increasing combustion efficiency and reducing NOx and SOx emission.

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