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Eulerian multi-fluid simulation of biomass gasification in circulating fluidized beds: effects of equivalence ratio

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Abstract. In this work, a three-dimensional Eulerian multi-fluid model (MFM) is developed to study the effects of equivalence ratio on the biomass gasification in a full-loop circulating fluidized bed (CFB). In the model, all phases are treated as interpenetrating continuum media in which the governing equations of mass, momentum, and energy of Navier-Stokes formulations are solved. The standard k- ε turbulence model, and common chemical reactions in biomass gasification are incorporated into the model. Moreover, the inter-phase heat transfer exchanges are also considered. The results are compared to existing experimental data and the effects of equivalence ratio are analysed. It is demonstrated that the model has good capability to predict syngas compositions of CO, CO_2, C_2H_4, and N_2 under different equivalence ratio. From this, hydrodynamics and heat transfer inside this complex system are analyzed. The results can be useful for better design and optimization of biomass gasification in CFBs.

1. Introduction

The decrease of available conventional energy sources, such as petroleum, natural gas, and coal, and the increase in energy demands to support the economic growth trigger the use of other alternative energies in order to secure the world's energy global. Biomass offers some advantages over conventional fossil energy such as low carbon emissions and abundant available supply. However, biomass has poor properties of grinding and flow abilities that make it difficult for handling, feeding and transporting. Therefore, the solid biomass needs to be converted to other liquid and gaseous forms to increase its handling and feeding capability. One method that is effective to convert solid biomass to gaseous energy form (or synthetic gas) is gasification. Circulating fluidized bed (CFB) is one of the most promising gasifier since it is characterized by excellent solid mixing and efficient heat and mass transfers. In recent years, experimental studies have been carried out to investigate aspects of biomass gasification in CFB, see for example: (1), (2), (3), and (4). Even though data and information obtained from these studies are useful in practice, they suffer from two drawback. Firstly, they are not comprehensive enough to describe the underlying mechanism of hydrodynamics, heat, and mass transfer in CFB. Secondly, these data and information are only valid for the range of operating variables and specific CFB geometry for which they were obtained. Therefore, in order to describe the behaviors of hydrodynamics, heat transfer, and chemical reaction using these data, it is necessary to replicate the

operating and geometry models.

With the development in computational technology, numerical approaches have become powerful methods generate comprehensive information on transport phenomena in CFB. In general, two numerical approaches are used to study transport phenomena in CFB: the multi- fluid model (MFM) and combined computational fluid dynamics and discrete element method (CFD-DEM). MFM is more comfortable to use for engineering applications in relation to process modeling while CFD-DEM approach is often used for fundamental research. Moreover, the MFM requires less computation than CFD-DEM. In MFM approach, all phases are treated as interpenetrating continuum media in a computational cell. In recent years, MFM has been frequently applied to the study of biomass gasification in fluidized beds, see for example: (5), (6), and (7). In our previous work, a 3D MFM approach has also been developed and validated for biomass gasification in a 3D full-loop circulating fluidized bed system (8). In the model, all heat transfer modes of interphases such as biomass-gas, sand-gas, and sand-biomass heat exchanges are considered. It has been demonstrated that the consideration of all heat transfer modes of interphases can increase the capability of the MFM approach to predict the syngas composition at the exit of CFB.

In this study, the proposed model is further developed to investigate the effects of equivalence ratio on the heat and mass transfer phenomena during the process of biomass gasification in a three-dimensional full-loop CFB is investigated by using a MFM approach. The simulation results are then validated in term of syngas composition to existing data from open literature and they are then analyzed to obtain better understanding on transport phenomena in such complex system.

2. Methods

2.1. Model Development

The MFM approach used in this work has been documented in the literature ((7, 9). For brevity, therefore, we only give a brief description of the method here. The governing equations of continuity, momentum, and energy are solved by well-known Navier-Stokes formulation. The kinetic theory of granular flow (KTGF), homogeneous and heterogeneous reactions, and standard k-ε turbulence model are considered and incorporated into the equations in order to describe the spatial velocity, temperature, and concentration for each phase and species.

Continuity equation

$$\frac{\partial \alpha_g \rho_g}{\partial t} + \nabla.(\alpha_g \rho_g v_g) = \dot{m}_{gs} \quad (1)$$

$$\frac{\partial \alpha_s \rho_s}{\partial t} + \nabla.(\alpha_s \rho_s v_s) = \dot{m}_{gs} \quad (2)$$

where g and s are the subscripts referring to the gas and solid phases, respectively. The variables of ρ, v, and α stand for density, velocity, and volume fraction, respectively. The source term of mass conservation due to chemical reactions is represented by m.

Momentum equation

$$\frac{\alpha_g \rho_g v_g}{\partial t} + \nabla.(\alpha_g \rho_g v_g v_g) = -\alpha_g \nabla p + \nabla.(\tau_g + \tau_g^t) + \alpha_g \rho_g g + \dot{m}_{gs} v_g + \beta(v_s - v_g) \quad (3)$$

$$\frac{\alpha_s \rho_s v_s}{\partial t} + \nabla.(\alpha_s \rho_s v_s v_s) = -\alpha_s \nabla p + \nabla.(\tau_s + \tau_s^t) + \alpha_s \rho_s g + \dot{m}_{sg} v_s + \beta(v_g - v_s) \quad (4)$$

where p is the pressure, and τ and τ^t are the viscous stress tensor and Reynolds stress tensor, respectively. β is the interactional momentum exchange coefficient.

Energy equation

$$\frac{\alpha_g \rho_g h_g}{\partial t} + \nabla.(\alpha_g \rho_g v_g h_g) = \nabla.(k_{eff,g} \nabla T_g) + S_g + Q_{sg} \quad (5)$$

$$\frac{\alpha_s \rho_s h_s}{\partial t} + \nabla.(\alpha_s \rho_s v_s h_s) = \nabla.\left(k_{eff,s} \nabla T_s\right) + S_s + Q_{gs} + Q_{ps} \quad (6)$$

where h is the specific enthalpy, k_{eff} is the effective thermal conductivity, T is the temperature, S is the source term of enthalpy change due to chemical reactions and thermal radiation, Q_{sg} and Q_{gs} are the intensity of heat exchange between the gas and solid phases, and $Q_{\text{sg}} = -Q_{\text{gs}}$. Q_{ps} is the heat exchange between solid phase 1 and 2.

Species transport equation

$$\frac{\partial \alpha_g \rho_g Y_{i,g}}{\partial t} + \nabla.\left(\alpha_g \rho_g v_g Y_{i,g}\right) = -\nabla.\left(\alpha_g J_{i,g}\right) + \alpha_g R_{i,g} + R \quad (7)$$

$$J_{i,g} = -\left(\rho_g D_{i,g} + \frac{u^t}{Sc_t}\right) + \nabla Y_{i,g} - D_{T,i} \frac{\nabla T}{T} \quad (8)$$

where Y_i J_i, R_i, D_i, $D_{T,i}$, Sc_t, and R are mass fraction, diffusion flux, net production rate for homogeneous reactions, mass diffusion coefficient, thermal diffusion coefficient for component *i*, turbulent Schmidt number, and net production rate for heterogeneous reactions, respectively.

In this study, the biomass pyrolysis decomposition expressed below is considered:

Biomass → char + volatile + moisture + ash.

The heterogeneous reactions included in the model are:

$$C + O_2 \rightarrow CO_2$$
$$C + CO_2 \rightarrow 2CO$$
$$C + H_2O \rightarrow CO + H_2$$
$$C + 2H_2 \rightarrow CH_4$$

Homogeneous reactions considered are as following:

$$CO + 0.5O_2 \rightarrow CO_2$$
$$H_2 + 0.5O_2 \rightarrow H_2O$$
$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
$$C_2H_4 + O_2 \rightarrow 2CO + 2H_2$$
$$CO + H_2O \rightarrow CO_2 + H_2$$

Inter-solid phase heat transfer

In this work, the direct solid-solid conduction trough contact area ($Q_{ps,dir}$) and solid-solid conduction through in-between fluid medium ($Q_{ps,flu}$) are incorporated into equation 6.

Direct solid-solid conduction

$$Q_{ps,dir} = n_s n_p (R_s + R_p)^2 \sqrt{8\pi(\Theta_s + \Theta_p)} x \frac{5.36(m/E)^{3/5}(R.V)^{7/10}.C}{(\rho_s C_{p,s}\lambda_s)^{-1/2} + (\rho_p C_{p,p}\lambda_p)^{-1/2}} (T_s - T_p) \quad (9)$$

$$R = \frac{R_s R_p}{R_s + R_{,p}} \quad (10)$$

$$m = \frac{m_s m_p}{m_s + m_p} \quad (11)$$

$$E = \frac{4/3}{(1-\gamma_s^2)/G_s + (1-\gamma_p^2)/G_p} \quad (12)$$

Solid-solid conduction through in-between fluid medium

$$Q_{ps,flu} = n_s n_p (R_s + R_p)^2 \sqrt{8\pi(\Theta_s + \Theta_p)} \, x \, \pi \frac{1}{b} \log\left(\frac{a - b\eta}{a - b\varphi}\right) (T_s - T_p) \quad (13)$$

$$a = \frac{1}{\min(R_s, R_p)} \left(\frac{0.5}{k_s} + \frac{0.5}{k_p} + \frac{1}{k_{g,eff}}\right) \quad (14)$$

$$b = \frac{1}{(k_{g,eff} \min(R_s, R_p))} \quad (15)$$

$$R_{ij} = 0.56 \min(R_s, R_p) (1 - \alpha_g)^{-1/3} \quad (16)$$

$$r_{sij} = \left(\frac{1.25mR}{E}\right)^{0.2} v_{ps}^{0.4} \quad (17)$$

Where *n*, *R*, Θ, γ , and *T* are the numbers of particles in the computational cell, particle radii, granular temperature, Young moduli, and temperature, respectively.

2.2. *Simulation Conditions*

Full-loop CFB geometry is applied in the simulation. There are four main components in a CFB loop: riser column, cyclone, standpipe, and return leg.

Table 1. Composition of biomass ((4))

Proximate analysis (wt%)	
Volatile matter	74.4
Fixed carbon	17.1
Ash	8.5
Ultimate analysis (wt%)	
C	52.7
H	7.2
N	1.6
S	0.07
Cl	0.37
O	38.1

Table 2. Parameters used in the simulation

Biomass diameter	1.89 mm
Sand diameter	0.5 mm
Equivalence ratio	0.41, 0.59, 0.73
Mesh number	263138
Simulation time	20 s

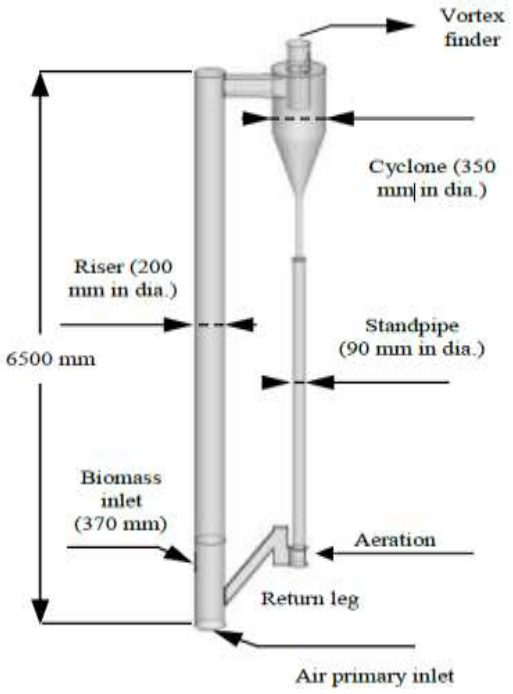

Figure 1. Geometry Model Representation Used in the Simulation

The geometry model representation is shown in Figure 1, whilst the compositions of biomass samples (on dry basis) and simulation conditions are presented in Tables 1 and 2 respectively. The sand material (with density, diameter, and volume of 2600 kg/m^3, 0.5 mm, and 0.019 m^3, respectively) is used as an inert material. The primary air is then imposed with uniform mass flow rate at the bottom of the riser column to fluidize the bed. At the top of the finder, atmospheric pressure condition is applied. All the walls are set to no-slip and adiabatic conditions

3. Results and Discussion

In this section, the simulation results for different equivalence ratio of 0.41, 0.59, and 0.73 are analyzed in terms of the capability of the proposed model to predict the syngas composition at outlet, spatial distributions of fluid temperature and velocity inside CFB.

Figure 2 describes the predicted syngas compositions (vol%) from simulation results and existing experimental data (Exp) of (4). As shown in the figure, the predicted syngas compositions of CO, CO_2, C_2H_4, and N_2 are in agreement with the experimental data with the greatest deviations are 34, 22, 38 and 3 %, respectively. However, for the components H_2 and CH_4 the deviations are quite large, i.e., 72 and 81 %, respectively. From this figure, it is demonstrated that the in general the model have a good capability to predict syngas composition at the outlet region.

Figure 3 illustrates spatial distributions of the average temperature of gas mixture under different equivalence ratio. As depicted in the figures, increasing the equivalence ratio results in the increase of area with higher temperature. For instance, at ER=0.41, the area with temperature of gas mixture higher than 1050 K is less than half of riser column while at ER=0.73, it occupies almost in all components of full-loop CFB except in standpipe. The increase of area with high temperature with the increase of ER might be due to the increase of the rate of chemical reactions during gasification process. The temperatures of gas mixture in the upper zone of the riser column are in agreement with those of existing experimental data of (4) which are around 1050 K. Figure 3 also depicts that at the bottom regions of the riser column and standpipe (with small area), the gas mixture has the lowest temperature.

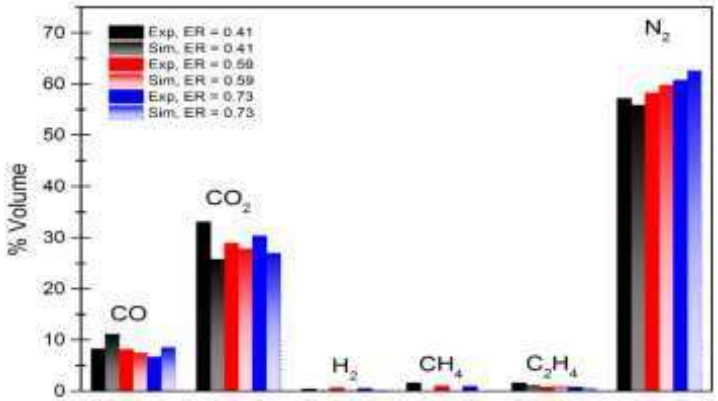

Figure 2. Comparison of syngas composition between simulation results (Sim) and experimental data (Exp) of García-Ibañez, Cabanillas (4)

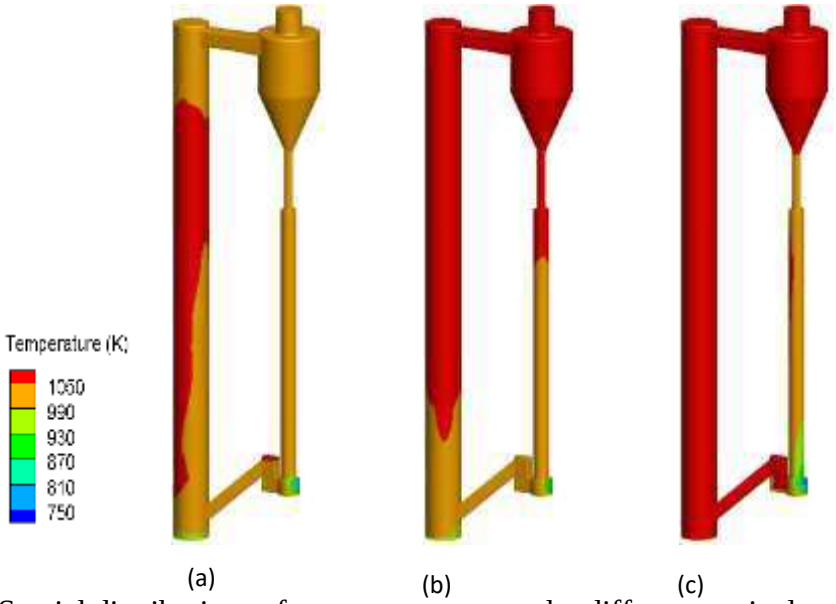

Figure 3. Spatial distributions of gas temperature under different equivalence ratio of (a) 0.41, (b) 0.59, (c) 0.73

Figure 4 describes spatial distributions of the velocity of gas mixture under different equivalence ratio. As shown in the figure, the area with higher velocity in the riser column and in the upper region of cylindrical cyclone increases with the increase of equivalence ratio. Whilst in the return leg and in the bottom region of standpipe, the velocity of gas mixture generally decreases as the increase of equivalence ratio.

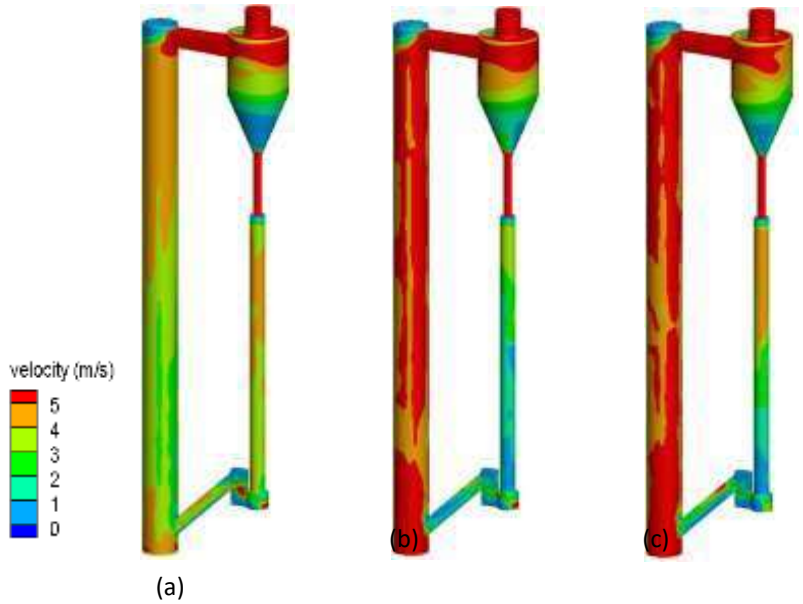

Figure 4. Spatial distributions of gas velocity under different equivalence ratio of (a) 0.41, (b) 0.59, (c) 0.73

4. Conclusion

In this work, a numerical method of MFM framework of biomass gasification in a 3D full- loop CFB has been developed to study the effect of equivalence ratio. In the model, inter-solid phase heat transfer (direct solid-solid conduction and solid-solid conduction

through an in- between fluid medium) is considered. The following conclusions are drawn: the model has good capability for predicting syngas composition of CO, CO_2, C_2H_4, and N_2 while it is still poor for H_2 and CH_4. It is demonstrated that increasing the equivalence ratio results in: (i) the increase of areas with higher temperature of gas mixture in most regions of full-loop CFB, and (ii) the increase of area of gas mixture with higher velocity at the riser column and the upper region of the cyclone.

5. References

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