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Prediction of bubble fluidisation during chemical looping combustion using CFD simulation

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ABSTRACT

Bubble fluidisation in the fuel reactor adopted in chemical looping combustion (CLC) has a siganificant impact on the operation efficiency. Although a variety of numerical modellings of fluid dynamic process in the fuel reactors have been conducted, studies on predicting the fluidised bubble behaviours in the cylindrical fuel reactor where the effect of the heterogeneous reaction is also considered are still lacking. In this paper, the use of correlations of fluid dynamic parameters to characterise the fluidised bubble formation in the fuel reactor was proposed. A correlation parameter relating the time-dependent fluidised bubbles to the local eddies was introduced by correlating the local gas velocity fluctuation with the pressure fluctuation. The existence of a strong correlation between the concentration of gaseous reactants or products and local vortices was also demonstrated. Three-dimensional multiphase CFD model coupled with the heterogenoeous reaction kinetics was employed to study the details of CLC process in the fuel reactor. The results clearly indicated that the approach used in the present work can effectively monitor the formation of fluidised bubble in the dense fluidised bed during the heterogeneous reaction and may be used in the CLC as an indicator for monitoring the reduction rate as the locally embedded large eddies are strongly associated with the fluidised bubble occurrance.

1. Introduction

The fact that chemical looping combustion (CLC) can be used as a potential alternative to reduce the industrial CO_2 emission has been well recognised. The inherent separation process of CO_2 from other combustion products like N_2 and extra O_2 involved in the CLC can effectively minimise the energy penalty encountered when using other CO_2 capture and storage (CCS) technologies (Adanez et al., 2012; Kvamsdal et al., 2007). Until very recently, the small scale CLC plants varying from 300W to 140 kW have been constructed for demonstration (Abad et al., 2006; de Diego et al., 2007; Kolbitsch et al., 2009a,b; Linderholm et al., 2008). The conventional design of CLC unit consists of a fuel reactor usually a bubbling fluidised bed (BFB) and an air reactor which is a circulating fluidised bed (Lyngfelt et al., 2001). It is found that the performance of the whole CLC system is largely affected by the behaviours of the fuel reactor such as the fluidised bubble formation and incomplete combustion of fuel. In order to improve the efficiency of a CLC system, various modifications and improvements on the geometry of the fuel reactor have been performed. Penthor et al. (2015) attempted to replace the BFB fuel reactor working at turbulent fluidised regime to reduce the bypass fluidising bubbles and to increase the gas-solid contact. However, compared with BFB, higher attrition rate and controllable issues of turbulent regime are still the drawbacks. Son and Kim (2006) investigated the performance of double loop circulating fluidised beds and found that despite better gas-solid contact in fuel reactor, higher temperature increasing the reaction rate of oxide carriers (OCs) was required to compensate for the larger gaseous fuel rate required in fuel reactor. The dynamic packed bed chemical looping combustion (Noorman et al., 2010) was originally proposed to avoid the insufficient separation of gas and particles encountered in the interconnected fluidised beds, considering the protection issues of the gas turbine and energy savings. The carbon deposition occurred in previous packed bed was suppressed by the addition of steam. Impressive improvements have been made and it has been recently demonstrated to be a high efficiencies and high CO_2 capture rate CLC unit (Gallucci et al., 2015; Spallina et al., 2015).

As the internal phenomena of the CLC fluidised flow cannot be observed directly in the experiments of CLC system, CFD modelling was adopted to investigate and provide the physical insight into the complicated phenomena of the fluidising flow encountered in the CLC system, assisting the scale up of the CLC process, especially

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Nomenclature

A_0	Cross-sectional area of the cylindrical fuel reactor [m^2]
C	Bulk concentration of gaseous reactant [Mol/m^3]
C_D	Drag coefficient of drag model [−]
C_{CH4_TGA}	CH_4 concentration in TGA [mol/m^3]
d_p	Diameter of particle [m]
D_{gs}	The interaction between the fluctuating gas velocity and the fluctuating particle velocity [m^2/s^2]
e	Coefficient of restitution [−]
e_w	Wall restitution coefficient [−]
E_0	Activation energy [kJ/mol]
g	Acceleration due to gravity [m/s^2]
g_0	Radial distribution function [−]
h_{ij}	Heat transfer coefficient between gas and solid phase [W/m^2K]
H	Enthalpy [J/kg]
I	Unit tensor [−]
I_{2D}	Second invariant of the deviatoric stress tensor [s^{-2}]
$J_{i,p}$	Diffusive mass flux [kg/m^2]
k	Thermal conductivity [W/mK]
k_0	Reaction pre-exponential factor [$mol^{1-n}m^{3n-2}s^{-1}$]
$k_{\theta s}$	Conductivity of fluctuation energy [kg/ms]
$\dot{m}_{ij}$	Interphase mass transfer due to heterogeneous reaction [$kgm^{-3}s^{-1}$]
Nu	Nusselt number [−]
Pr	Prandtl number [−]
p	Gas pressure [N/m^2]
P_s	Solid pressure [N/m^2]
p'	Pressure fluctuation [N/m^2]
Q_{ij}	Interphase heat transfer from the i phase to j phase [W/m^2]
r_g	Mean radius of the grain [m]
R	Universal gas constant [$JK^{-1}mol^{-1}$]
Re_p	Renolds number of particles [−]
Re_t	Multi-particle Renolds number under terminal velocity condition [−]
Re_{ts}	Single particle Renolds number under terminal settling conditions [−]
R_{he}	Heterogeneous reaction rate [$kmol/m^3s$]
$R_{\overline{Y}_{CH_4}S_{AI}}$	Correlation between outlet CH4 concentration and gas-solid apparent interfacial area [−]
$R_{p'u'g}(\tau,z)$	Area-weighted time correlation between pressure fluctuation and gas phase velocity fluctuation [−]
$R_{\varepsilon'\varepsilon'}(\tau,z)$	Area-weighted time auto-correlation for gas-phase volume Fraction [−]
R	Universal gas constant [$JK^{-1}mol^{-1}$]
S_{AI}	Apparent gas-solid interfacial area [m^2]
S_i	Heat released due to chemical reaction [W/m^2]
$\boldsymbol{u}$	Instantaneous velocity [m/s]
u'_s	Solid velocity fluctuation [m/s]
u'_g	Gas velocity fluctuation [m/s]
U_{sl}	Slip velocity [m/s]
$u_{r,s}$	Terminal velocity correlation in syamlal-O'Brein drag model [−]
X	Conversion of oxygen carrier [−]
$Y_{i,p}$	Mass fraction of species p in phase i [−]

Special characters

ε	Volume fraction [−]
ε'_g	Gas-phase volume fraction fluctuation [−]
ρ	Density [kg/m^3]
ρ_m	Molar density of the particle [mol/m^3]
μ_i	Dynamic viscosity for gas phase or solid shear viscosity [$N.s/m^2$]
$\mu_{s,col}$	Solid collision viscosity [kg/ms]
$\mu_{s,kin}$	Solid kinetic viscosity [kg/ms]
$\mu_{s,fr}$	Solid frictional viscosity [kg/ms]
β_{ij}	Interphase drag coefficient [kg/m^3s]
λ_i	Bulk viscosity [$N\ s/m^2$]
τ_i	Stress tensor of i_{th} phase [N/m^2]
Θ_s	Granular temperature [m^2/s^2]
$\boldsymbol{\Phi}$	Exchange of fluctuation energy [kg/ms^2]
γ	Dissipation rate [kg/ms^3]
ξ	Angle of internal friction [−]
$\boldsymbol{\tau}$	Time increment in time-dependent correlation [s]
$\boldsymbol{\tau_i}$	Gas or solid phase stress tensor [N/m^2]

Subscripts

i or j	Gas or solid phase
dense	Dense phase
thin	Dilute phase

in the FR as evidenced in (Deng et al., 2008, 2009; Harichandan and Shamim, 2014; Jung and Gamwo, 2008; Kruggel-Emden et al., 2011). Wang et al. (2015) conducted a 2-D CFD model to simulate the CLC flow in a DCFB coupled with heat transfer. The results showed that good agreement with the experimental data was obtained and the variation of gas concentration in the axial direction was larger in dense phase than dilute phase. The radial variation of both the gas species concentration and the gas-solid fluidised flow, however, were not revealed because of the constraint of the intrinsic features of 2D geometric models. Peng et al. (2014) conducted full 3-D simulations based on cold flow model of the full CLC system using CFD-DEM approach to investigate the effects of operation parameters on the performance of CLC system and found that the fluctuations of solid circulating rate was resulted from the turbulent regime in the air reactor. Wang et al. (2011) conducted a 3D simulation on a bubbling fluidised bed fuel reactor with a rectangular cross section to study the hydrodynamic and chemical kinetic behaviours of the CLC process. It was founded that decreasing gas superficial velocity or particle diameter could increase the fuel conversion efficiency and less concentration of gas products were found in the bubble phase compared with the emulsion phase in the fuel reactor. Parker (2014) developed a 3-D Computational Particle Fluid Dynamics (CPFD) model coupled with the chemical reactions to predict the first 50 s of the hydrodynamics and chemical kinetic performance of a full CLC loop with coal as the fuel where solid particles were modelled by Lagrangian method and Eulerian approach for gas phase. The fluid hydrodynamics were well described by the simulation and parameters affecting CLC operations like efficiencies of air and fuel reactors (57% and 23%) for designed gas flow rates, the solid circulation rate and temperature profiles are obtained.

Based on the open literatures, most of the improvements focus on improving the gas-solid contact in fuel reactors through altering the configurations of CLC systems so as to increase the reduction efficiency. Limited researches are found to reveal the relationships between the local fluid dynamics, mass transfer and those fluidising bubbles occurring in the fuel reactor. Busciglio et al. (2008) experimentally studied the bubbling behaviours of 2D gas-sold fluidised bed with CCD camera. Matlab Image Processing Toolbox was employed to process the image to obtain bubble properties. Followed by the experimental study, they also conducted the CFD simulation of 2D fluidised bed. Bubbling behaviours were