



A rigorous model for the simulation of chemical reaction in gas-particle bubbling fluidized bed: II. Application to gas combustion case

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ABSTRACT

Simulation of gas combustion process in bubbling fluidized beds (BFB) using the model proposed in Part I is carried out. The predictions are compared against the experimental measurements and good agreement is observed. It demonstrates that the turbulent Schmidt number is changing throughout the BFB. Therefore, the conventional way of using constant turbulent Schmidt number for the simulation of BFB is questionable.

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1. Introduction

The BFB gas combustors have been often applied in industry uses, i.e., calcinations of solids and incinerations of sludge [1], due to their simplicity of construction, versatility in handling a multitude of fuels with little retrofitting, and high efficiency at low temperature what reduces NO_x emission [2]. With the remarkable benefit mentioned above, gas combustion process in BFB has been investigated extensively through experiments. For instance, Hayhurst et al. [3–6] presented their experiments on combustions of mixtures of air with carbon monoxide, methane and propane. Zukowski et al. [7,8] and Dounit et al. [1,9] studied the combustion processes of natural gas. The previous experimental studies of gaseous combustions involved not only aliphatic, but also aromatic hydrocarbons, alcohols, ketones and esters [10].

In recent years, the computational fluid dynamics (CFD) simulation based on two-fluid model (TFM) has been proven to be able to give more detailed information on the hydrodynamic, heat, and mass transfer in fluidized bed (FB). Many studies involving chemical reactions in BFB have been carried out [11–18] including those on gas combustion. However, the prediction of species concentration is still relying on empirical method (e.g. guess a turbulent Schmidt number for the determination of turbulent mass diffusivity) which will no doubt increase

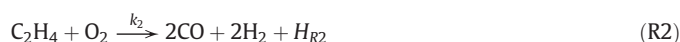
uncertainty of simulation. To avoid the use of Sc_t , a numerical model composed by the momentum, energy, and mass transfer equations, with their $k_g - \varepsilon_g - k_p - \varepsilon_p - \Theta$ [19], $t^2 - \varepsilon_t$ and the recently developed $\overline{c^2} - \varepsilon_c$ closing formulations [20] was proposed for simulating reactive multiphase flow in a BFB in part I of this work.

In this second part (Part II), the numerical model is introduced for simulating the combustion of air-propane mixture in a BFB. The present work includes the simulation of axial and radial profiles of species concentrations and the profiles of gas/solid velocities, and also the gas phase temperature. Then, the simulated results are compared with the published experimental measurements [21].

2. Model implementations

2.1. Simulation target

The object of the simulation is a combustion process of air-propane mixture in BFB. In the present study the following reaction scheme for the combustion is considered [22]:



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Nomenclature

D_g	molecular diffusivity, $\text{m}^2 \text{s}^{-1}$
$D_{t,g}$	turbulent mass diffusivity, $\text{m}^2 \text{s}^{-1}$
h_{gs}	heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$
H_{Rn}	heat of reaction, kJ kmol^{-1}
k_n	reaction rate, $\text{kmol m}^{-3} \text{s}^{-1}$
Nu_s	Nusselt number of the solid phase
S_{Ci}	net mass increase of species n
Sc_t	turbulent Schmidt number
$S_{T,g}$	gas phase thermal source term, $\text{kJ m}^{-3} \text{s}^{-1}$
$S_{T,s}$	solid phase thermal source term, $\text{kJ m}^{-3} \text{s}^{-1}$
t	time, s
T_{wall}	wall temperature, K
T_b	bed temperature, K
T_g	gas phase temperature, K
T_s	solid phase temperature, K
\vec{u}_g, \vec{u}_s	gas and particle velocity vectors, m s^{-1}
U_g	gas phase superficial velocity, m s^{-1}
H	total height of the BFB reactor, m
h	height of the BFB reactor from the bottom inlet, m
α_g, α_s	gas and solid volume fraction, respectively
λ_g	molecular thermal diffusivities of gas, $\text{m}^2 \text{s}^{-1}$
λ_s	thermal conductivity of solid, $\text{W m}^{-1} \text{K}^{-1}$



where the reaction rates, k_n , and the heat of reactions, H_{Rn} , are summarized in Table 1 [23].

Experimental data for comparisons with the model predictions are taken from the work of Hesketh and Davidson [21]. Their experimental conditions are as follows: the bubbling fluidized bed gas combustor is of 69.3 mm in diameter and 300 mm in height and is surrounded by an electrically heated furnace. The air-propane mixture with certain composition, temperature and speed is injected from the bottom of the combustor through a gas distributor. Properties of the solid particle and main operation conditions of the experiment are listed in Table 2. More detailed information are available in literature reported by Hesketh and Davidson [21].

2.2. Determination of source terms

The numerical model applied is that described in Part I. And the source terms in model equations should be determined so as to realize the simulation.

- (1) The source term S_{Ci} . The source term S_{Ci} represents the net increase rate of each species due to the combustion, and can be calculated according to the reaction rate summarized in Table 1 and the reaction stoichiometry. For example, the net increase rate of

Table 2

Solid particle properties and main operating conditions [21].

Particle size d_p (μm)	410
Particle density ρ_s (kg m^{-3})	2650
Expanded bed height H_{mf} (m)	0.098
Initial bed void ($-$)	0.45
Minimum fluidization velocity U_{mf} (m s^{-1})	0.058
Inlet propane concentration C_0 (vol%)	2.5
Gas superficial velocity U_g (m s^{-1})	0.278
Inlet gas temperature T_{g0} (K)	773
Bed temperature T_b (K)	1023–1223

propane in the gas phase could be determined by $S_{C, C_3H_8} = -k_1$; while for those of carbon dioxide and oxygen, the formulations of $S_{C, CO_2} = k_3$ and $S_{C, O_2} = -k_2 - \frac{1}{2}k_3 - \frac{1}{2}k_4$ are used.

- (2) The source terms $S_{T, g}$ and $S_{T, s}$. The thermal source term $S_{T, g}$ includes the heat from inert particles and the heat produced by the combustion:

$$S_{T, g} = h_{gs}(T_s - T_g) + \sum_{n=1}^4 k_n(-H_{Rn}) \quad (1)$$

The thermal source term $S_{T, s}$ represents the heat transferred from gas to the inert particles:

$$S_{T, s} = h_{gs}(T_g - T_s) \quad (2)$$

In which h_{gs} denotes the heat transfer coefficient $h_{gs} = 6\lambda_g\alpha_g\alpha_sNu_s/d_p^2$, where Nusselt number of the solid phase is determined by [24] $Nu_s = 2.0 + 0.6Re_p^{0.5}Pr^{0.33}$.

2.3. Computational domain and boundary conditions

The computational domain and boundary arrangement are shown in Fig. 1.

2.3.1. Inlet conditions

The gas is induced to the BFB from the bottom, and the inlet conditions are set to be [19,25]:

Gas phase:

$$\begin{aligned} \overline{U_{g, in}} &= U_g; k_g = 0.004\overline{U_{g, in}^2}; \varepsilon_g = 2k_{g, in}^2/(\kappa d_{col}); \\ \overline{C_{gn, in}} &= C_{gn, in}; \overline{c_{gn}^2} = (0.082\overline{C_{gn, in}})^2; \varepsilon_{cn} = R_\tau \left(\frac{\varepsilon_{g, in}}{k_{g, in}} \right) \overline{c_{gn}^2}; \\ \overline{T_{g, in}} &= T_{g, in}; \overline{t^2} = (0.082\overline{T_{g, in}})^2; \varepsilon_t = R_\tau \left(\frac{\varepsilon_{g, in}}{k_{g, in}} \right) \overline{t^2}; \end{aligned}$$

Solid phase:

$$\overline{U_{s, in}} = 0; k_s = 0; \varepsilon_s = 0; \Theta = 0.0001.$$

where the time scale ratio R_τ is set to be 0.73 [26].

Table 1

Reaction rate and heat of reaction [23].

Reaction	Reaction rate	Heat of reaction	Activation energy	
	k_n ($\text{kmol m}^{-3} \text{s}^{-1}$)	H_{Rn} (kJ kmol^{-1})	E_n (kJ kmol^{-1})	T_{bed} (K)
R1	$k_1 = 2.57 \times 10^{13} C_{C_3H_8}^{0.5} C_{O_2}^{1.07} C_{C_2H_4}^{0.4} \exp(-E_1/RT_g)$	1.834×10^8	204	1023
R2	$k_2 = 3.71 \times 10^{12} C_{C_3H_8}^{0.9} C_{O_2}^{1.18} C_{C_2H_4}^{-0.37} \exp(-E_2/RT_g)$	-2.735×10^8	214	≥ 1073
			212	1023
			218	1073
			230	≥ 1123
R3	$k_3 = 1.3 \times 10^{11} C_{CO}^{0.5} C_{H_2O}^{0.5} \exp(-E_3/RT_g)$	-2.820×10^8	126	-
R4	$k_4 = 2.45 \times 10^{11} C_{H_2}^{0.83} C_{O_2}^{1.42} C_{C_2H_4}^{0.56} \exp(-E_4/RT_g)$	-2.418×10^8	172	-

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