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Three-dimensional full loop simulation of solids circulation rate in an interconnected fluidized bed

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Abstract

3-D full loop CFD simulation of solids circulation rate is conducted in a complicated circulating-fluidized bed, which consists of a riser, a bubbling bed, a cyclone and a loop-seal. The effects of operating gas velocity, particle diameter and total solids inventory on the solids circulation rate are investigated based on the system pressure balance of an interconnected fluidized bed. CFD results indicate that the gas velocity in the riser plays a dominant role in controlling the solids circulation rate, whilst the gas velocity in the pot-seal influences in a narrow operating range. The solids circulation rate is strongly influenced by particle diameter and total solids inventory, but becomes insensitive to the operating conditions in the bubbling bed as the gas velocity is higher than the minimum fluidization velocity.

Key words: 3-D full loop; CFD simulation; Solids circulation rate; Interconnected fluidized bed; Chemical looping combustion

1. Introduction

Chemical looping combustion (CLC) is a novel and economic technology for CO_2 capture, which has been intensively investigated over the past twenty years [1,2]. Comparing with other CO_2 capture strategies, oxygen is transferred from air to fuel through oxygen carriers in a CLC plant, avoiding direct contact between air and fuel [3,4]. Generally, a CLC system consists of two separate reaction zones, as shown in Fig.1. Metal (Me) particles are oxidized to metal oxide (MeO) particles in air in the oxidation zone, which is then transferred to the reduction zone where the fuel reduces them into CO_2 and H_2O. There is no or little energy loss for the separation of CO_2 in the CLC process [5], because the relatively pure stream of CO_2 can be obtained after condensing and purifying H_2O. The circulation of oxygen carriers between the two reaction zones not only plays an important role in transporting oxygen needed for the combustion, but also maintains the system heat balance. The heat carried by the oxygen carriers from the oxidation reaction zone is supplied to the endothermic reaction in the reduction zone. Thermodynamically, the total amount of heat from the two reactions is the same as that from conventional combustion, where the fuel is in direct contact with air [6]. Stable circulation of oxygen carriers between the two reaction regions is critical to achieve a high thermal efficiency and high CO_2 capture efficiency.

Fig. 1. Schematic of chemical looping combustion process

Quite a few CLC configurations have been proposed [6-11]. The interconnected fluidized bed configuration, which is based on the principle of circulating fluidized bed including a high-velocity riser (air reactor) and a low-velocity bubbling bed (fuel reactor), has been identified as one of the promising choices [6,12,13]. For this design, a higher particle residence time for the reduction reaction and a lower particle residence time for oxygen reaction can be achieved based on the oxygen carrier reactivity [14]. It can provide excellent gas-solids contact in each reactor, and also handle particles at an adjustable circulation rate between the two reactors. However, the gas leakage between the air reactor and the fuel reactor is a major problem, which decreases the reliability and efficiency of CLC systems. As the gas leakage is closely related to the solids circulation rate [15], it is essential to understand the solids circulation behaviour and the influence of various operating conditions in order to achieve better design and operational efficiency for any interconnected fluidized bed.

Computational fluid dynamic (CFD) is regarded as a promising technology for predicting the complex hydrodynamics and related characteristics in a fluidized bed. Some efforts have been carried out on the CFD simulation of chemical looping combustion processes [10,16-29]. However, only a few investigations have been focused on the full loop simulation of the interconnected fluidized bed, due to the complexities in geometry and flow physics, which requires large computational resources [1,28]. Kruggel-Emden et al. [20] applied the exchanges of mass, momentum, heat and species sinks through time-dependent inlet and outlet boundaries to couple the fuel reactor and air reactor. Seo et al. [10], Wang et al. [21] and Nguyen et al. [24] conducted 2-D full loop simulation of the interconnected fluidized bed to investigate the hydrodynamic behaviours and compared with experimental data. However it is questionable to apply 2-D simulation data to a 3-D operation due to the influences of the bed walls and geometry of non-symmetric flow [30,31]. For 3-D full loop simulation of the chemical looping combustion process, Parker et al. [26] predicted the gas-solids hydrodynamics, thermal characteristics and reaction efficiency by the computational particle fluid dynamics (CPFD) method. Very recently, a 3-D full loop simulation was conducted to investigate the solids circulation in a dual circulating fluidized bed composed of a riser and a turbulent bed [29]. In our previous work, the Eulerian-Eulerian method was employed to predict the hydrodynamics in a 3-D full-loop interconnected fluidized bed for CLC applications, and the coupled effect of operational conditions on the fluid dynamics was explored between the riser and the bubbling bed [28]. The work compared the effect of various drag models, and revealed a non-uniform distribution of the solids volume fraction in the riser and bubbling bed, without considering the detailed information on solids circulation rate, which is essential to prevent gas leakage and achieve a reliable operation for any CLC plant. Continuing from our previous work, this study is focused on the solids circulation rate in a 3-D full loop interconnected fluidized bed, where detailed solids circulation characteristics and the influence of solids property and operational condition, including particle diameter, total solids inventory and operating gas velocity, were simulated. Predicted results were carefully analysed based on the system pressure balance in the interconnected fluidized bed, and the implication to the CLC operation was revealed.

2. CFD simulation

2.1. CFD modelling

The Eulerian-Eulerian model together with the kinetic theory of granular flow (KTGF) is used to predict the gas-solids flow in the interconnected fluidized bed. In the two-phase model, the gas and solids phases are mathematically treated as interpenetrating continua with appropriate interaction terms. The volume fraction represents the space occupied by each phase, and the conservation equations of mass and momentum for each phase are derived with similar structures. Table 1 gives details of the conservation equations. Eqs. (1) and (3) are the continuity conservation equations for gas and solids phases, respectively. Here, α is the volume fraction (α_g+α_p=1), ρ is the density and $\vec{u}$ is the velocity vector. The gas phase momentum conservation equation is expressed by Eq. (2), where β is the gas-solids inter-phase momentum transfer coefficient, $\vec{g}$ is the acceleration due to gravity, and $\bar{\bar{\tau}}_g$ is the gas phase stress-strain tensor and expressed by Eq. (6). The standard k-ε turbulent model is used for modelling turbulence of gas phase where μ_{gt} is the turbulent viscosity; k and ε represent the turbulent kinetic energy and dissipation rate of turbulent kinetic energy. The constants in Eqs. (9) and (10) are C_μ = 0.09, C_1 = 1.44 and C_2 = 1.92 respectively. The turbulent Prandtl numbers for k and ε are σ_k =1.0 and σ_ε =1.3. G_k is defined as the generation of turbulent kinetic energy due to the mean velocity gradients.

Eq. (4) is the solids phase momentum equation, where p_p is the solids pressure and $\bar{\bar{\tau}}_p$ is the solids stress-strain tensor. The kinetic theory of granular flow is used to describe the rheology of the particle phase. Eq. (5) is solved to account for the conservation of solids fluctuating energy. The two terms on the left hand side of Eq. (5) describe the accumulation and convection of kinetic fluctuation energy, respectively. The first term on the right hand side describes the production of kinetic fluctuation energy due to irreversible deformation of the velocity field, the second term describes the conductive transport of kinetic fluctuation energy, the third term represents the fluctuation energy dissipation due to inelastic particle-particle interactions, and the last term represents the exchange of fluctuation energy due to interphase momentum transport. The solids pressure p_p, which represents the normal force due to particles interaction, is calculated by the expression from Lun et al. [32].

The first term on the right hand side of Eq. (13) is the kinetic term and the second term represents the particle collisions. The solids shear viscosity is defined as the sum of the collisional viscosity, kinetic viscosity and frictional viscosity as expressed in Eqs. (14)-(17). The bulk viscosity for the particle phase accounts for the resistance of granular particles to compression and expansion, and the Lun et al. [32] expression is used in this work. The radial distribution function of solids phase takes into account the probability of collisions of the particles, and expressed by Eq. (21). The drag force is more important than other types of inter-phase forces due to the large difference between the gas and particle phases, and the drag force acting on a particle in a gas-particle system can be represented by the product of a momentum transfer coefficient and the slip velocity between the fluid and solid phases. The correlation given by Gidaspow [33] is used in this study (Eqs. (23)-(26)), which combines the Ergun equation (Eq. (23)) and the Wen-Yu model (Eq. (24)) to calculate the inter-phase momentum transfer coefficient (β) in the dense phase and dilute phase.

Table 1 Conservation equations of gas-solids flow

Table 2 Constitutive equations for momentum

A three-dimensional (3-D) geometry of the interconnected fluidized bed, including riser, bubbling bed, pot-seal and cyclone for chemical looping combustion, was selected as the simulation object (Fig. 2). The geometry was the same as the experimental configuration in Johansson et al. [15]. Silica sand was adopted as the solids phase with density of 2600 kg/m^3 and mean diameter of 150 μm, and air was used as the gas phase with density of 1.19 kg/m^3 and viscosity of 1.81×10^{-5} Pa·s. The velocity boundary conditions were selected for the inlets of the riser, the bubbling bed and the pot-seal; the pressure conditions were specified at the outlets of the bubbling bed and the cyclone outlets. For the walls of the riser and bubbling bed, the no-slip condition was assumed for the gas phase, the partial-slip condition proposed by Johnson and Jackson [34] was applied for the particle phase. A grid system including 482,465 computational cells was employed based on the grid independency analysis. A time step of 1×10^{-3}s was selected for this study. Detailed description of the numerical process was provided in our previous work [28].

Fig. 2 Layout of the interconnected fluidized bed for chemical looping combustion

2.2. Simulation conditions

Accurate knowledge of the minimum fluidization velocity (u_{mf}) is fundamental in understanding the hydrodynamic behavior of a fluidized bed. Generally, the operating gas velocity in proportion to the minimum fluidization velocity was investigated to explore its effect on solids circulation rate in the interconnected fluidized bed [10,35-37].

The minimum fluidization velocity is the superficial gas velocity at which particles are just suspended in the fluid [38]. The onset of fluidization occurs when the drag force by the upward moving gas is equal to the weight of particles. If the effect of friction between the gas/particles and wall is ignored, the following equation can be obtained based on the static analysis

$$\Delta p A_c = H_{mf} A_c [(1-\varepsilon_{mf})\rho_p g + \varepsilon_{mf}\rho_f g] \tag{27}$$

By combined Eq. (27) and the Ergun equation for packed bed [39], the expression at the minimum fluidization condition is given by

$$\frac{1.75}{\phi_s {\varepsilon_{mf}}^3}\left(\frac{d_p u_{mf}\rho_f}{\mu}\right)^2 + \frac{150(1-\varepsilon_{mf})}{{\phi_s}^2 {\varepsilon_{mf}}^3}\left(\frac{d_p u_{mf}\rho_f}{\mu}\right) = \frac{d_p^3 \rho_f(\rho_p-\rho_f)g}{\mu^2} \tag{28}$$

where Φ_s is the particle sphericity.

For different fluid-solids systems, Wen and Yu [40] obtained the following approximate relationships

$$(1-\varepsilon_{mf})/{\phi_s}^2{\varepsilon_{mf}}^3 \cong 11 \tag{29}$$

$$1/(\phi_s{\varepsilon_{mf}}^3) \cong 14 \tag{30}$$

The quadratic to determine the minimum fluidization velocity is obtained by combined Eqs. (28), (29) and (30)

$$\frac{d_p u_{mf}\rho_f}{\mu} = \left[C_1^2 + C_2\frac{d_p^3\rho_f(\rho_p-\rho_f)g}{\mu^2}\right]^{\frac{1}{2}} - C_1 \tag{31}$$

Grace [41] suggested that C_1=27.2 and C_2=0.0408 were more suitable for gas-solids systems in Eq. (31), which was widely employed to calculate the minimum fluidized velocity for Geldart type B particles [42-45]. To investigate the effect of operating gas velocity on the solids circulation rate, the minimum fluidization velocity was calculated as 0.02367 m/s according to Eq. (31) in this study. Table 3 summarizes the operating conditions examined in the simulations.

Table 3 Operating conditions for simulations

A preliminary study was initially conducted to determine the time-averaged solids behaviour. Fig. 3 shows the solids volume fraction along the bed height in the riser. In the first 20 seconds, the time-averaged solids volume fraction decreased in the lower part of the riser with increasing the simulation time. When the simulation time was increased to 30 s, the 20-30 s time-averaged result was closed to that of 30-40s. This implied that the time-averaged results in the range of 20-30 s could be regarded as the steady-state conditions, which were used in the following discussions.

Fig. 3. Axial profiles of time-averaged solids volume fraction in the riser

3. Results and discussion

3.1. Pressure balance analysis

The pressure balance is one of the key issues for the interconnected fluidized bed system to prevent gas leakage and ensure solids circulation between the riser (air reactor) and the bubbling bed (fuel reactor). As presented in Fig. 4, the pressure balance in the full loop of the interconnected fluidized bed can be expressed as

$$\Delta P_{riser} + \Delta P_{duct} + \Delta P_{cycl} + \Delta P_{dc1} + \Delta P_{dc2} = 0 \tag{32}$$

where ΔP_{riser} is the pressure drop in the riser between the centerlines of particle returning leg and the exit of riser, ΔP_{duct} is the pressure drop of the exit duct, ΔP_{cycl} is the pressure drop in the cyclone, ΔP_{dc1} and ΔP_{dc2} are the pressure drop in the bubbling bed downcomer and pot-seal downcomer, respectively.

In order to ensure solids transportation and minimize the gas leakage between different compartments, two particle seals, i.e., one separated pot-seal and one seal at the bottom of the bubbling bed, were used in the interconnected fluidized bed. The flow of solids through the downcomer was considered as a moving bed flow, and the solids were transported by the overflow effect in the pot-seal. The pressure drop in the downcomer could be divided into two parts: a dilute zone with little particles and a dense zone containing high solids column (Fig. 4). Generally, the pressure in the former region was neglected. However, it must be pointed out that the dense zone in the downcomer was a key part for the interconnected fluidized bed due to the high pressure in this region, and they were also responsible for the closure of the system pressure balance [46]. Fig. 5 shows that the pressure in the cyclone was lower than those in the pot-seal and lower part of the riser. The pressure in the bubbling bed was higher than that of the cyclone, whilst lower than that in the riser and the pot-seal. This was consistent with the experimental observations [15].

Fig. 4. Pressure balance in the interconnected fluidized bed

Fig. 5. Pressure profile in the interconnected fluidized bed

3.2. Effect of gas velocity in the riser

Fig. 6 shows the variation of solids circulation rate (G_s) by varying the superficial gas velocity in the riser ($u_{g,r}$). The solids circulation rate increased significantly with increasing gas velocity $u_{g,r}$ due to the decreased pressure drop in the riser. This trend indicated that the gas velocity in the riser provided the momentum to the upward transportation of the solids, which, in turn, controlled the solids circulation between the riser and the bubbling bed. The flow pattern could directly affect the gas-solids mixing as well as heat and mass transfer in the bubbling bed [47]. Our previous studies have shown that the higher solids circulation rate produced a higher bed height and solids volume fraction, promoting the mixing of solids and gas in the bubbling bed [28]. However, further increase in the $u_{g,r}$ would lead to a higher leaving rate of particles than the return rate in the riser, which led to the blockage in the pot-seal. As a result, the system pressure balance was broke due to insufficient total solids inventory in the riser. This was the reason why a decrease in solids circulation rate occurred at $u_{g,r}$=2 m/s.

Fig. 6. Effect of the superficial gas velocity $u_{g,r}$ on solids circulation rate in the riser

3.3. Effect of gas velocity in the pot-seal

Non-mechanical valve of pot-seal was used in a hot prototype investigated in this study, which has the advantage of operation in high temperature and pressure conditions [10]. In this study, the pot-seal was operated in the bubbling fluidization regime. When the gas was introduced to the pot-seal, a portion of gas flowed into the downcomer to develop the necessary pressure seal, and then the friction effects among particles were reduced by means of the airflow. The solids flow back into the riser by means of an overflow orifice. With the increase in gas velocity $u_{g,p\text{-}t}$, the bubbles caused the bed to expand further over the outlet of the pot-seal. As a result more particles overflow into the recycle pipe, resulting in a higher solids circulating rate. This is clearly shown in Fig. 7 at different gas velocity of the pot-seal. The solids circulation rate increased gradually from 62 $kg/m^2 \cdot s$ to 98 $kg/m^2 \cdot s$ as the gas velocity increased from u_{mf} to 4 u_{mf} (i.e, u_{mf}=0.02367 m/s). Slight decrease in solids circulation rate was obtained when the superficial gas velocity $u_{g,p\text{-}t}$ reached 0.12 m/s, which was due to the slug occurred in the standpipe and the bubble motions hindered the particle flow, resulting in a reduced solids circulation rate. However, to compare with the hot prototype [15], the pot-seal was not scaled in this study (Fig.2), and the effect of $u_{g,p\text{-}t}$ was amplified in the simulation. For a practical setup where the pot-seal will be smaller in scale, the effect of pot-seal on the solids circulation rate shall be much smaller. In addition, the gas leakage issue would become serious at higher gas velocities [15]. Consequently, a proper gas velocity shall be used in the pot-seal, where in practice a velocity slightly exceeding the minimum fluidization velocity is adopted, by considering the combined effect of solids circulation and gas leakage

Fig. 7. Effect of the superficial gas velocity $u_{g,p\text{-}t}$ on solids circulation rate in the pot-seal

3.4. Effect of gas velocity in the bubbling bed

The effect of superficial gas velocity in the bubbling bed ($u_{g,b}$) on the solids circulation rate (G_s) is shown in Fig. 8. It was observed that the solids circulation rate increased from 38 kg/m^2·s to 85 kg/m^2·s with increasing superficial gas velocity $u_{g,b}$ from 0.015 m/s to 0.024 m/s. This was because both the solids volume fraction and pressure drop in the bubbling bed increased with increasing $u_{g,b}$, which increased the pressure head in the downcomer to push more solids into the riser through the pot-seal. However the solids circulation rate become insensitive to the gas velocity when the gas velocity $u_{g,b}$ was greater than the minimum fluidization velocity u_{mf}; the values of solids circulation rate were maintained at almost constant ~85 kg/m^2·s. This phenomenon could be explained by the change of pressure drop corresponding to the gas velocity in the bubbling bed. When the gas velocity $u_{g,b}$ was lower than u_{mf}, the pressure drop in the bubbling bed increased with increasing volumetric flow rate of air, and more particles flowed into the riser through the pot-seal. As $u_{g,b}$ was higher than u_{mf}, a constant pressure drop was established resulting in stable solids circulation rates. This observation was consistent with the previous experimental observations in dual fluidized beds [10,35]. On the other hand, Jung et al. [16], Deng et al. [17] and Wang et al. [25] observed that the high weight fraction of unburned fuel in the flue gas was detectable due to fast, large bubbles rising through the fuel reactor (bubbling bed). Therefore, it must be careful in determining the operational gas velocity of the bubbling bed in a hot unit.

Fig. 8. Effect of the superficial gas velocity $u_{g,b}$ on solids circulation rate in the bubbling bed

3.5. Effect of particle diameter

Fig. 9 shows the effect of particle diameter (d_p) on the solids circulation rate (G_s)

when the operating gas velocities were fixed. Smaller particles diameter resulted in higher solids circulation rates as expected. It was attributed to a smaller particle settling velocity, resulting that particles accelerated upward in the riser and then more particles flowed from the bubbling bed to the pot-seal form the solids circulation loop. In addition, a decrease in particle diameter could decrease the bubble size, which, in turn, would increase the gas-solids contact area and the conversion of fuel particles in the reactor [16,25]. However, it shall be cautious to decrease particle size. Abad et al. [48] found the increase in the solids circulation flow actually caused a decrease in the char conversion, possible due to reduced residence time, and CO_2 capture efficiency was subsequently reduced. Cleary both the fluidization behavior and the chemical reaction characteristics of the oxygen carrier need to be taken into account in determining the appropriate particle diameter.

Fig. 9. Effect of the particle diameter d_p on solids circulation rate

3.6. Effect of total solids inventory

Fig. 10 shows an example of the influence of the total solids inventory. As the total solids inventory increased, the hydrostatic pressure, which pushed particles from the bubbling bed to the riser through the pot-seal, increased, and increased the particle elutriation in the riser. Moreover, the extension of the dense zone in the riser was observed due to a higher solids inventory, which was consistent with the experimental observations [49-51].

As summarized in Table 4, higher total solids inventory resulted in higher solids circulation rate for a given operating gas velocity, and the trend was more obvious at higher gas velocity in the riser. This was because the pressure in the interconnected fluidized bed, including the riser, the cyclone, the bubbling bed and the pot-seal, increased with increasing the total solids inventory. Hence the corresponding pressure in the standpipe was increased to balance the pressure change of other parts.

Fig. 10. Solids volume fraction distribution with different total solids inventory (d_p = 150 μm, $u_{g,r}$ = 1.5 m/s, $u_{g,b}$ = 0.12 m/s, $u_{g,p\text{-}t}$ = 0.087 m/s)

Table 4 Effect of total solids inventory on solids circulation rate

4. Conclusions

A 3-D full-loop CFD simulation was conducted to investigate the effect of physical property and operating conditions on the solids circulation rates (SCR) in an interconnected fluidized bed for chemical looping combustion applications. Simulated results were analyzed based on the full-loop pressure drop and the main results can be summarized as:

- The superficial gas velocity in the riser was identified as the main parameter to control the SCR, which increased significantly with the increase of gas velocity in the riser.
- The SCR was independent of the superficial gas velocity in the bubbling bed as the gas velocity was higher than the minimum fluidization velocity.
- For the effect of the pot-seal, higher gas velocity resulted in higher SCR in the gas velocity range of u_{mf} to $4u_{mf}$.
- The SCR became smaller for larger particles and but increased with increasing total solids inventory under different operating conditions.

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Nomenclatures

C_μ, C_1, C_2	coefficients in turbulence model
C_D	particle drag force coefficient

d_p	particle diameter (m)
e_{ss}	restitution coefficient
$\vec{g}$	acceleration due to gravity (m/s^2)
$g_{0,ss}$	radial distribution function
G_s	solids circulation rate (kg/m$^2\cdot$s)
H	static bed height (m)
I_s	total solids inventory
k	turbulent kinetic energy (m^{2}s^{-2})
k_{Θ_p}	diffusion coefficient for granular energy
P	pressure (Pa)
p_p	particle pressure (Pa)
r	radial position (m)
R	radius (m)
Re	Reynolds number
t	time (s)
$\vec{u}$	velocity vector (m/s)
u	superficial gas velocity (m/s)
u_{mf}	minimum fluidized velocity (m/s)
z	height (m)

Greek letters

α	volume fraction
β	inter-phase momentum transfer coefficient
μ	shear viscosity (Pa$\cdot$s)
λ	bulk viscosity (Pa$\cdot$s)
ρ	density (kg/m^3)
σ_k, σ_ε	Prandtl number
ε	dissipation rate of turbulent kinetic energy (m^{2}s^{-3})
ϕ_{gp}	energy exchange between gas and particle phase
φ	specularity coefficient
Υ_{Θ_p}	collisional dissipation of energy
Θ	granular temperature (m^{2}s^{-2})
$\bar{\bar{\tau}}$	stress-strain tensor (Pa)

Subscripts

g	gas phase
p	particle phase
r	riser
b	bubbling bed
p-t	pot-seal