A computational study of the effects of O$_2$/CO$_2$ ratios on the oxy-fuel combustion process within a circulating fluidized bed.

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1. Introduction

Circulating fluidized bed reactors (CFB) have attracted significant interests since last 2 decades and implemented in a number of industrial process including power generation. Its excellent operating performance gives huge advantages over the traditional pulverized coal (PC) boilers. In CFB reactors, the fuel burns in a fast fluidized bed regime and gas velocity is found sufficiently high to blow all solids up of the furnace. The majority of solid phases are separated by the cyclone separator and recirculated back to the bed [1]. The main advantages of circulating fluidized bed reactors in contrast to pulverized coal boilers are low greenhouse gases (GHG) emission, high combustion efficiency, fuel flexibility, turndown capacity and load-following capability [2, 3, 4]. Introduction of oxy-fuel combustion technology to circulating fluidized bed tends to lower the flame temperature of the bed that consequently simplifies the temperature control of the reactor [3].

Computational fluid dynamics (CFD) has become a practical tool for simulation of different number of processes. It provides with essential outputs and performs a comprehensive study on fluid flow, heat transfer, chemical reactions and multiphase flow modelling. In multiphase flow applications, CFD modelling studies are mainly applied by two types of approaches that are Eulerian-Eulerian two-fluid model (TFM) and Eulerian-Lagrangian models [5, 6]. Eulerian-Eulerian TFM method is found as one of the most applied approach in literature for simulation of heat transfer and hydrodynamic models. In Eulerian-Eulerian method, the solid and gas phases are considered to be interpenetrating continuous fluid and interacting with the fluid phase [7], while Eulerian-Lagrangian method is a discrete$^1$ method simulates each particle dynamics where explicit motion of the interphase is neglected. In this method continuous phase is modelled by Eulerian framework and the trajectories of individual solid particle are simulated in Lagrangian framework [8].

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Combustion process in circulating fluidized bed reactor is found as turbulent model and most of oxy fuel combustion CFD studies available in literature for circulated fluidised bed and pulverized reactors are mainly applied with k-ε modelling approach. CFD numerical simulation tool also has capability to implement the kinetic theory of granular flow (KTGF) with Eulerian method to model the motion of the particles. Two fluid flow model combined with kinetic theory of granular flow has advantages in predicting of gas-solid hydrodynamics in CFB risers due to its less CPU and memory requirements than trajectory. This model has also been used in bubbling fluidized bed combustors for modelling coal gasification processes. The granular particle temperature is found as the main concept for solving kinetic theory of granular flow [7].

Most of numerical studies of CFB are limited with only the riser modeling and do not consider the recirculation of solids to the combustor, therefore it resembles the scope of fluidized bed. In present paper, a CFD model was used to model gas-solid flow circulation in a circulating fluidized bed considering both riser and recirculating loop under different oxidant injection. The fluid dynamics, heat transfer and mass transfer phenomena are taken into account. O₂/CO₂ ratios that ranges from: (air-21% O₂/79% N₂); (oxy fuel-21% O₂/RFG 79%); (oxy fuel-28 % O₂/RFG 72%) and (oxy fuel-35% O₂/RFG 65%). The pressure drop in the reactor, residence time of solids, effect of fluidizing velocity, main coal gasification chemical reactions, and other important combustion characteristics will be analysed.

2. Modeling approach

2.1. Experimental setup

The small-scale circulating fluidized bed reactor experiment is designed to study coal combustion characteristics under different O₂/CO₂ atmospheres. The experimental and modelling investigation reported by references [9, 3] in a 50 kW pilot CFB combustion reactor at the Southeast University of China. The small-scale experiment facility consists of CFB riser, gas-solid separator cyclone, fuel feeding system, recycled flue gas duct and primary/secondary air supply as shown in Fig 1; 2D reactor model has been applied for investigation of numerical simulation of hydrodynamics in a circulating fluidized bed under oxy-fuel combustion. Height of the rig is 4.2 m with diameter of 0.150 m. The part flue gas product is recycled to bed and supplied as recycled flue gas (RFG) in oxy-fuel combustion cases.

Table 1. Colombian coal properties [10].

<table>
<thead>
<tr>
<th>Proximate analysis (wt%)</th>
<th>Ultimate analysis (wt%)</th>
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<tbody>
<tr>
<td>Moisture</td>
<td>C</td>
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<td>Volatile matter</td>
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<td>Fixed carbon</td>
<td>O</td>
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<td>Ash</td>
<td>N</td>
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<tr>
<td>Proximate analysis (wt%)</td>
<td>S</td>
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<tr>
<td>2.6</td>
<td>75.3</td>
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<td>41.8</td>
<td>5.4</td>
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<tr>
<td>54.1</td>
<td>15.6</td>
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<tr>
<td>1.5</td>
<td>1.8</td>
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<td></td>
<td>0.4</td>
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</tbody>
</table>
2.2. Chemical reaction

Main coal gasification heterogeneous and homogeneous reactions are implemented for analysis of coal combustion processes that taken from ref [6].

Devolatilization process of coal is represented as:

1 kg coal $\rightarrow$ $Y_c$ kg (char) + $Y_v$ kg (volatile matter) + $Y_w$ kg (H$_2$O) + kg (ash)

The kinetic reaction rate is calculated by

$$k_i = A_i \exp \left(-\frac{E_i}{RT}\right);$$

where $k_i$ is given in the Arrhenius form, $E$ is activation energy, $R$ is universal gas constant, $A$ is constant of pre-exponential factor ref [11].

2.3. Basic assumptions:

- In order to simplify the model and its convergence time, a two-dimensional planar geometry is created to describe coal combustion processes. Gas density is taken as incompressible ideal gas law. Particles are assumed isothermal, inelastic and smooth spheres.
- Mass, momentum and energy conversion equations are applied for each phase and species conservation equations are solved for each species.
- Simulated air flows supplied from the bottom of the riser.
- 4 cases are considered for coal combustion oxidant as: (air-21% O$_2$/79% N$_2$); (ox-21% O$_2$/RFG 79%); (ox-28 % O$_2$/RFG 72%); (ox-35% O$_2$/RFG 65%).

Interaction forces as lift force, thermophoretic force, Brownian force, virtual mass forces are neglected. Energy transfer due to pressure stress work, viscous dissipation and species diffusion are not considered.

3. Discussion

Flow characteristics of gas and solid mixture are to be modelled under different O$_2$/CO$_2$ concentrations and validated with experimental work made by references [10]. First of all a cold model will be studied under different oxidant atmospheres, then steeply expand to complex model. For simplification two–dimensional geometry is designed with mesh number of around 10000 quadrilateral cells and with solving conversion time steps that set up as $1 \times 10^4$. The development of full paper is expected to follow as indicated below:

1. Simulate the hydrodynamic characteristics of gas and solid phases in cold two-dimensional model with different O$_2$/CO$_2$ atmospheres and result validation with available literature results.
2. Heat transfer modelling between different phases.
3. Gas-solid mixture analysis in CFB and analysis of flue gas composition in the outlet of the CFB.
4. Implementation of chemical reactions into cold gas-solid hydrodynamic model.
5. Impacts of recycled solids to CFB.

4. Conclusion

A computational study of the effects of O2/CO2 ratios on the oxy-fuel combustion process is expected to be analysed within a circulating fluidized bed. 2D-CFD model of gas-solid flow will be developed for simulating coal combustion behaviour using KTGF approach. The results of the paper will be validated with experimental and
modelling data from [9, 3]. Four different oxidant atmospheres will be implemented to CFB combustor to simulate coal gasification process as ranges from:

1) (air-21% O₂/79% N₂);
2) (oxy-fuel: 21% O₂/RFG 79%);
3) (oxy-fuel: 28% O₂/RFG 72%);
4) (oxy-fuel: 35% O₂/RFG 65%);

The pressure drop in the reactor, residence time of solids, effects of fluidizing velocity, main coal gasification chemical reactions, and other important combustion characteristics are expected to achieve.

5. References