Prediction of Flue Gas Composition in Coal Combustor: CFD Approach

Deeksha Gupta*, Dr. S Prasad**

*PG Scholar, Madhav Institute of Technology & Science, Gwalior (MP)
**Associate Professor, Department of Chemical Engineering, M.I.T.S. Gwalior (MP)

Abstract: **The present work is based on the software ANSYS FLUENT Workbench 15.0. This approach aims to provide an improved prediction of flue gases composition from combustion of pulverized coal when the coal was injected pneumatically. The mathematical models used for the combustion of pulverized coal includes realizable K-ε model for turbulent flow, species transport model and discrete phase model. For the purpose of simulating the combustion process, 2D mesh was adapted. The composition of O_2 and CO_2 is good agreement with literature.**

Key Words :CFD, pulverized coal, speciestransport model

I. INTRODUCTION

Reliable, efficient and clean energy supply is one of the basic needs of humankind. Today our energy supply system is under-going a long term transition from its conventional form to a more sustainable and low carbon style, especially addressing greenhouse gas (H_2O, CO_2, CH_4, Nitrogen oxide, CFC & aerosol) emissions into the atmosphere.

Pulverized coal is an important fuel for electricity production and will continue to be important for decades. [1]

Pulverized coal combustion is a very complicated physical and chemical process, which is related to gaseous turbulent two-phase flow involving solid particles, homogenous gaseous reactions, heterogeneous surface reactions, radiation heat-transfer, etc. [2]Combustion chamber designers endeavor to achieve optimum operating conditions that give maximum combustion efficiency together with minimum pollutant formation rate. [1]

The application of CFD technology and other advanced mathematical methods offer opportunities for analysis, optimization and options examination in order to increase the overall efficiency of the energy facilities. This method, in which the governing equation of the combustion field are developed using a computer is capable to provide the detailed information on the distributions of temperature and chemical species and the behavior of pulverized coal particles over entire combustion field that cannot be obtained by experiments. In addition, it facilitates the repeated review in arbitrary conditions for the properties of pulverized coal and the flow field at a relatively low cost. It is therefore strongly expected that the CFD becomes a tool for the development and design of combustion furnaces and burners.

II. MECHANISM OF COMBUSTION OF PULVERIZED COAL

The ignition temperatures of the naturally occurring solid fuels, namely, wood, peat, lignite, coal, etc. are appreciable higher than the initial temperature of active decomposition. These fuels also contain appreciable quantities of moisture. Therefore, they undergo drying and decomposition before actual combustion takes place. The volatile matter, thus evolved, contains combustible gases, vapors, and also minute droplets of tarry substances. The combustion of these solid fuels consequently involves the combustion of the volatile matter and the combustion of the solid carbonaceous residue. The composition of the volatile matter and hence its burning process, varies widely. The residue is essentially carbon. However, its reactivity depends on the type of fuel and hence its ignition characteristics also vary. The flame of a solid fuel is due to the combustion of the volatile matter and the carbon monoxide produced during the combustion of carbon. The visible indication of the combustion of carbon is a bright glow of the burning piece.

Carbon furnishes a typical case of heterogeneous combustion, i.e. combustion between two different phases. The fuel is in the solid state and the oxidant in the gaseous state. This heterogeneous process has two basic components: *(i)* delivery of the gaseous reactant to the surface of the solid by diffusion and *(ii)* chemical reaction of the solid and gas at the surface.

The combustion of pulverized fuel is simulated by the combustion of carbon particles; the overall kinetics of a single particle is given by

$$\frac{1}{R_t} = \frac{1}{k_0 p_o} + \frac{1}{k_2 p_o} \qquad (i)$$

Where,

$$k_0 = \frac{D}{r}$$

This bears out the enormous effect of size reduction in accelerating the process. [4]

III. PROBLEM DESCRIPTION

The problem description was as following:
The coal combustion system considered in this problem is a simple 10m×1m two-dimensional duct as shown in Figure1. Only half of domain width is modeled because of symmetry. The inlet of the 2D duct is split into two streams. A high-speed stream near the center of the duct enters at 50 m/s and spans 0.125 m. The other stream enters at 15m/s and spans 0.375 m. Both streams are air at 1500 K. Coal particles enter the furnace near the center of the high-speed stream with a mass flow rate of 0.1 kg/s (total flow rate in the furnace is 0.2 kg/s). The duct wall has a constant temperature of 1200 K. The Reynolds number, based on the inlet dimension and the average inlet velocity is approximately 100,000. Thus the flow is turbulent.

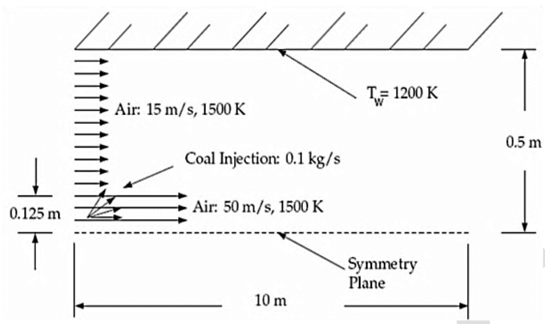

Figure 1: Problem Schematic

IV. COMPUTATIONAL APPROACH

A medium volatile coal was combusted for which the proximate and ultimate analysis was given in Table 1 & 2.

Table 1: Proximate Analysis (%)

Moisture	0.6-1.5
Ash	18-42
Volatile	17-28
Fixed Carbon	50-60

Table 2: Ultimate Analysis (%)

C	90-93
H	5.4-5.8
O	3.9-7.5
N	1.7-2.2
S	0

The governing equations used in the simulation of pulverized coal combustion process were taken as below:

- *K-$\mathcal{E}$ equation for air flow:*

$$-\rho u_i u_j = \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3}\left(\rho_k + \mu_t \frac{\partial u_k}{\partial x_k} \right)$$

- *Energy Equation:*

$$\frac{\partial \bar{T}}{\partial t} + \bar{u}\frac{\partial \bar{T}}{\partial x} + \bar{v}\frac{\partial \bar{T}}{\partial y} + \bar{w}\frac{\partial \bar{T}}{\partial z} = \alpha \left(\frac{\partial^2 \bar{T}}{\partial x^2} + \frac{\partial^2 \bar{T}}{\partial y^2} + \frac{\partial^2 \bar{T}}{\partial z^2} \right) - \left(\frac{\partial \overline{u'T'}}{\partial x} + \frac{\partial \overline{v'T'}}{\partial y} + \frac{\partial \overline{w'T'}}{\partial z} \right)$$

- *RANS continuity equation:*

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = 0$$

V. PROCEDURE OF COMPUTATION

The simulation of pulverized coal was carried out using ANSYS FLUENT 15.0.The solving procedure is based on a fully conservative structured finite volume formulation employing Cartesian vector and tensor components. Equations deduced for the models are solved. The rate of production of volatile gases is given by a 1st order reaction and the rate constant is expressed in an Arrhenius form.

Discrete phase model was used to model the discrete phase of coal particles. Then we set the properties for our combusting particle and the data is tabulated as following:

Table 3: Coal parameters

Parameter	Value
Density (kg/m^3)	1300
C_p(j/kg-K)	1000
Volatile Component Fraction (%)	28
Binary Diffusivity (m^2/s)	5e-4

- *Boundary Conditions:*

Once the problem was defined, the establishment of the boundary conditions is required. The necessary boundary conditions for the present simulation were taken as given in the table 4, 5, 6 and 7.

1. Boundary Conditions for Primary Inlet

Table 4: Primary Inlet Parameters

Parameter	Value
Velocity Magnitude	50 (m/s)
Specification Method	Intensity & Hydraulic Diameter
Turbulence Intensity	10%
Hydraulic Diameter	0.75 m
Temperature	1500 K
Species mass fraction	$O_2 = 0.23$

2. Boundary Conditions for Secondary Inlet

Table 5: Secondary Inlet Parameters

Parameter	Primary inlet-1	Primary inlet-2
Velocity Magnitude	20 (m/s)	15 (m/s)
Specification Method	Intensity & Hydraulic Diameter	Intensity & Hydraulic Diameter
Turbulence Intensity	5 %	5 %
Hydraulic Diameter	0.25 m	0.25 m
Temperature	1500 K	1500 K
Species mass fraction	$O_2 = 0.23$	$O_2 = 0.23$

3. Boundary Conditions at Wall

Table 6: Wall parameters

Temperature	1200

4. Boundary Conditions at Outlet

Table 7: Outlet Parameter

Parameter	Value
Specification Method	Intensity & Hydraulic Diameter
Backflow Turbulence Intensity	5%
Backflow Hydraulic Diameter	1 m
Backflow Total Temperature	2000 K

VI. RESULTS & DISCUSSION

The parameter was computed by ANSYS FLUENT 15.0 by varying the excess air is given in the table 8 and 9.

Table 8: Excess air parameters

Secondary air (m/s)	Excess air (%)
20	40
15	12.5

Resultant figures are obtained at 15 m/s secondary air velocity and are given below:

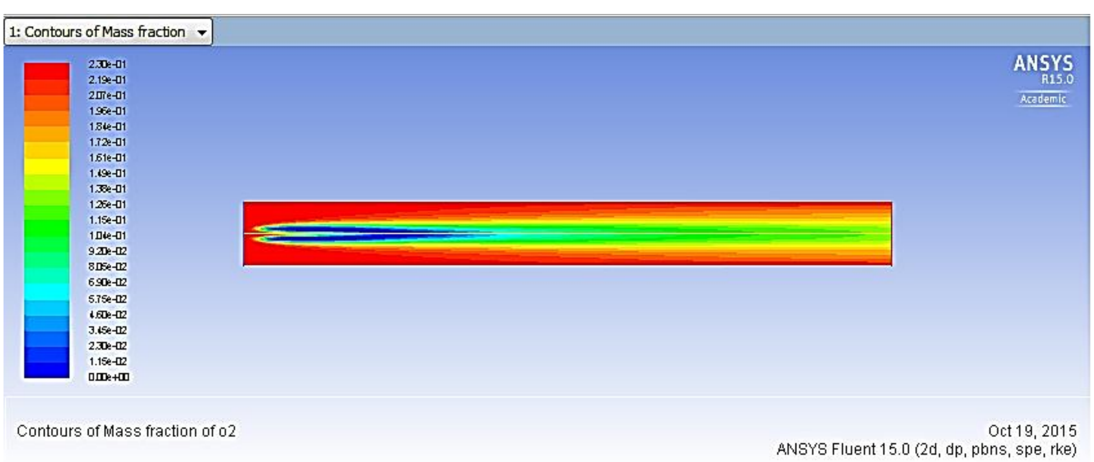

Figure 2: Contours of mass fraction of Oxygen (O_2)

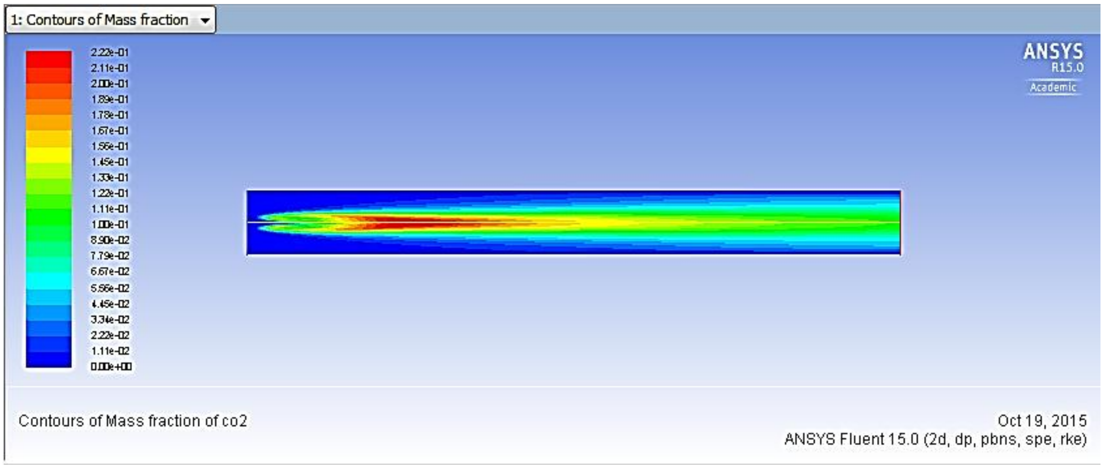

Figure 3: Contours of mass fraction of Carbon dioxide (CO_2)

Composition of flue gases O_2 and CO_2 were calculated from the contours of O_2 and $CO_2$was taken as given in table 9:

Table 9: Composition of flue gases inside the combustion chamber

Excess Air	O_2 (%)	CO_2 (%)
12.5	3	17.8

VII. CONCLUSION

The objective of this simulation is to have a good reference base-case. This has been accomplished for a situation of nominal operating conditions at full load and the validation has been carried out. Once the reference case-base is ready, new simulation for different operating conditions can be carried out in order to study possible strategies aiming at improving combustion efficiency.

The flue gas analysis is carried out by Orsat apparatus. It gives status of combustion in coal fired systems. It is very difficult to find out CO_2 and O_2 composition inside combustion chamber, but by the application of ANSYS FLUENT 15.0 we are able to determine CO_2 and O_2 composition inside the combustion chamber. The CO_2 and O_2 composition can be determine at any location of the combustion chamber because CFD provides the facility to estimate the point value at any location. By this we can improve the combustion efficiency of a combustion system.

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Mathematical Symbols

R_t= total rate of reaction per unit area of external surface
k_0 = velocity constant for diffusion across the boundary layer
k_2 = rate of decomposition of the surface complex
p_0 = oxygen partial pressure in the main stream
D = diffusion coefficient
ρ = density
u_i,u_j = velocities in x, y direction
μ_t = turbulent viscosity
w = weight fraction (cumulative)
dp = size of the coal in that fraction
dp^* =dispersion coefficient
n = distribution parameter