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Mathematical Simulation of Pulverized Coal Combustion

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Abstract: Two different computational fluid dynamic models for the combustion of species were applied for the study of the combustion of pulverized coal in a drop tube. The drop tube is available in the department of energy research of the technical university of Ostrava. The purpose of this work is to find out the main characteristics of the combustion of pulverized coal using data gathered at the laboratory where the drop tube is installed. Some characteristics studied were the total heat transfer involved in the combustion, highest temperature and pressure gradients. A 2d mesh of the drop tube was created in gambit pre-processor and the simulations were performed using the CFD program Ansys fluent. The simulations were performed with double precision (dp mode) in order to get accurate results. In order to simulate the pulverized coal combustion, it was necessary to study turbulence, turbulence models (RNG k–ε), combustion models (species transport and non-premixed model) as the modeling in gambit and the setting up of a case in Ansys Fluent. The main goal was to get similar results in the simulations using distinct approaches (different methods of studying the combustion) in Ansys Fluent and the results were satisfying. The total amount of heat transfer results, for example, was quite similar in both experiences.

Keywords: Pulverized coal combustion, particles, species, coal.

1. Introduction

A three-dimensional multi-phase model was developed in a blast furnace tuyere using Eulerian approach to simulate the coal transfer process of heat, devolatilization, and combustion. Information including the field of velocity, temperature distribution, and combustion characteristics was obtained in detail and the effect of carbon diameter, coal injection was presented on the pulverized coal combustion process [1]. The predicted results show that the size of carbon particles, the Pulverized coal, and coal injection affect the inside tuyere process of coal combustion [2]. The volatile matter released from the coal faster for the smaller carbon particle diameter. This leads to a higher carbon burnout at the tuyere exit. The coal burnout is dependent on the volatile matter content of the coal; the coal with a higher volatile matter content will obtain a higher carbon burnout [3]. The injection of coal affects the flow pattern within the tuyere, resulting in a different process of pulverized coal and burning [4].

The drop tube is available at the Ostrava Technical University's Department of Energy Research [5, 6]. The aim of this work is to identify the main characteristics of pulverized coal combustion using data collected in the laboratory where the drop tube is installed. The total heat transfer involved in the combustion, highest temperature, and pressure gradients were some of the characteristics studied [7].

In Ansys pre-processor a 2D mesh of the drop tube was created and simulations were conducted using the ANSYS FLUENT CFD program [8].

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To simulate the combustion of pulverized coal, it was necessary to study turbulence, turbulence models (RNG $k-\varepsilon$), combustion models (non-premixed model) as the Ansys model and the ANSYS FLUENT case set-up [9].

2. Mathematical model of combustion

2.1. Mathematical Model of Pulverized Coal Particles Burnout In FLUENT

The movement of solid particles (coal particles) is based on a multi-phase model defined by the concept of Lagrangian. The gaseous phase of access in Lagrangian is defined as a continuous phase. Real gas flow equations (Navier-Stokes equations, mass conservation equations, and energy equation) solve this phase [10]. The second phase consists of spherical particles (which can be taken for representation, droplets or bubbles) dispersed throughout the continuous phase. FLUENT calculates the trajectories and heat and mass transfer to/from these discrete phase entities [11]. It is possible to include the coupling between the phases and their impact on the discrete phase trajectories as well as the continuous phase flow [12]. FLUENT can then include hydrodynamic drag solution, gravity force, discrete phase heating/cooling, combustion particles, including volatile evolution and char combustion to simulate coal combustion [13, 14].

2.2. Definition of the Non-Premixed Approach

All the details of the Non-Premixed Approach definition will be described in this chapter: general details, boundary conditions, and flow particles [15].

The input of coal properties is the same as those described above:

- *The program automatically calculates values such as Empiric Fuel Specific Heat and Empirical Fuel Lower Calorific Value of the coal.*
- *The oxide is not pure air, it is a mixture with a CO_2 mass fraction of 0.004079 (1) that has been prepared before. Consequently, CO_2 is added to the Oxidizer Boundary table and its value 0.792 (1) is input.*
- *The fuel temperature is 293 K and the Oxide temperature is 1.200 K.*
- *The PDF table is generated in the tab table after this data is entered.*
- *The reaction is defined as a one-step reaction and the SO_2 is present in the reaction (this way the information on the "S" component in the coal composition can be entered).*

Density is defined in this menu as pdf, calorific power as mixing law, thermal conductivity as pdf mixing law, velocity as pdf mixing law, and mass diffusivity are automatically calculated using turbulent velocity.

The input properties for coal are presented in the following tables (the input information is the detailed chemical information of the coal samples used at the VSB Technical University of Ostrava's Energy Research Centre) [15].

The volatile, ash, moisture and fixed percentage of mass fraction carbon as well as the detailed chemical characteristics of the coal used in the simulations (Table 1).

Table 1: Coal Calculator

Proximate Analysis of Coal		Ultimate Analysis of Coal	
Component of coal	*Percentage*	*Elemental analysis of coal*	*Percentage*
Volatiles	26.27%	C	84.26%
Ash	21.27%	H	5.26%
Fixed carbon	51.23%	O	8.3%
Moisture	1.23%	N	1.36%
		S	0.82%

The program automatically generates mixture templates in materials with the following materials after inputting these data into the coal calculator: carbon-volatile, sulfur dioxide, nitrogen, water vapor, carbon dioxide, oxygen, and the following equation for the gas phase reaction.

2.3. Discrete Phase

The discrete phase (particles) is activated as the Continuous Phase Interaction. The maximum number of steps in the tracking tab is equal to 1000 and the remaining option is the default.

Table 2: Coal Injection

Coal Physical properties	
Density ($kg \cdot m^{-3}$)	1.400
Specific heat ($J \cdot kg^{-1} \cdot K^{-1}$)	1.680
Thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$)	0.00454

The type of injection is set up with 20 particle streams and "combusting" as a group injection (see Figure 1). The following table presents information on the physical properties of coal and coal placing the injection, its temperature, mass flow rate, and size parameters.

The Specification Method is *Intensity and Hydraulic Diameter* with Turbulent Intensity equal to 0.5%

and Hydraulic Diameter 0.033m (half of the real value because symmetry is used to speed up the simulations).

Species

Coal-volatiles: $1e^{-6}$ (1)

O_2: 0.049 (1)

CO_2: 0.792 (1)

H_2O: $1e^{-6}$ (1)

S_2O: $1e^{-6}$ (1)

These values are obtained from the laboratory of Research of Energy of The Technical University of Ostrava. Values in mass fraction form.

The values for Coal-volatiles, H_2O and S_2O are computed, during the simulation, by ANSYS Fluent, therefore, they are defined as with the value $1e^{-6}$ because it's a small value, negligible.

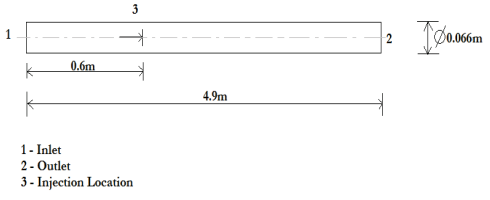

Figure 1: Scheme of the drop tube configuration and injection positioning

The definition of the boundary conditions is very simple, without operating conditions (the operating conditions will be defined in ANSYS FLUENT and described in the future)

The defined boundary conditions non-premixed combustion;

- ***Wall** boundary condition is defined as a stationary **Wall;***
- ***Inlet** Boundary condition is defined as a mass-flow **Inlet;***
- ***Outlet** Boundary conditions are defined as a pressure **Outlet;***
- ***Symmetry** boundary condition, defined as an **Axis;***
- *Default interior boundary condition, defined as an interior.*

2.4 Boundary Conditions

Inlet

» *The inlet is defined as a mass-flow-inlet, with a mass Flow Specification Method Mass Flow Rate of air. The value of the Mass Flow Rate is 0.004079 (kg/s) and the Mode of Direction Specification is Normal to Boundary.*

» *The Specification Method is Intensity and Hydraulic Diameter with Turbulent Intensity equal to 0.5% and Hydraulic Diameter 0.033m (half of the real value because it uses symmetry to speed up simulations.*

» *The total temperature of 1200 K.*

Outlet

– *The outlet is defined as an outlet for pressure.*

– *Specification Method: Hydraulic diameter and intensity.*

– *Turbulent intensity (percentage) equal to 0.5 as the flow is turbulent but with a low number of Reynolds.*

– *Diameter hydraulic (m): 0.033.*

– *The species are defined in the H_2, N_2, and O_2 where they were defined.*

– *The total temperature of 1200 K.*

– *The simulation is initialized with the value 0 for Axial Velocity, Turbulent Kinetic Energy and Turbulent Dissipation Rate after all these details have been entered.*

– *Double precision is used to calculate the simulation.*

Wall

– *The wall is isolation.*

– *Heat flux is 0.*

The table 3 below presents information on injection placement, temperature, total mass flow rate, and coal size parameters. The carbon particle size distribution follows Rosin- Rammler's model.

Table 3: Diameter Distribution

Diameter Range (μm)	*The mass fraction in Range (μm)*
0-70	0.05
70-100	0.10
100-120	0.35
120-150	0.30
150-180	0.15
180-200	0.05

Minimum Diameter - this is the size distribution's smallest diameter to be considered.

Maximum Diameter - this is the biggest diameter in the size distribution to be considered.

Linear Diameter - this diameter is also same as Rosin-Rammler's. So, we can use constant Diameter.

3. Results and its Discussion

The results of the simulation will be presented in this section. The discussion will focus on the temperature, pressure drop, velocity, and mass flow rate distribution.

The tube's orientation is in the X direction, and gravity acceleration in that direction has been applied. Obviously, the real case has the tube in the Y direction, but the simulations were carried out in X direction with the tube to facilitate the presentation of the results.

Due to its dimensions, the results will be presented as partial pictures of the drop tube

profile. The drop tube is very long, but its diameter is small (as compared to the length), so the only way to show the results is to focus the images on the tube's most important areas, depending on the aspect being studied and analyzed.

By giving the above parameter as input values we get below results in Pressure (Pa), Temperature (K), Species (1), Velocity ($m.s^{-1}$) and so on (Figure 2).

3.1 Basic parameter

Inlet

Q = 0.00454 ($kg.s^{-1}$)

T = 1200 (K)

Outlet

P = 0 (Pa)

T = 1200 (K)

Wall - isolation

Injection:

Qm = 5.5555e^{-6} ($kg.s^{-1}$)

D = 0.0066 (m)

T = 293 (K)

U = 0 ($m.s^{-1}$)

By giving the above parameter as input values we get below results in Pressure (Pa), Temperature (K), Species (1), Velocity ($m.^{s-1}$) and so on.

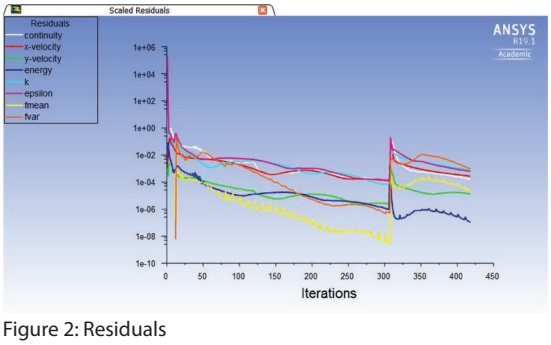

Figure 2: Residuals

In these cases, the initial setting of temperature was equal to 293 (K) and velocity is 0, but higher velocity increases in the approach. In the Non-Premixed case, the velocity distribution appears to be more linear. But is also not as low in areas closer to the drop tube wall (Figure 3).

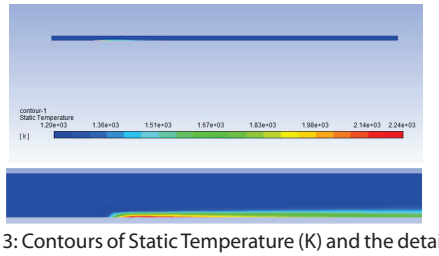

Figure 3: Contours of Static Temperature (K) and the detail near the injection.

The Distribution of contour Static Temperature is shown on above Figure 3. Here have same get a given result are minimum 1.200K to maximum 2.240K. The Temperature distribution is shown on Figure 4 is says give all details about the Temperature of after injections point higher Temperature to lower Temperature. Here is also explain the details in Static Temperature using XY plot in the show in Figure 4.

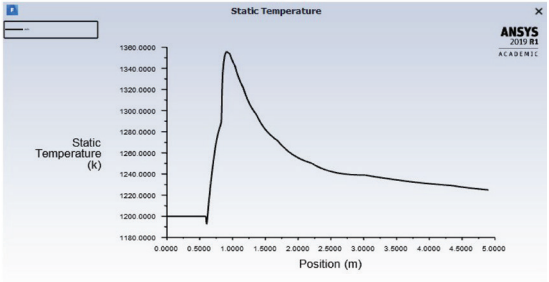

Figure 4: XY plot Static Temperature

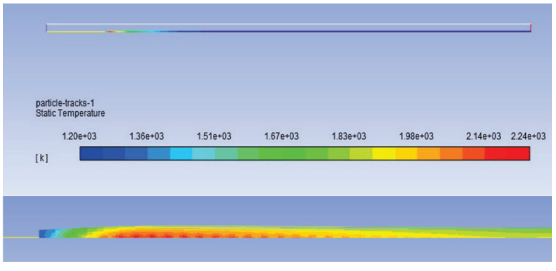

Figure 5: Particle Tracks Colored by Temperature (K) and details. The Distribution of Particles Tracks Colored Static Temperature is shown on above Figure 5. Here have same get a given result are minimum 1.200 K to maximum 2.240 K.

4. Conclusions

A pulverized coal combustion was performed with air flow field interacting with a discrete phase of carbon particles. Simulated the devolatilization of coal injected into the field of gas phase flow. The Non-Premixed model (mixture fraction / PDF model) simulated reactions between the discrete phase and the continuous phase. The Non-Premixed model was developed specifically for turbulent flames and offers many advantages over the other mathematical model for combustion studied. The Non-Premixed model allows for intermediate effects of species formation and dissociation, so the results obtained with this method are theoretically more realistic than the other approach in oxygen concentration and char burnout rate. The Non-Premixed model does not perform a large number equation solution, which is why it is more efficient

computationally. The results were satisfactory–in terms of average temperature and total heat transfer, both simulations resulted in similar outlet results. To know if the results are like the actual results of life obtained in the laboratory, it would be necessary, for example, to have the results of the laboratory at the outlet for the mass fraction of species. The outlet's final temperature is the only result obtained at the Ostrava Energy Research Center. The value is approximately 1205 K, but the information is not complete and therefore finding a comparison of this value with the values obtained in the simulations is complicated.

The outlet average temperature values were approximately 1.204 and 1.206 K in testing the in fluent mass flow of particles and mass flow air and so on. In conclusion, because of its overall similarity, the results seem very satisfying.

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