Shape Effect of the Riser Cross Section on the Full-Loop Hydrodynamics of a Three-Dimensional Circulating Fluidized Bed

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ABSTRACT: In this work, numerical simulation is carried out in a three-dimensional full-loop pilot-scale circulating fluidized bed to explore the shape effect of the riser cross section on the typical flow characteristics of the bed via the multiphase particle-in-cell (MP-PIC) method. The gas and solid phases are modeled with the large eddy simulation and Newton’s law of motion in the Eulerian and Lagrangian frameworks, respectively. The proposed model has been well validated with experimental data, followed by evaluating the typical flow behavior and regime, polydispersity, cluster property, and internal effects. Due to its relatively coarse resolution, the TFM has been widely adopted for investigating flow characteristics in the CFB, such as the effect of ring baffles, flow behavior and regime, polydispersity, cluster property, and flux distribution. However, limited by the resolution for the solid phase, the particle-scale information cannot be obtained through this method. Another weakness of this approach is its disadvantage of incorporating the wide particle size distribution.

1. INTRODUCTION

Circulating fluidized beds (CFBs) have been widely employed in many industrial applications, such as coal combustion, ore roasting, biomass gasification, and fluid catalytic cracking (FCC), due to their excellent gas–solid mixing, increased throughput, and excellent fuel flexibility. A CFB always consists of a riser for gas–solid processing, a cyclone for separating the bed material, a standpipe for material inventory, and a loop seal for transporting the particles into the riser. The geometrical complexity of the CFB gives rise to the significant distinctive flow characteristics of the gas and solid phases in the different components of the system and also many operation difficulties (e.g., agglomeration, gas refluxing, solid back-mixing). Thus, a detailed understanding of the underlying flow mechanisms behind the complex flow patterns of the solid phase in the bed is exceptionally critical for the successful and reliable design, operation, and scale-up of this kind of apparatus.

Until now, lots of experimental studies have been conducted to explore the typical flow structure and important hydrodynamics in the CFB, such as solid velocity distribution, cluster behavior, solid circulation rate, polydispersity, segregation, annulus flow behavior, multiple cyclones, and internal effects.

Restricted by the opaque nature of solid motion in the bed, experimentally exploring the CFB is often difficult and expensive. During the last two decades, the significant advancement of computational hardware has resulted in making numerical simulation a powerful and cost-effective tool for exploring the dense gas–solid flow in fluidized beds as it can provide a detailed local gas–solid flow (e.g., solid concentration, particle-scale information, and gas–solid interactions). In general, the numerical methods available can be divided into three types based on the resolution chosen for the solid phase. The first one is the two-fluid model (TFM), which resolves gas and solid phases at the computational cell level in the Eulerian–Eulerian framework. Due to its relatively coarse resolution, the TFM has been widely adopted for investigating flow characteristics in the CFB, such as the effect of ring baffles, flow behavior and regime, polydispersity, cluster property, and flux distribution. However, limited by the resolution for the solid phase, the particle-scale information cannot be obtained through this method. Another weakness of this approach is its disadvantage of incorporating the wide particle size distribution.

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The second one is computational fluid dynamics coupled with the discrete element method (CFD-DEM),\textsuperscript{18–21} which tracks the solid phase at the particle-scale level and handles particle collision events through a soft-sphere collision model.\textsuperscript{22} However, this high-fidelity numerical method requires numerous computational resources for tracking the solid phase, and thus the majority of the available studies have been carried out for small-scale risers of the CFB with a limited particle number.\textsuperscript{23–27}

The third method is the recently developed multiphase particle-in-cell (MP-PIC), which is a Eulerian–Lagrangian model and resolves the particle collision through the normal stress model.\textsuperscript{28–30} Compared with the TFM, this approach provides more accurate tracking of the solid phase and also has the ability to handle the wide particle size distribution. As compared with the CFD-DEM, this approach resolves the particle collision through the particle stress gradient instead of accurately determining the collision process. Thus, the MP-PIC method can provide a fast solution to the large-scale dense fluidizing apparatus, becoming more and more popular for modeling the dense two-phase flow currently.\textsuperscript{31–35} Lan et al.\textsuperscript{36} numerically explored solid back-mixing in a CFB riser with the MP-PIC method and found that solid back-mixing in the dilute phase transport regime can be attributed to the downward flow of the solid phase near the wall. The numerical work conducted by Chen et al.\textsuperscript{37} demonstrated that the drag force in computational particle fluid dynamics is overestimated. Shi et al.\textsuperscript{38} numerically explored the solid residence time in the riser of a CFB with the MP-PIC method and observed the nonuniform distribution of solid residence time along the radial and axial directions. Via the MP-PIC method, Ma et al.\textsuperscript{39} numerically simulated a three-dimensional full-loop high-density CFB, and the results demonstrated that the solid residence time distribution in the standpipe exhibits a feature of an early peak with an extended tail.

Although there exist plenty of experimental and numerical reports for the gas–solid flow characteristics in the CFB, three aspects should be highlighted. (i) Many of the past studies have mainly focused on the riser of the CFB for the purpose of reducing geometrical complexity and computational cost. The dense gas–solid flow is highly chaotic and nonlinear, giving rise to the dynamic variation of full-loop pressure in the apparatus. Thus, only simulating the riser fails to predict the low-frequency variation of pressure fluctuation in the bed. Furthermore, only exploring the riser part cannot provide a complete screen of the flow dynamics in the whole apparatus. The full-loop simulation of the entire CFB is treated as the most accurate and valuable approach for the design and optimization of this apparatus. There was a growing interest in simulating the three-dimensional full-loop dynamics of the CFB in the past several years.\textsuperscript{40–43} (ii) As the main part for the processing of gas–solid flows, the riser geometry among nearly all of the reports is square or circular. Different riser geometries result in the appearance of different flow dynamics (e.g., the radial distribution of the solid phase, the back-mixing intensity), thus further impacting the system performance of the whole system. Until now, reports on the effect of riser cross section on the gas–solid flow characteristics of the CFB have been rare. Only Tu and Wang \textsuperscript{44} numerically studied the influence of riser geometry on gas–solid flows in the CFB and found that fluidization was less disordered in the rectangular riser. In-depth investigation of the shape effect of the riser cross section on the full-loop gas–solid flow characteristics in the CFB is essential for the design, optimization, and scale-up of the CFB. (iii) Owing to the inherent multiscale flow characteristics of the dense gas–solid flow, deeply exploring the particle-scale information of the solid phase provides essential knowledge on the flow dynamics of solid materials in the components of the CFB. Unfortunately, reports on this kind of information are extremely limited. The effect of riser geometry on this is still unavailable.

Therefore, the current work was numerically conducted via the MP-PIC method to simulate the dense gas–solid flow in a pilot-scale full-loop circulating fluidized bed with the aim of exploring the effect of riser geometry on the essential flow characteristics in this apparatus. Specifically, the gas motion is solved with the large eddy simulation under the Eulerian framework, while the solid phase is solved with the numerical parcel concept in the Lagrangian framework. First, the proposed numerical model is validated with the experimental data, in terms of the radial and axial distributions of the solid concentration. Then, the shape effect of the riser cross section on the full-loop characteristics (e.g., gas and solid fluxes, core–annulus structure, and solid back-mixing) in the CFB is explored, followed by investigating the nonuniformity of solid properties along the radial and axial directions of the riser. Finally, the effect of riser shape on the particle-scale information of the solid phase in different parts of the CFB is discussed.

### 2. RESULTS AND DISCUSSION

#### 2.1. General Full-Loop Behavior of the CFB

Figure 1 gives the general flow behavior of the solid phase in the CFB with different shapes of the riser. Particles in the lower part of the riser are dragged upward by rising gas introduced from the riser bottom. After the rising process, the particles reach the riser top and then are directed horizontally by a crossover channel, followed by tangential injection into the cyclone. Then, the particles spiral downward around the inner cyclone surface, resulting in the separation of gas and solid phases in this component. The separated gas exits through the top of the cyclone, while the particles fall into the standpipe under the effect of gravity. Gas streams aerated from the bottom of the standpipe transport the solid material into the riser, and then a full-loop cycle of the solid material is completed. This cycle keeps repeating; thus, a continuous circulation of the solid phase around the CFB loop is established.

![Figure 1](https://dx.doi.org/10.1021/acsomega.9b03903)
As illustrated in Figure 1a, the height of the solid inventory in the standpipe of the square-shaped CFB is higher compared with that in the circular one because the square riser has a stronger circulation intensity of particles. The fundamental reasons for this phenomenon can be explained via the particle-scale characteristics of the solid phase, which will be given in the following sections. It is noted that the circular riser has a higher solid concentration compared with the square one. As presented in Figure 1b, the particles are chaotic in the dense region of the riser, demonstrating the drastic gas–particle interaction intensity. Particles have positive horizontal velocities (Ux) in the top channel between the riser exit and the cyclone entrance and negative horizontal velocities in the incline part of the loop seal. It is noted from Figure 1c that the axial particle velocity (Uz) is negative in the circular riser, indicating that the solid back-mixing phenomenon takes place. In the square riser, particles rise and leave with intense kinetic energy, leading to a stronger circulation intensity of particles than that in the circular riser.

2.2. Effect of Riser Shape on Flux Distribution. Gas and solid fluxes in the CFB are the key parameters to assess gas and solid transport intensities, which should be thoroughly investigated. Figure 2 shows gas and solid fluxes in the central slice (y/Y = 0) of the CFB with different riser shapes. x, y, and z represent the dimensions along width, depth, and height, respectively. The gas or solid flux is a combination of gas/particle density, gas/particle volume fraction, and gas/particle velocity.\(^2^4\) In general, the axial gas and solid fluxes are 1 order of magnitude larger than the radial ones. Besides, the solid flux is about 10 times larger than the gas flux.

Gas flow spirals downward around the inner surface of the cyclone and moves upward in the core region of the cyclone. The square riser gives a more drastic secondary flow under the vortex finder and wake vortex in the lower part of the cyclone. For the Y-component gas flux (Gg_y), it is noted that the center of flow is not in coincidence with the axis of the cyclone. This flow pattern of the gas phase is defined as the “fishing tail” phenomenon, which has been proved by plenty of experiments and simulations.\(^4^5\)−\(^4^8\) In contrast to the gas flow, particles spin around the cyclone wall and are separated into the standpipe. It is clearly observed that the axial gas flux (Gg_z) and the axial solid flux (Gs_z) are quite different between the square riser and the circular one. Specifically, many particles fall back around the periphery of the circular riser, while a small number of particles resides in the sidewalls of the square riser. To illuminate this phenomenon, a specific cross section located at the height of z/Z = 0.5 of the riser is extracted with the axial gas and solid fluxes presented in Figure 3. It is noted that the axial gas flux is significant in the core region and small in the four corners of the square riser. However, the axial solid flux pattern is not symmetric, ascribed to the introduction of auxiliary gas flow from the left side of the riser (x/R = 0), which causes the nonuniform distribution of gas–solid flow. For the circular riser, the gas flux shows a hatlike pattern with a large value in the core and a small value in the periphery. Attributed to the single-side introduction of auxiliary gas flow, particles tend to back-mix near the left-side wall (x/X = 0).

2.3. Effect of Riser Shape on the Core–Annulus Structure. Figure 4 shows the profiles of the solid volume fraction in two perpendicular lines (i.e., X-line and Y-line) passing through the center of cross sections (slice z = 1.0, 3.0, and 5.0 m) with different bed heights. In general, the profiles of the solid volume fraction present a parabolic curve pattern. Due to the single-side refeed structure, the profiles of the X-line are unsymmetrical, which are more evident in the square riser. The solid volume fraction is lower in the left side of the riser where the auxiliary gas flow is introduced. However, the profiles of the Y-line are symmetric, even if they are just above the recycling port of the riser (Figure 4a,d). The difference between the X-line and Y-line is slight in the core region and significant in the annulus region. Thus, the radial particle concentration is comparatively low in the central core region and increases sharply near the wall in the riser, which represents the so-called typical core–annulus structure. The core–annulus structure mainly results from the solid back-mixing phenomenon in the riser. It is noted that the solid back-mixing intensity and the thickness of the solid back-mixing layer are reduced along the riser height. At any height, the solid volume fraction is lower in the square riser than that in the circular one. Interestingly, it is noted that solid back-mixing tends to concentrate in the four corners of the square riser, while it is not obvious far away from this region, which is demonstrated in the experiment and called the “wall-sheltering” phenomenon.\(^3^9\)

Figure 5 gives the surface plots of the solid volume fraction in the vertical cross section (slice x/X = 0). It is noted that the solid volume fraction decreases as the height increases. The core–annulus structure is observed along the whole riser, which diminishes along the bed height. The change of solid volume fraction in the circular riser is more significant than that in the square riser, which is large in the bottom (z < 1.0 m) and the top (z > 6.0 m) of the riser. The former tendency is because of the
dense region where particle agglomeration occurs. The latter is due to the "L-type" abrupt exit, which makes particles accumulate in the top region.

The centerline from the vertical cross section is extracted to quantitatively compare the solid volume fraction between the square riser and the circular riser. As presented in Figure 6, the solid volume fraction in the bed bottom first increases to a maximum value and then decreases along the bed height and finally rises in the bed ceiling. The maximum value for the square riser is about 0.09, while for the circular riser it is about 0.18. In the lower region, the circular riser gives rise to a larger solid volume fraction. In the developed region (3.0 m < z < 5.0 m), the shape of the riser has a slight influence on solid volume fraction distribution.

2.4. Axial Mass Distribution. The typical characteristics of the solid phase in the riser are the presence of the nonuniform distribution of the solid phase along the radial and axial directions. The mass distribution in the bed is extremely critical for successful operation and also performance improvement as this parameter is strongly related to the heat transfer and the reaction behavior inside the riser. To explore the nonuniformity along the axial direction, the fraction distribution of the total mass combined with the rising and falling mass along the axial direction is evaluated. Specifically, the riser is uniformly divided into 100 sections along the axial direction, followed by evaluating the mass fraction of the solid phase distributed in each region with regard to the total mass in the riser.

Figure 7a illustrates the mass fraction of the total mass distributed in the riser. The largest mass fraction of the solid phase appears in the bottom region of the riser, which is attributed to the addition of the circulating particles transported from the loop seal. Along the bed height, the decreasing mass of the solid phase reflects the dilute distribution of the particles, which is due to the fact that many of the particles dragged by the rising gas continuously fall back along the axial direction. The apparent large mass of the solid phase near the riser outlet results from the strong back-mixing of the rising particles after colliding with the riser top. Compared with the square riser, a larger mass fraction of the solid phase appears in the lower part of the circular riser, demonstrating more vigorous nonuniformity of

Figure 3. Axial gas and solid fluxes in a specific cross section with the height of z/Z = 0.5, where r represents the dimensions along the X or Y directions: (a, b) axial gas flux (Gg_z) and axial solid flux (Gs_z) in the square riser; (c, d) axial gas and solid fluxes in the circular riser.
the mass distribution of the solid phase along the axial direction in the circular riser.

In the riser, many of the particles rise upward while others fall downward near the riser wall. To quantitatively reflect the distribution characteristics of the rising and falling particles in the riser, Figure 7b presents the axial distribution of the mass fraction of the rising and falling mass along the bed height. Continuous decrease of the rising and falling mass of particles can be observed along the axial direction, reflecting the more and more dilute distribution of particles in the upper part of the bed. Steep distribution of the mass fraction appears for the CFB with a circular riser, demonstrating that more significant nonuniformity of the rising and falling mass of particles can be observed for the circular riser. As expected, the vigorous falling mass of the solid phase exists near the riser top due to the restriction effect of the abrupt exit on the particle flow.

2.5. Rising and Back-Mixing Intensity. The solid backmixing significantly impacts the performance of the CFB as this has a strong relationship with the reaction process underway, the reaction rate, and also the solid residence time. In this work, solid flux is adopted to quantitatively evaluate the flow intensity of the rising and falling behavior of the solid phase in the bed. Figure 8 quantitatively presents the spatial distribution of the

Figure 4. Radial particle solid volume fraction in the cross sections with different heights of the riser: (a–c) square riser with slice \( z = 1.0, 3.0, \) and 5.0 m; (d–f) circular riser with slice \( z = 1.0, 3.0, \) and 5.0 m.

Figure 5. Surface plots of the solid volume fraction in the vertical cross section (slice \( x/X = 0 \)) of the riser: (a) square riser; (b) circular riser.

Figure 6. Axial distribution of the solid volume fraction in the riser with a different shape.

Figure 7b.
flux fraction of the rising and falling fluxes of the solid phase along the radial (a) and vertical (b) directions of the CFB with different riser cross sections. Specifically, the radial and axial distributions of the solid flux are obtained by horizontally dividing the riser into 10 and 100 parts along these two directions, respectively. Then, the time-averaged rising and falling fluxes of the solid phase in each part are obtained, followed by calculating the total flux magnitude of the solid phase in each part. Subsequently, the fraction of the rising and falling fluxes in each part can be obtained by dividing the total flux magnitude in this region.

Figure 8a illustrates the radial distribution of the flux fraction of the rising and falling particles in the riser. For these two systems, the nonuniform radial distribution of both the rising and falling solid fluxes can be observed. The rising solid flux mainly appears in the central region as the rising particles are dragged by the rising gas flow. Significant falling solid flux appears in the near-wall region, which corresponds to the
vigorous solid back-mixing in this region. Furthermore, the Table 1. Comparison of the Particle-Scale Information of the Solid Phase in Different Components of the CFB with Different Riser Shapes

|                | Ux (m/s) | Uy (m/s) | Uz (m/s) | drag | slip velocity (m/s) | Dx (10^{-4} m^2/s) | Dy (10^{-4} m^2/s) | Dz (10^{-4} m^2/s) |
|----------------|----------|----------|----------|------|---------------------|-------------------|-------------------|-------------------|
| riser of square geometry | 0.17     | 0.10     | 1.89     | 1.61 | 419                 | 6.23              | 47.7              | 11.6              | 3026              |
| cyclone of square geometry | 1.26     | 1.04     | 1.46     | 1.04 | 210                 | 3.15              | 1930              | 550              | 1217              |
| standpipe of square geometry | 0.027    | 0.014    | 0.37     | 2.3  | 41.2                | 0.61              | 4.5               | 2.7               | 337               |
| riser of circular geometry  | 0.13     | 0.106    | 1.96     | 1.73 | 360                 | 5.35              | 26.8              | 12.9              | 3500              |
| cyclone of circular geometry | 1.23     | 1.0      | 1.51     | 0.86 | 146                 | 2.34              | 1720              | 520               | 1289              |
| standpipe of circular geometry | 0.043    | 0.024    | 0.54     | 2.6  | 73.7                | 1.09              | 7.2               | 4.9               | 823               |

distribution pattern. However, the square riser gives rise to a large horizontal velocity along the radial direction, demonstrating its effect of enhancing the solid exchanging velocity between the core and annulus regions. Figure 9b shows the axial distribution of the sectional-averaged horizontal and axial velocities of particles. The largest horizontal solid velocity appearing in the lower part of the bed mainly results from the effect of the horizontal particle stream introduced from the loop seal. Along the axial direction, the horizontal velocity sharply decreases in the lower part but smoothly in the upper region of the bed. Near the riser exit, the noticeable large horizontal solid velocity results from the horizontal transportation of particles from the riser exit. Regarding the axial solid velocity, continuous increases of the solid velocity along the bed height exist, which is mainly due to the acceleration effect of the rising gas phase. After being fully accelerated, the decrease of solid velocity in the region near the riser top is attributed to the intensive collision of the rising particles with the falling ones, restricted by the riser top. Obviously, the riser shape does not change the distribution tendency of both the radial and axial solid velocities but gives rise to a minor difference for both the velocities along the axial direction.

2.6. Radial and Axial Distribution of Solid Information. Tracking the solid phase in the Lagrangian framework provides the possibility of evaluating the solid property in a specific region. The horizontal motion of the solid phase pushes the particles from the central region to the riser wall. Similar to the method chosen for the mass distribution, the whole domain is divided into 10 and 100 parts along the radial and axial directions, respectively, to evaluate the lateral and vertical distributions of the solid phase.

Figure 9 presents the radial (a) and axial (b) distributions of the magnitudes of the horizontal (Ux) and axial (Uz) velocities of particles in the riser of the CFB. Obvious nonuniform distribution of solid velocity appears along both the radial and axial directions. Along the radial direction (Figure 9a), the horizontal velocity of the solid phase is the largest in the central region of the riser and continuously decreases along the radial direction. The horizontal transportation velocity is nearly 1 order of magnitude smaller than the vertical one. Meanwhile, the largest vertical solid velocity appears in the central part of the bed. The riser shape does not obviously alter the general patterns of the distribution pattern. However, the square riser gives rise to a large horizontal velocity along the radial direction, and also the drag force exerted on the solid phase. The drag force strongly affects the solid transport and the internal circulation of the solid phase in the system. In the literature, there exist empirical correlations for the one-dimensional (1D) analysis of the slip factor and drag force and also the utilization of the slip velocity for determining the solid residence time. Figure 10 presents the radial (a) and axial (b) distributions of the drag force and slip velocity of the solid phase, which are calculated as the sectional-averaged particle-scale information of the solid phase. Nonuniform distribution of the slip velocity appears along the radial direction (Figure 10a), with the appearance of large slip velocity in the central core region of the riser and small ones near the sidewalls of the bed. Large slip velocity in the...
central core region results from the large gas velocity in this part. Near the riser wall, the wall restriction on the gas flow gives rise to a comparatively smaller slip velocity in this region. Along the axial direction, the slip velocity in the square riser is obviously larger than that of the circular riser. Moreover, along both the radial and axial directions, a similar distribution tendency of the slip velocity appears for the CFB with different risers. The square riser gives rise to a larger slip velocity along the radial direction of the riser, as compared with the circular riser. However, the circular riser gives rise to a larger drag force on the particles along the radial direction, and also in the lower part of the riser, as compared with the square riser. The inconsistency of the drag force with the slip velocity is due to the fact that the drag force is determined by several factors despite the slip velocity.

2.7. Comparison of Particle-Scale Information in Components. The complex geometry of the CFB gives rise to different flow characteristics of both the gas and solid phases in different components of the system. To give a general comparison of the solid motion, the time-averaged information of the solid phase evaluated through the particle-scale level is provided in Table 1.

Several tips can be obtained. (i) The axial solid velocity in the riser is obviously larger than the horizontal one. However, the solid velocity along three directions is at the same magnitude scale in the cyclone. Extremely small solid velocity exists in the standpipe. As compared with the square riser, the circular riser gives rise to a larger horizontal solid velocity but a smaller axial one for the solid motion in both the riser and cyclone. (ii) Among the three components of the riser, the drag force, the particle Reynolds number, and the slip velocity of the solid phase in the riser are the largest, followed by the cyclone, and finally the standpipe. The circular riser gives rise to a larger slip velocity and drag force in the riser, as compared with the square one. (iii) The axial dispersion intensity of the solid phase in the riser is extremely larger than the horizontal one for both CFBs investigated. However, the horizontal dispersion intensity of the solid phase is the largest due to the spiral flow of particles along the cyclone’s inner surface. The weakest dispersion of the solid phase in the standpipe can be observed. As compared with the circular riser, the horizontal dispersion intensity of the solid phase is slightly larger than that in the square riser, reflecting the enhanced horizontal transportation of the solid material between the core and annulus regions of the riser. However, the axial dispersion intensity of the solid phase in the square riser is smaller than that in the circular one.

3. CONCLUSIONS

Based on the multiphase particle-in-cell method, the full-loop gas—solid flow in a three-dimensional circulating fluidized bed is numerically simulated. After validating the numerical results with experimental data, the effect of riser shape on the typical gas—solid hydrodynamics (e.g., the core—annulus structure and the nonuniform distribution property) in the bed is explored. Furthermore, the radial and axial distributions of the particle-scale information of the solid phase in the riser are comparatively investigated. Based on the numerical results, the following tips can be drawn.

(1) The square riser gives rise to a higher solid inventory in the standpipe, owing to the stronger circulation intensity in the square riser, as compared with that in the circular one. Solid back-mixing occurs in the periphery of the circular riser, and the thickness of the solid back-mixing layer reduces along the riser height. Interestingly, the solid back-mixing tends to concentrate in the four corners, while it is not obvious near the sidewalls of the square riser. As compared with the circular riser, the square riser gives rise to a smaller mass fraction distributed in the lower part and a comparatively uniform distribution of the solid mass combined with the rising and falling mass fractions along the axial direction.

(2) The square riser gives rise to a larger rising solid flux along the axial direction. Nonuniform distribution of the particle-scale information of the solid phase (velocity, slip velocity) in the riser along the radial and axial directions can be observed. The riser shape does not obviously alter the general distribution pattern along both directions. The square riser results in a large horizontal transportation velocity between the core and annulus regions and a smaller drag force on the solid phase.

(3) The largest drag and slip velocity of the solid phase can be observed in the riser, followed by the cyclone. The square riser results in a larger horizontal velocity and a horizontal dispersion coefficient of the solid phase in the riser.

In view of the inherent complex gas—solid flow hydrodynamics of the CFB, the study regarding the effect of riser geometry on the gas—solid hydrodynamics in the CFB operating with different parameters (e.g., the superficial velocity, the particle diameter, the aeration velocity of the L-valve) will be the focus of our following work. In general, the insights emanating from this study are expected to be valuable for the in-depth understanding of the extremely complex and critical hydrodynamic behaviors of both the gas and solid phases in the full-loop circulating fluidized bed, further contributing to the design and optimization of a high-efficiency large-scale commercial system in practical industrial applications.

4. NUMERICAL METHODS AND SETTINGS

4.1. Mathematical Model. The gas phase is treated as a continuous medium, and its motion is tracked at the computational cell scale in the Eulerian framework. The governing equations for gas continuity and momentum can be formulated as

\[
\frac{\partial (\varepsilon \rho g)}{\partial t} + \nabla \cdot (\varepsilon \rho g u_s) = 0
\]

\[
\frac{\partial (\varepsilon \rho g u_s)}{\partial t} + \nabla \cdot (\varepsilon \rho g u_s u_s) = -\nabla p_g + \nabla \cdot (\varepsilon \tau) + \varepsilon \rho g g - F_g
\]

where \( \varepsilon \rho g u_s \) and \( \rho g \) denote the voidage, density, velocity, and pressure of the gas phase, respectively. \( t \) and \( g \) are the time instant and gravitational acceleration, respectively. \( F_g \) represents the gas—solid momentum exchange rate per unit volume and will be discussed later. \( \tau \) is the gas stress tensor, for which the constitutive equation can be formulated as

\[
\tau = \mu_s \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu_s \frac{\partial u_i}{\partial x_k} \frac{\partial u_k}{\partial x_i}
\]

Here, \( \mu_s \) stands for the shear viscosity of the gas phase, which consists of the laminar viscosity and the turbulent viscosity. In this work, the turbulent viscosity is modeled through the Smagorinsky model described as
The transport equation for the PDF $f_s$ can be formulated as

$$\frac{df_s}{dt} + \frac{\partial(f_s u_s)}{\partial t} + \frac{\partial(f_s \Gamma_s)}{\partial u_s} = \frac{f_D - f_s}{\tau_D}$$

where $f_D$ and $\tau_D$ are the PDFs for the local mass-averaged particle velocity and collision damping time, respectively, and the details can be found in the literature.\(^{(29,60)}\) $\Gamma_s$ is the particle acceleration due to the aerodynamic drag, the pressure gradient, the gravity, and the interphase interactions, which can be given as\(^{(61)}\)

$$\Gamma_s = \frac{du_s}{dt}$$

$$= \beta(u_s - u) - \frac{1}{\rho_s} \nabla p_s - \frac{1}{\rho_s} \epsilon_s \nabla \epsilon_s + g + \frac{\rho - \rho_s}{2\tau_D}$$

where $\tau_s$ is the particle normal stress adopted to model the collision force acting on a numerical particle. It is evaluated through the Harris and Crighton model,\(^{(62)}\) which is expressed as

$$\tau_s = \frac{P_s}{\max(\epsilon_s - \epsilon, \alpha(1 - \epsilon_s))}$$

where $P_s$, $\epsilon$, and $\gamma$ are the model parameters. $\alpha$ is a minimum value chosen to remove the singularity at the close-packing state of the solid phase. $\epsilon_s$ in eq 7 is the solid concentration, which can be evaluated from the PDF $f_s$ as

$$\epsilon_s = \iiint \frac{m_s}{\rho_s} d\rho_s d\epsilon_s du_s$$

$\beta$ in eq 7 represents the interphase momentum exchanging coefficient evaluated with a combination of the Wen–Yu\(^{(63)}\) and Ergun\(^{(64)}\) drag models. It can be formulated as

$$\beta = \begin{cases} \beta_1 & \text{if } \epsilon_s < 0.7\epsilon_s \text{ or } \epsilon_s > 0.85\epsilon_s \\ \beta_2 & \text{if } 0.75\epsilon_s \leq \epsilon_s \leq 0.85\epsilon_s \\ \beta_3 & \text{if } \epsilon_s > 0.85\epsilon_s \end{cases}$$

$$\beta_1 = 3 \frac{C_D \rho_s \rho_g \epsilon_s - \rho_s u_s}{\rho_s d_s}, \quad \beta_2 = \left( \frac{180\epsilon_s}{\epsilon_s \text{Re}_s} + 2 \right) \frac{\rho_g \epsilon_s - \rho_s u_s}{\rho_s d_s},$$

$$\beta_3 = \frac{24}{\text{Re}_s} (1 + 0.15 \text{Re}_s^{0.687}) \epsilon_s^{-2.65} \text{Re}_s < 1000$$

$$0.44 \epsilon_s^{-2.65} \quad \text{Re}_s \geq 1000$$

$$\text{Re}_s = \frac{\rho_g \epsilon_s u_s}{\mu_g d_s}$$

where $d_s$ stands for the particle diameter.

The interphase momentum exchanging rate $F_{\text{ex}}$, which is related to the particle probability distribution function, can be expressed as
\[ F_g = - \iiint \rho \left[ \rho (u_g - u_p) - \frac{\nabla P}{\rho} \right] d\mathbf{V} d\mathbf{q} d\mathbf{u} \quad \text{(14)} \]

4.2. Numerical Validation. The simulation is carried out on the platform of the open-source software package OpenFOAM, in which the MP-PIC solver (i.e., MPPICFoam) is available. The MP-MPIC method used in the present work is validated with the experimental data from a pilot-scale cold CFB apparatus, which has a rectangular riser with a cross-section area of 1000 mm \( \times \) 300 mm. The height of the riser is 8.5 m, and the exit is L-type abrupt. For simplification, the external circulation system is omitted in the simulation, which is virtually represented by a boundary condition connection technique. Specifically, all particles escaped from the riser exit are automatically returned from the loop seal to loosen and transport the particles to the riser, whose cross-section area is 177 mm \( \times \) 177 mm and an angle of 45°. Moreover, the particles are assumed to be 100% recycled to maintain a constant particle inventory during the whole simulation. Sand is used as the bed material, which has a density of 2600 kg/m\(^3\) and a surface mean diameter of 140 \( \mu \)m. Gas flow is introduced from the bottom distributor with a superficial gas velocity of 4.0 m/s. The density and viscosity of the gas are 1.18 kg/m\(^3\) and 1.5 \( \times \) \( 10^{-5} \) kg/(s-m), respectively. The grid size along the width, depth, and height is, respectively, assigned as 35 mm \( \times \) 22.5 mm \( \times \) 55 mm, which has been proved to be reasonable by Hartge et al.\(^{37}\) The details of operating parameters can be found in the literature.\(^{37}\)

The experimental data available in Schlichthärl\(^{65}\) is quite limited. Only the axial solid volume fraction along the riser height is presented. It is noted from Figure 11a that the numerical results agree well with the experimental data along the bed height, especially in the medium and upper parts (i.e., \( z > 3.0 \) m). The reason is that the medium and upper parts of the riser are dilute suspension regions, where the homogeneous gas–solid flow is suitable to be described using the Wen–Yu and Ergun drag model. In contrast, the lower part of the riser (i.e., \( z < 3.0 \) m) is a dense region, where the heterogeneous gas–solid flow should be captured using the advanced drag model with heterogeneity considered, such as the EMMS drag model.\(^{67}\) Therefore, there is a slight discrepancy between numerical results and experimental data in the lower part of the riser. However, this discrepancy is acceptable in the pilot-scale CFB simulations to some extent. In the experiment, the solid inventory and pressure drop are set, and the external solid mass flux \((G_s)\) is 20 kg/(s-m\(^2\)).\(^{37,65,66}\) As illustrated in Figure 11b, the external solid mass flux obtained from the simulation fluctuates around a mean value of 18.9 kg/(s-m\(^2\)), which is in accordance with the experimental data of 20 kg/(s-m\(^2\)).

In summary, the proposed MP-PIC method is reliable and reasonable to investigate gas–solid flow characteristics in the three-dimensional full-loop CFB.

4.3. Numerical Settings. A three-dimensional CFB model is built according to the experimental test rig.\(^{66}\) The CFB is extracted from a 0.3 MW\(_{th}\) pilot plant system, which includes three main parts: (i) feeding system; (ii) primary and secondary gas flow; and (iii) external circulation system including a cyclone and a recycling system. For the feeding system, a rotating screw feeder is used to control the feed rate of solid fuels. The current work focuses on cold gas–solid hydrodynamics in the CFB; thus, the process of feeding solid fuels is neglected. The air supplying system provides primary and secondary air to the CFB, which is composed of a compressor, the main valve, and two flowmeters. The primary air is introduced from the distributor located at the bottom of the riser to fluidize the bed materials, while the secondary air is fed into the system to assist in the solid circulation and control the equivalent ratio. The heart of the plant system is a CFB with a total height of 6500 mm, as shown in Figure 12. X, Y, and Z represent the directions along the width, depth, and height of the CFB, respectively. The origin of the coordinates is the center of circular and square cross sections. In the experiment, the cross section of the riser is circular with a diameter of 200 mm. To explore the shape effect on the full-loop gas–solid flow dynamics, a square riser is adopted with the same cross-section area as the circular one. Thus, the side length of the square cross section is 177 mm. The cyclone with a diameter of 350 mm separates particles from gas–solid flows. The standpipe with a diameter of 120 mm is used to store solid materials. The computational domain of the CFB with a circular and square riser is divided into 142 576 and 147 840 grid elements, respectively. Besides, the number of parcels is 105 679 and 101 775 for the circular system and square system, respectively.

The primary air is introduced into the riser with a superficial gas velocity \((U_g)\) of 7.0 m/s and a temperature of 298 K. The auxiliary air is provided from the feed inlet, which is located 370 mm above the bottom distributor with a mass flow rate \((Q_s)\) of 0.04 kg/s. The aeration air is introduced from the bottom of the loop seal to loosen and transport the particles to the riser, whose mass flow rate \((Q_a)\) is 0.04 kg/s. The particle diameter and density are 488 \( \mu \)m and 2600 kg/m\(^3\), respectively. Details of gas–solid properties and operating parameters are listed in Table 2.

For the velocity, the primary, auxiliary, and aeration inlets are assigned as a velocity/mass flow boundary condition, while the top of the vortex finder (i.e., outlet) is set as a zero-gradient boundary condition. Besides, the walls are set as a no-slip boundary condition. For the pressure, the outlet is assigned as a fixed pressure boundary condition, 1.01 \( \times \) \( 10^5 \) Pa. The simulation is focused on the cold model of the CFB without chemical reactions. Thus, the time step can be large enough to complete a fast calculation. In the present simulation, the time step is set as 5.0 \( \times \) \( 10^{-4} \) s and the particles are first packed in the
bottom of the riser, loop seal, and standpipe with an initial solid volume fraction of 0.56.

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**Notes**
The authors declare no competing financial interest.

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| Table 2. Details of Gas–Solid Properties and Operating Parameters Used in the Current Work |
|-----------------------------------------------|
| parameter | value |
|---|---|
| Solid Phase (Sand) | --- |
| diameter (μm) | 488 |
| density (kg/m³) | 2600 |
| close-packing volume fraction | 0.60 |
| restitution coefficient | 0.95 |
| Gas Phase (Air) | --- |
| density (kg/m³) | 1.205 |
| viscosity (kg/(m·s)) | 1.8 x 10⁻⁵ |
| temperature (K) | 298 |
| superficial gas velocity (Uₚ, m/s) | 7.0 |
| auxiliary gas flow rate (Qₐ, kg/s) | 0.04 |
| aeration gas flow rate (Qₑ, kg/s) | 0.04 |
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