

THREE-DIMENSIONAL COAL COMBUSTION SIMULATION OF CIRCULATING FLUIDIZED BED BY EULERIAN-EULERIAN METHODS

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Abstract – The circulating fluidized bed (CFB) combustion, due to its unique advantages like high fuel flexibility, excellent heat transfer and low pollutant emission, has become a prosperous and competitive technology. However, due to the complexity of the CFB system, the deep theoretical research and experimental study of the CFB is of great difficulty. The numerical simulation by the computational fluid dynamics (CFD) has become a significant method to study the complicated characteristics of the CFB. Based on the pilot-scale circulating fluidized bed combustor, this paper develops a comprehensive three-dimensional CFB combustion model by the Eulerian-Eulerian approach. The profile of hydrodynamic, temperature and gas composition is analyzed, and good resemblance is observed between the simulated results and the experimental data. The simulation in this paper helps to have a better understanding of the CFB combustion system and enriches its investigation method.

NOTATION

H	bed height, mm
d_p	surface to volume mean diameter, mm
x_i	mass fraction, %
d_i	particle diameter, mm
r	reaction rate, kmol/(m ³ s)
C	concentration, kmol/m ³

1. INTRODUCTION

The circulating fluidized bed (CFB), as a chemical reactor, has attained great attention due to its unique advantages of high fuel flexibility, excellent heat transfer and low pollutant emission. Nowadays, it is under rapid development and has been widely used in the chemical processes like the coal combustion and gasification. However, due to the complicated mechanism of multiphase flow in the CFB, the deep theoretical analysis and experimental study of the CFB becomes extremely difficult. Computational fluid dynamics (CFD) provides an economical and effective way for a better understanding of the CFB study. It is considered as one of the most feasible options for predicting some critical parameters that are difficult to be obtained by the experimental study. Therefore, the numerical simulation by CFD exhibits great potential to replace the conventional empirical or semi-empirical models for the industrial-scale CFB design in future.

Based on the pilot-scale CFB combustor in the Southeast University of China, a three-dimensional CFD coal combustion model by the Eulerian-Eulerian method is developed in this paper. The simulation aims to achieve the following: (1) to establish a comprehensive model involving the gas-solid flow, heat and mass transfer, as well as various homogeneous and heterogeneous reactions; (2) to reach a stable coal combustion condition with a detail insight into the CFB's behavior including fluidization, thermal and chemical characteristics; (3) to achieve good resemblance on some parameters between the simulated results and the experimental data.

2. MODEL CONFIGURATION

Geometry of the CFB riser is shown in Fig.1. The riser is divided into three different zones, namely, a dense zone (0-800mm), a transition zone (800mm-1000mm) and a dilute zone (1000mm-4200mm). The inner diameters of the dense zone and the dilute zone are 122mm and 150mm. The riser consists of a primary air inlet at the bottom, a coal inlet at the bed height H=700mm, a secondary air inlet at the bed height H=900mm, a solid circulating inlet at the bed height H=200mm and a furnace outlet at the bed height H=3500mm.

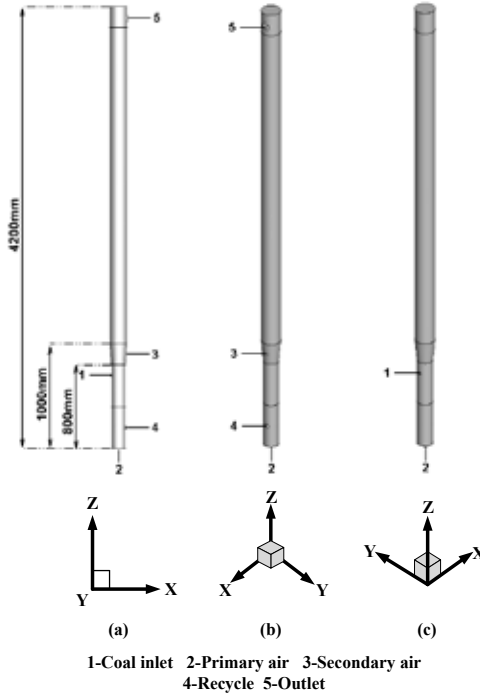


Fig. 1. Geometry of the CFB riser from different angles.

To ensure the good convergence and save the computational time, some assumptions are adopted as follows:

(1) The surface to volume mean diameter is used to represent the average diameter of the particles, which is calculated by,

$$d_p = 1 / \sum_i \frac{x_i}{d_i} \quad (1)$$

Where d_p is the surface to volume mean diameter; x_i is the mass fraction of particles with diameter of d_i .

(2) Simulation in the high-temperature cyclone and the solid circulating system is ignored on the assumption that no chemical reactions occur in these parts. The solid flow rate and species composition of the solid circulating inlet are the same as those of the furnace outlet. Besides, the solid temperature of the solid circulating inlet is determined by considering the temperature drop in the high-temperature cyclone and the solid circulating system.

3. KINETIC MODEL

The coal combustion in the CFB is an exothermic process at a relatively high temperature. When the coal is fed into the furnace, it dries at first (R₁) and experiences the volatile pyrolysis (R₂), in which a wide range of gaseous products are generated. The released gaseous products undergo the homogeneous reactions (R₃-R₆) whereas the remaining char undergoes the heterogeneous reactions (R₇-R₉). Besides, the pollutant formation of NO_x and SO₂ are accompanied.

In this paper, the pyrolysis process is based on the MGAS (METC Gasifier Advanced Simulation) model (Syamlal et al, 1992). The released gaseous products contain CH₄, H₂, CO₂, CO, H₂O(g), tar, NH₃ and H₂S. Based on the mass balance of each component, the molecular formula of volatile (C_{2.2}H_{8.22}O_{1.036}N_{0.109}S_{0.1}) and tar (C_{10.79}H_{11.43}O_{0.18}) and the stoichiometric coefficients of pyrolysis products are determined. The char oxidation rate is determined by the combination of oxygen transfer to the particle surface and the surface kinetic reaction. For the pollutant formation, the sulfur and nitrogen is partitioned between the volatile form (C_{2.2}H_{8.22}O_{1.036}N_{0.035}S_{0.032}) and the char form (CN_{0.008}S_{0.0075}), and the mass fraction in the volatile is identical

to that in the dry, ash-free original coal (Fan et al, 1998). The volatile form is devolatilized into H₂S and NH₃ in the pyrolysis process, whereas the char form is oxidized into SO₂ and NO. Besides, it is assumed that NO is the only form of NO_x. The oxidation of H₂S and NH₃, together with NO/CO/char/NH₃ reduction reactions, is introduced.

The main reactions in this paper are shown as follows, with the reaction rates (Syamlal et al, 1992) listed in Table 1.

Table.1: The reaction rates for the coal combustion.

$(R_1): H_2O(l) \rightarrow H_2O(g)$	$r_1 = \varepsilon_s k_1 C_{H_2O(l)}$
$(R_2): Volatile \rightarrow \alpha_1 Tar + \alpha_2 CO + \alpha_3 CO_2 + \alpha_4 CH_4$ $+ \alpha_5 H_2 + \alpha_6 H_2O(g) + \alpha_7 NH_3 + \alpha_8 H_2S$	$r_2 = \varepsilon_s k_2 C_{Volatile}$
$(R_3): CH_4 + 1.5O_2 \rightarrow CO + 2H_2O(g)$	$r_3 = \varepsilon_g k_3 C_{CH_4}^{0.2} C_{O_2}^{1.3}$
$(R_4): CO + 0.5O_2 \rightarrow CO_2$	$r_4 = \varepsilon_g k_4 C_{CO}^{0.25} C_{H_2O}^{0.5}$
$(R_5): H_2 + 0.5O_2 \rightarrow H_2O(g)$	$r_5 = \varepsilon_g k_5 C_{H_2} C_{O_2}$
$(R_6): Tar + 13.5574O_2 \rightarrow 10.79CO_2 + 5.7146H_2O(g)$	$r_6 = \varepsilon_g k_6 C_{Tar} C_{O_2}$
$(R_7): CN_{0.008}S_{0.0075} + \left(\frac{1}{\phi} + 0.0115\right)O_2 \rightarrow$ $\left(2 - \frac{2}{\phi}\right)CO + \left(\frac{2}{\phi} - 1\right)CO_2 + 0.008NO + 0.0075SO_2$	$r_7 = \frac{6\varepsilon_s \rho_s Y_{char}}{d_p \rho_c} k_c C_{NO}$ $k_c = \frac{RT / w_c}{(1/k_d) + (1/k_7)}$
$(R_8): CN_{0.008}S_{0.0075} + 1.023CO_2 \rightarrow 2.023CO$ $+ 0.008NO + 0.0075SO_2$	$r_8 = \frac{k_8 C_{CO_2}}{1 + aC_{CO_2} + bC_{CO}}$
$(R_9): CN_{0.008}S_{0.0075} + 1.023H_2O(g) \rightarrow 1.023H_2 + CO$ $+ 0.008NO + 0.0075SO_2$	$r_9 = \frac{k_9 C_{H_2O(g)}}{1 + aC_{H_2O(g)} + bC_{H_2} + cC_{CO}}$
$(R_{10}): H_2S + 1.5O_2 \rightarrow SO_2 + H_2O(g)$	$r_{10} = \varepsilon_g k_{10} C_{H_2S}^{0.2} C_{O_2}^{1.3}$
$(R_{11}): NH_3 + 1.25O_2 \rightarrow NO + 1.5H_2O(g)$	$r_{11} = \varepsilon_g k_{11} C_{NH_3} C_{O_2}$
$(R_{12}): CN_{0.008}S_{0.0075} + 1.015NO \rightarrow CO$ $+ 0.5115N_2 + 0.0075SO_2$	$r_{12} = \frac{6\varepsilon_s \rho_s Y_{char}}{d_p \rho_c} k_{16} C_{NO}$
$(R_{13}): CO + NO \rightarrow CO_2 + 0.5N_2$	$r_{13} = \varepsilon_g k_{13} \left(\frac{aC_{NO}(bC_{CO} + c)}{aC_{NO} + bC_{CO} + c} \right)$
$(R_{14}): NO + NH_3 + 0.25O_2 \rightarrow N_2 + 1.5H_2O(g)$	$r_{14} = \varepsilon_g k_{14} C_{NH_3}^{0.5} C_{O_2}^{0.5} C_{NO}^{0.5}$

4. PARAMETER SETTING

In this paper, the gas phase consists of 12 species (methane CH₄, oxygen O₂, carbon dioxide CO₂, carbon monoxide CO, water vapor H₂O(g), hydrogen H₂, sulfur dioxide SO₂, tar C_{10.79}H_{11.43}O_{0.18}, ammonia NH₃, nitric oxide NO, hydrogen sulfide H₂S and nitrogen N₂) and the solid phase consists of 4 species (volatile C_{2.2}H_{8.22}O_{1.036}N_{0.109}S_{0.1}, char C, moisture H₂O(l) and ash). The gas density is calculated based on the ideal gas state equation. The specific heat of each gas component is the piecewise-linear function of temperature and the viscosity follows the power law. The physical properties of mixtures obey the volume/mass-weighted mixing law. Properties of the volatile, ash and tar are estimated by the method proposed by Eisermann et al. (1980). Besides, the enthalpy of the volatile is determined based on the low heating value (LHV) of coal, whereas the enthalpy of ash is set as zero.

For the boundary conditions, all the inlets (the primary air inlet, the secondary air inlet, the coal feed inlet and the solid recirculating inlet) adopt the velocity-inlet type, while the furnace outlet adopts the pressure-outlet type. The no-slip boundary is used for the gas phase while the partial slip boundary is used for the solid phase. At the initial time, the gas composition is air and the ash particles are stacked up to 400mm with the solid volume fraction set to be 0.55. Temperature of the gas and the solid phase is 1123K. Some main parameters used in this simulation are shown in Table 2.

Table.2: Main parameters used in this simulation.

Parameter	Value	Parameter	Value
Coal feed rate	8kg/h	Secondary air ratio	0.3
Excess air coefficient	1.2	Coal distributing air ratio	0.05
Primary air temperature	298K	Material returning air ratio	0.05
Secondary air temperature	298K	Particle diameter	0.35mm
Coal distributing air temperature	298K	Restitution coefficient	0.95
Material returning air temperature	700K	Wall thickness	300mm
Primary air ratio	0.6	Furnace outlet pressure	-50Pa

A time-step of 1.0×10^{-4} with 50 iterations per time step is used. The phase-coupled SIMPLE algorithm and the first-order upwind scheme are used to discretize the governing equations. Besides, some relaxation factors are adjusted to ensure the numerical stability.

5. RESULTS AND DISCUSSION

The simulated O_2 and CO_2 outlet volume fraction with time is shown in Fig.2. Various reactions of the coal combustion are accompanied by a decrease of O_2 and an increase of CO_2 . The whole simulation is run for 50s. Besides, it can be observed that the result reaches a steady value from about 25s, which indicates the stable condition in the furnace. The time-averaged value of the simulated results under the stable condition is compared with the experimental data in the following study.

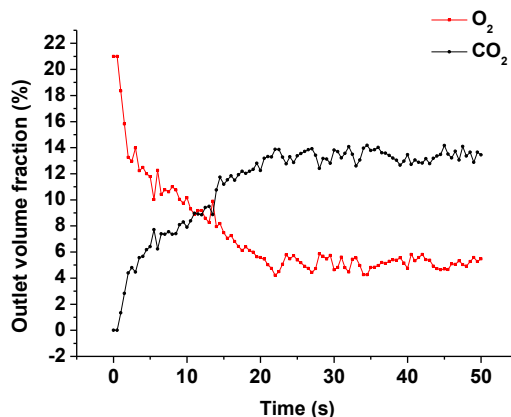


Fig. 2. The simulated O_2 and CO_2 outlet volume fraction with time.

5.1 HYDRODYNAMIC

The time-averaged pressure and solid volume fraction profile of the simulated results, based on the EMMS drag model, is compared with the experimental data in Fig.3 and Fig.4. The riser is obviously separated into a lower dense region and an upper dilute region, with the simulated results showing a good agreement with the experiment data.

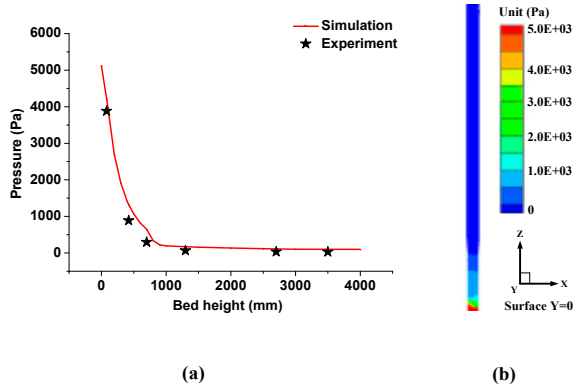


Fig. 3. The pressure profile (a) time-averaged curve (b) transient contour.

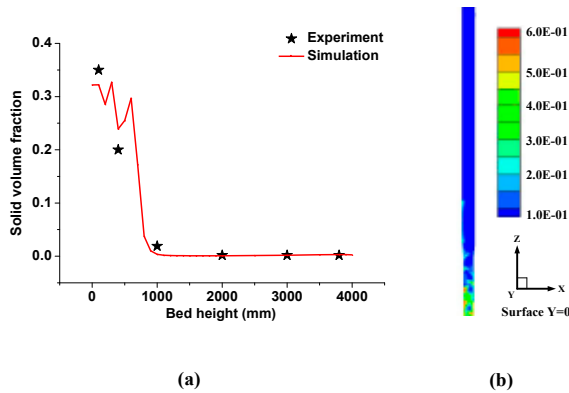


Fig. 4. The solid volume fraction profile (a) time-averaged curve (b) transient contour.

5.2 TEMPERATURE

The time-averaged axial gas temperature and the transient contour are shown in Fig.5. In the dense zone, the cold primary air is heated and the temperature increases due to the exothermic reactions of the char oxidation and the pyrolysis products oxidation. When a large amount of the cold secondary air is injected in the transition zone, the temperature greatly reduces. With the further oxidation of the pyrolysis products, the temperature in the dilute zone increases with the bed height at first and reaches the maximum at a position where the pyrolysis products almost burn out, then begins to cut down due to heat dissipation through the wall. Compared to the experimental data, the simulated results successfully predict the axial gas temperature distribution with the maximum deviation of about 50K. Temperature in the dense zone is underestimated, whereas temperature in the lower part of the dilute zone is overestimated. The deviation lies in the fact that the wide size distribution of the coal particles in the experiment is replaced by a single particle diameter in the simulation, and the heat released by the pyrolysis products oxidation is intensified in the lower part of the dilute zone, leading to a higher combustion fraction in this area.

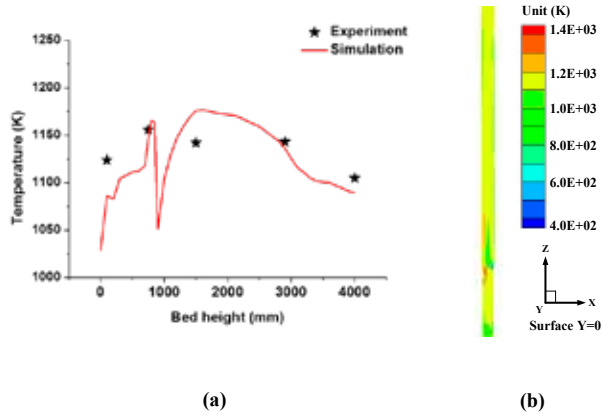


Fig. 5. The axial gas temperature (a) time-averaged curve (b) transient contour.

5.3 GAS COMPOSITION

The time-averaged outlet gas volume fraction is compared in Fig.6. Results show a good agreement between the simulation results and the experimental data, indicating that the selected chemical reaction models are acceptable.

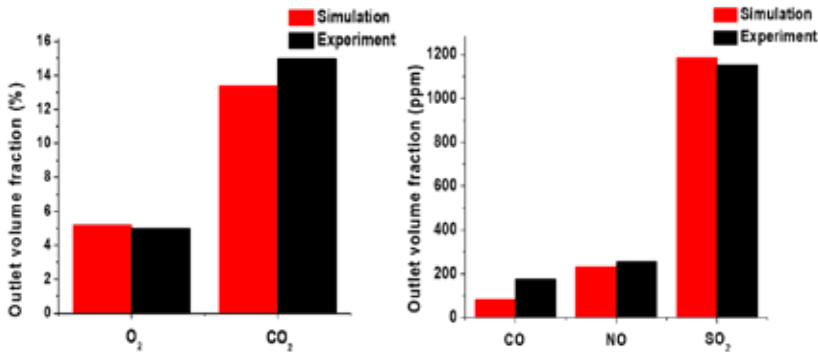


Fig. 6. The solid volume fraction profile (a) time-averaged curve (b) transient contour.

The time-averaged axial gas distribution and the transient contour are shown in Fig.7. The mass fraction of O₂ and CO₂ is studied in this section.

In the dense zone, O₂ in the primary air is consumed and its concentration decreases due to the char oxidation and the pyrolysis products oxidation. The injection of the secondary air increases the O₂ concentration in the transition zone. With the further oxidation of the pyrolysis products, the O₂ concentration begins to fall down and reach a steady value when the pyrolysis products almost burn out. The CO₂ distribution shows an opposite tendency with its concentration symmetrical to O₂.

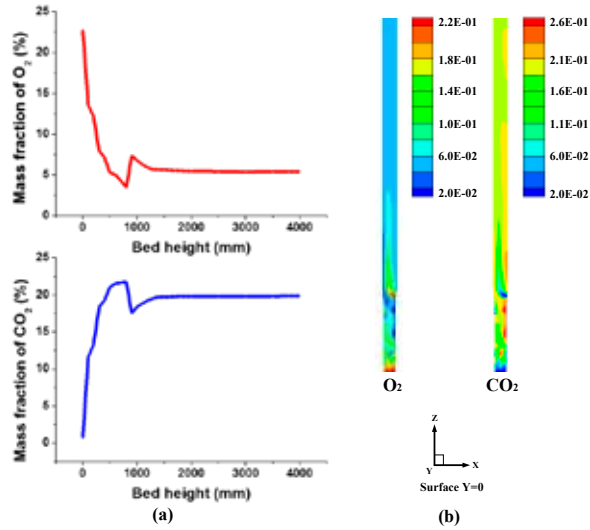


Fig. 7. The solid volume fraction profile (a) time-averaged curve (b) transient contour.

6. CONCLUSION

The three-dimensional computational fluid dynamics simulation is conducted for a CFB combustor under the Eulerian-Eulerian framework. The established model couples the gas-solid flow with heat transfer, mass transfer, as well as various homogeneous and heterogeneous chemical reactions. The whole simulation is run for 50s and it takes about 25s to reach the stable condition of coal combustion. The hydrodynamic, temperature and gas composition profile is analyzed in detail. The simulated results show a good agreement with the experimental data and provide a unique way for a better understanding of the coal combustion in the pilot-scale CFB combustor, which not only enriches its investigation method, but also exhibits great potential to replace the conventional empirical or semi-empirical models for the industrial-scale CFB design in future.

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