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Prediction of formation of gas-phase bubbles correlated by vortices in the fuel reactor of chemical looping combustion

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ABSTRACT

Chemical looping combustion (CLC) as a potential CO_2 capture technology has been considered as a promising and likely alternative to traditional combustion technology to mitigate the CO_2 emission due to its prosecution of CO_2 sequestration at a low cost. Although a number of studies on the hydrodynamic behaviours of the CLC process in fuel reactor have been documented in the open literature, there have been rare studies on the correlation between the bubble formation and the local particulate volume fraction. This paper aims to investigate the CLC process in a fuel reactor using the CFD modelling, coupled with the heterogeneous reactions, the hydrodynamics and reaction kinetics occurring in the fuel reactor. A parameter correlating the occurrence of bubble and dynamic properties is proposed. The parameter may be acted as an indicator of time-dependent bubble evolution with a potential to be adopted in the CLC for controlling the bubbling phenomena since the occurrence of the bubbles at specific positions is highly correlated with the local large eddies embedded in the flow. The results obtained clearly indicate that the CFD model developed in the current study reasonably forecasts the hydrodynamic behaviours and important phenomena observed in the fuel reactor.

1. Introduction

Chemical looping combustion (CLC) has been considered as a promising alternative to traditional combustion technology to mitigate the CO_2 emission due to the potential of CO_2 sequestration at a very low cost. According to the estimation, a coal-fired power plant needs to consume around 20% of the total electricity generated to separate and compress the produced CO_2 in the combustion while CO_2 separation process is responsible for almost three-fourths of the whole energy consumed in the process [1,2]. In addition, coal combustion causes enormous environmental problems. Thus, the application of the CLC may partially resolve the problem. In a CLC, solid oxygen carriers, usually highly-reactive metal particles, are introduced to transfer the oxygen necessary for the combustion from air through the initial oxidation in air reactor and to subsequently realize the reduction in fuel reactor. Until very recently, most of the adopted CLC reactors are based on fluidised bed technology due to its distinct benefits of uniformed particle mixing and temperature gradients together with the continuous operation mode in the fluidised bed reactor. Meanwhile, the bubbling fluidised bed is usually acted as the fuel reactor due to the benefits of controllable handling of particles, high heat flow and relatively high rate of gas–solid reaction due to the large gas–solid contact area [3]. So far, the most common type of CLC reactor is composed of a conventional circulating fluidised bed operated as the air reactor and a bubbling fluidised bed acted as the fuel reactor. It should be noticed that the use of the packed [4], moving [5,6] or circulating fluidised bed [7] to operate as the fuel reactor has also received attention and has been investigated to assess their capabilities. A schematic of the typical CLC unit is shown in Fig. 1 [8].

Development of oxygen carriers, fundamental design of the CLC reactor and the CLC system analysis has been documented [9–11]. Experimental studies on the CLC systems operated with different types of fuels in the range from 300 W to 140 kW have been performed [12–16], with the findings being summarised in the literature [10,11]. Kolbitsch et al. assessed the capability of Ni-based oxygen carriers within a 120 kW dual circulating fluidised bed reactor system [12] and the authors found that the oxygen reduced in both syngas and methane conversion processes when using such system is significantly improved. It was identified that besides high reactivity and oxygen transport capacity, no tendency to agglomeration is presented by Ni-based oxygen carriers except for NiO/TiO_2 [17]. The studies [18,19] have reported that high fuel conversion up to 98–99% without gas leakage was observed within the long-term run of the 10 kW CLC unit using Ni-based oxygen carriers. When other oxygen carriers are used, Garcia-Labian et al. revealed that the sulfur compound like H_2S in fuel gas deactivates the reactivity of Ni-based particles and reduces the combustion efficiency because of the formation of nickel sulfide [20].

Compared with the experimental approach for investigation of the CLC, computational fluid dynamics (CFD) approach can be easily

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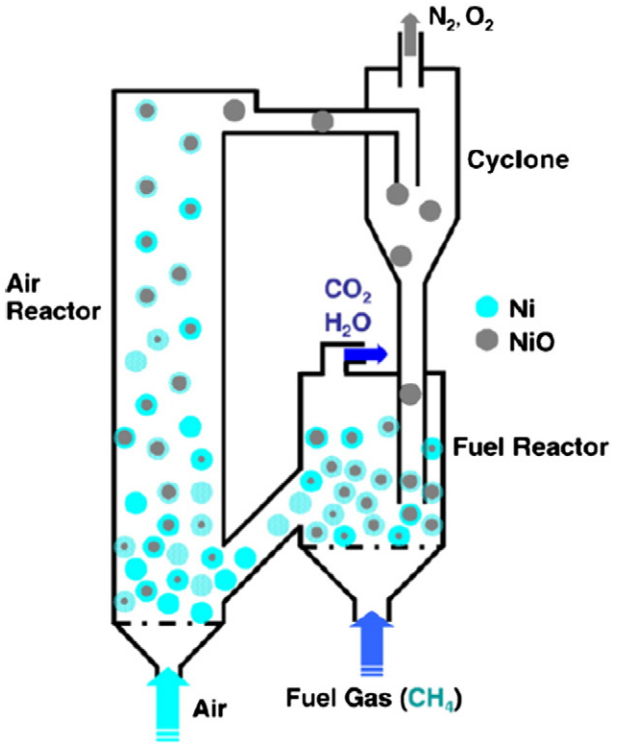

Fig. 1. Schematic of two interconnected CLC reactors [8].

conducted to investigate the interactions between hydrodynamics and chemical kinetics of the CLC process with a compromise between the level of accuracy and the computational cost. In CFD modelling of the CLC process, both gas and solid phases are treated as continuous and interpenetrating phases in the time and phase averaged Navier–Stokes equations. Wang et al. and Seo et al. investigated, respectively, the hydrodynamic behaviours of the full CLC loop using the simplified two-dimensional cold-flow model [21,22]. CFD modelling of the flow behaviours and reactive characteristics of different oxygen carriers in the fuel reactors was also reported [8,23,24] and the predictions were in reasonable agreement with the experimental results. Kruggel-Emden et al. developed a 2-D interconnected multiphase CFD model using a buffer which can maintain a stable and sufficient solid flow rate in the fuel reactor. In their CFD modelling, the air reactor and the fuel reactor are simulated separately, involving an exchange of solid flow by using the time-dependent sinks and specifying the suitable boundary conditions [25]. Wang et al. studied the CLC process in the DCFB reactors using CFD code — a revised K-FIX programme with implementation of the reaction kinetics [26] into the simulation. A reasonable agreement between the simulation and experimental results was claimed. Although these studies have provided to some extent the physical insights into the fluid dynamics involved in the CLC process, there are many fundamental problems that remained to be resolved, e.g. how the bubble formation correlates with large vortices in the fuel reactor. In the present study, an attempt to develop a CFD model coupled with heterogeneous reaction for analysing the CLC process in the fuel reactor will be made, aiming at partially answering the above question. Methane is chosen as fuel gas while NiO coated on $NiMgAl_2O_4$ particles will be used as the oxygen carrier, similar to the work reported in [27,28].

The paper will be organised in such a way. Section 2 will present the mathematical modelling adopted in the current study while Section 3 will present the simulation results and discussion, focusing on bubble formation and distributions of reactants and products in the fuel reactor and characterisation of the bubbling using the correlation between the velocity fluctuations and local volume fraction. Section 4 will present the conclusions derived from the study.

2. Mathematical modelling

This study assumes the solid particles in the fuel reactor to be spherical and uniform in size and density. The commercial CFD software ANSYS FLUENT was employed to carry out the simulation. Eulerian–Eulerian two-fluid model was used to describe the continuity, exchange of momentum, heat and mass transfer between gas–solid flows while the kinetic theory of granular flow was adopted to model the solid phase. The governing equations are described below:

2.1. The continuity equations

For gas phase

$$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_g\right)=S_{gs}. \tag{1}$$

For solid phase

$$\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\right)+\nabla\cdot\left(\varepsilon_s\rho_s\boldsymbol{u}_s\right)=S_{sg} \tag{2}$$

where $S_{gs}=-S_{sg}$ accounts for the mass transfer between gas and solid phases due to heterogeneous reactions; and ε, ρ, and $\boldsymbol{u}$, are the volume fraction, density and instantaneous velocity respectively. The sum of the volume fraction of each phase must be equal to one.

2.2. Momentum balance equations

The momentum equations for both phases are given respectively by Eqs. (3) and (4):

$$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\boldsymbol{u}_g\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_g\boldsymbol{u}_g\right)=-\varepsilon_g\nabla p+\nabla\tau_g+\varepsilon_g\rho_g\boldsymbol{g}-\beta\left(\boldsymbol{u}_g-\boldsymbol{u}_s\right)+S_{gs}\boldsymbol{u}_g \tag{3}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\boldsymbol{u}_s\right)+\nabla\cdot\left(\varepsilon_s\rho_s\boldsymbol{u}_s\boldsymbol{u}_s\right)=-\varepsilon_s\nabla p+\nabla\tau_s-\nabla P_s+\varepsilon_s\rho_s\boldsymbol{g}+\beta\left(\boldsymbol{u}_g-\boldsymbol{u}_s\right)+S_{sg}\boldsymbol{u}_s \tag{4}$$

where β is the interphase drag coefficient, $\boldsymbol{g}$ is the gravity, p is the gas pressure and P_s is the solid pressure. Constitutive closure models are adopted to provide the constitutive equations which are essential for the closure of the governing equations. The gas and solid tensors are given by Eqs. (5) and (6)

$$\boldsymbol{\tau}_g=\mu_g\left(\left(\nabla\boldsymbol{u}_g+\left(\nabla\boldsymbol{u}_g\right)^T\right)-\frac{2}{3}\left(\nabla\cdot\boldsymbol{u}_g\right)\boldsymbol{I}\right) \tag{5}$$

$$\boldsymbol{\tau}_s=\mu_s\left(\left(\nabla\boldsymbol{u}_s+\left(\nabla\boldsymbol{u}_s\right)^T\right)-\frac{2}{3}\left(\nabla\cdot\boldsymbol{u}_s\right)\boldsymbol{I}\right)+\lambda_s\left(\nabla\cdot\boldsymbol{u}_s\right)\boldsymbol{I} \tag{6}$$

where, μ_g is the dynamic viscosity for gas phase and μ_s is the solid shear viscosity which will be discussed in the latter section. λ_s represents the solid bulk viscosity, and $\boldsymbol{I}$ is the unit tensor.

2.3. Energy equations

The energy balance equations of gas and solid phases are given by:

$$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_gH_g\right)+\nabla\cdot\left(\varepsilon_g\rho_g\boldsymbol{u}_gH_g\right)=\nabla\cdot\left(k_g\nabla T_g\right)+Q_{gs}+S_{sg}H_g \tag{7}$$