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Research article

Modeling of biomass pyrolysis in a bubbling fluidized bed reactor: Impact of intra-particle heat conduction

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ABSTRACT

Biomass fast pyrolysis in a fluidized bed reactor is studied numerically by a three-fluid model where the biomass thermal decomposition is introduced with multi-step kinetics. Different superficial velocities of fluidizing gas are defined to investigate the hydrodynamics of the fluidized beds and the consequent influence on the yield fractional distribution of end-products. Heat conduction inside particles is considered indirectly through modifying the rate constants of biomass reaction scheme. The simulation results show that superficial velocity has to be designed carefully based on balancing the char-removal efficiency and biomass heating up rate; compared to the experimental data, the modified reaction scheme can be employed to describe the intra-particle heat penetration, qualitatively, but the accuracy of predicting the end-product yields needs to be improved.

1. Introduction

Fast pyrolysis of biomass has been studied extensively due to the interests on the primary end-product, namely tar or bio-oil. A series of works on biomass pyrolysis mechanism have been reported [1,2] and the end-products are analyzed [3,4]. Numerical simulation is a useful tool to aid the design of biomass pyrolysis reactors. The product yields of biomass pyrolysis are predicted by the two-fluid model (TFM) coupling with the multi-component reaction scheme and the simulation results are validated experimentally [5,6]. The Boltzmann equation accounting for the collisional transfer between particles in a fluidized bed has been introduced into the modeling of biomass thermal degrading. The improved prediction of the fractional distribution of end-products can be expected [7]. One or several biomass particles are identified in the computational fluid dynamics-discrete element method (CFD-DEM) modeling of biomass fast pyrolysis to study the flow characteristics of fluidized beds and the yields of end-products. Although the number of the traced particles is limited, the evolution of the reacting particles has been studied in detail such as intra-particle heat conduction, particle shrinkage and particle entrainment in gas flow [8–11]. Two different reaction schemes including the single-component model and the detailed chemistry scheme are introduced into the 3D simulations. In the latter scheme, biomass can be written as $C_6H_{8.46}O_{3.9}$ while the products of the primary reaction are addressed with the reference species including Phenol, Acetone, Acrylic-acid, etc. [12,13]. Different reaction schemes have been employed into the simulations of biomass fast pyrolysis meanwhile the parametric study reveals the effect of biomass particle type and size on the yields of the products [14]. Modeling of red oak pyrolysis in a bubbling fluidized bed is reported and the impact of hydrodynamics of bubbling fluidized bed on tar yield is investigated numerically by changing the sand size and sand bed height [15]. Particle size distribution (PSD) is investigated through Eulerian-Eulerian CFD modeling in which the PSD model would be more realistic than the mono-particle size model on describing the motion of real particles [16]. For large particles, the temperature gradient due to the intra-particle heat conduction cannot be neglected and will lead to the variation of local reaction rate. To consider the heat penetration process, thermal conductivity of wood has been specified by an effective thermal conductivity which is a function of temperature, density and moisture [17]. It is clear that the representation of mass and heat transfer on the particle scale is practical by Lagrangian approaches whereas the direct inspection is impossible for Eulerian approaches. Hence incorporating empirical correlation into chemical kinetics is proposed to describe the effect of intra-particle heat conduction on the product yields [18]. As the intra-particle heat penetration is seldom considered in the modeling of biomass pyrolysis, the present work is trying to employ the Eulerian approaches to investigate the corn stalk fast pyrolysis in a bubbling fluidized bed. Meanwhile the impact of intra-particle heat penetration is considered by the modified chemical kinetics and the simulation results are validated with the experimental data.

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2. Model setup

2.1. Model geometry

The 2D geometry is set up with the diameter of 100 mm and height of 600 mm (Fig. 1). Sand particles are pre-loaded above the bottom distributor with the initial bed height of 50 mm and packing rate of 0.63. Sand and biomass particles are defined as perfect spheres with the uniform diameter of 0.4 mm. PSD of the real samples is not emphasized in the current work. Biomass samples are injected by hot nitrogen from the side-inlet point (inlet 1) and the sand particles are fluidized by hot nitrogen from the bottom distributor (inlet 0). Biomass composition is followed with the analysis of corn stalk samples: cellulose of 37.6 wt.%, hemi-cellulose of 21.6 wt.% and lignin of 18.4 wt.% [19]. As no extractives is presented in the simulations, the mass fractions of the three pseudo-components are translated to 48.5 wt.%, 27.8 wt.% and 23.7 wt.%, approximately. The gas and solid physical properties are given in Table 1.

2.2. Numerical model setup

In the current work, a three-fluid model is constructed including one gas phase and two solid phases of sand and biomass. All of the solid phases are treated as interpenetrating continua with individual volume fractions. The gas phase is a mixture of n_2, tar and syngas. Meanwhile one of the solid phases, s_1, is a mixture of biomass and char with the initial fractions of 1 and 0, respectively. The other solid phase, s_2, is sand. The multi-step kinetics of biomass fast pyrolysis is shown in Fig. 2 and the relevant reaction constants are given at Table 2 [7].

2.3. Mathematical model setup

The three-fluid model is extended by two-fluid model (TFM) with an additional solid phase. The governing equations have to be completed with the consideration of interactions between solid phases. The momentum exchange between the gas and solid phases is calculated by Gidaspow model [20] meanwhile that between solid phases is considered by Syamlal model [21]. The mass transfer in reactions is defined by the mass changes of different species. The consequent variations are presented in the momentum and energy conservation equations. The governing equations are summarized as follows.

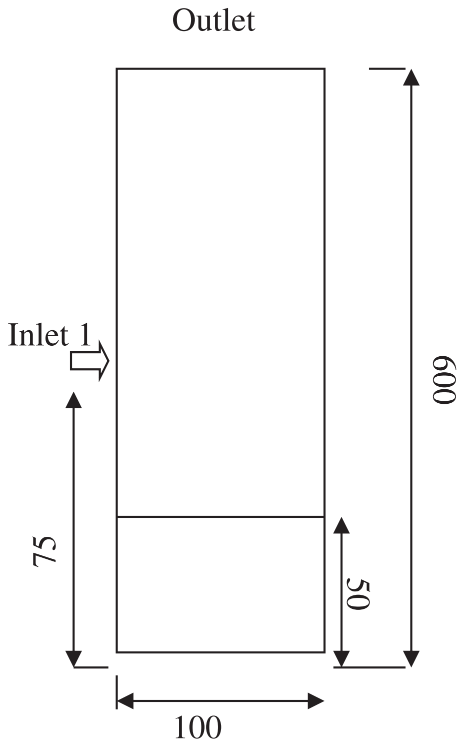

Fig. 1. Schematic of the fluidised bed reactor.

Table 1
Gas and solid physical property.

Property	Value	Unit	Comment
ρ_{bio}	400	kg/m^3	Biomass density
ρ_{cha}	200	kg/m3	Char density
ρ_{san}	2500	kg/m3	Sand density
Cp_{cha}	1100	J/kg · K	Heat capacity
Cp_{san}	835	J/kg · K	Heat capacity
μ_{n_2}	3.58e − 5	Pa · s	Viscosity
λ_{bio}	0.105	W/m · K	Heat conductivity
λ_{cha}	0.071	W/m · K	Heat conductivity
λ_{san}	0.35	W/m · K	Heat conductivity
d_{bio}	0.4	mm	Diameter
d_{san}	0.4	mm	Diameter

2.3.1. Gas phase

The species mass fraction is solved separately to represent the species mass balance:

$$\frac{\partial}{\partial t}\left(\alpha_g\rho_g Y_i\right)+\nabla\cdot\left(\alpha_g\rho_g v_g Y_i\right)=\dot{M}_i \tag{1}$$

where α_g, ρ_g, $\mathrm{Y_i}$, v_g, $\dot{\mathrm{M}}_\mathrm{i}$ are the local mass fraction, density, velocity of gas and the net production rate of species i, i = 1, 2, …, n, respectively.

The mass conservation of gas phase is written as

$$\frac{\partial}{\partial t}\left(\alpha_g\rho_g\right)+\nabla\cdot\left(\alpha_g\rho_g v_g\right)=\sum_{i=1}^{n}\dot{M}_i \tag{2}$$

The momentum conservation equation of gas phase is given with additional terms considering interphase interactions and momentum exchange by mass transfer. I is the momentum exchange due to

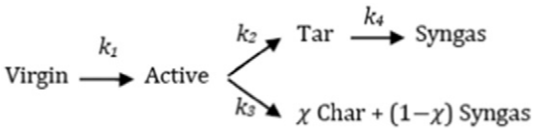

Fig. 2. Reaction sheme of biomass fast prolysis.

Table 2
Reaction constants of chemical kinetics of biomass pyrolysis [7].

Rate constant	$A_i(^1/_s)$	$E_i(J/kmol)$	Char yield (%)
$k_{1,cel}$	2.8×10^{19}	2.424×10^{8}	
$k_{2,cel}$	3.28×10^{14}	1.965×10^{8}	
$k_{3,cel}$	1.30×10^{10}	1.505×10^{8}	
χ_{cel}			0.35
$k_{1,hem}$	2.10×10^{16}	1.867×10^{8}	
$k_{2,hem}$	8.75×10^{15}	2.024×10^{8}	
$k_{3,hem}$	2.60×10^{11}	1.457×10^{8}	
χ_{hem}			0.6
$k_{1,lig}$	9.60×10^{8}	1.076×10^{8}	
$k_{2,lig}$	1.50×10^{9}	1.438×10^{8}	
$k_{3,lig}$	7.70×10^{6}	1.114×10^{8}	
χ_{lig}			0.75
k_4	4.28×10^{6}	1.08×10^{8}	