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<td><strong>Author(s)</strong></td>
<td>Li, Xiaofei; Wang, Lei; Jia, Lei; Cai, Wenjian</td>
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</table>
Numerical and Experimental Study of a Novel Compact Micro Fluidized Beds Reactor for CO₂ Capture in HVAC

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Abstract: In order to reduce the pressure drop and increase the adsorption performance for the CO₂ capture using solid adsorbents in Heating, Ventilation and Air Conditioning (HVAC), a novel Compact Micro Fluidized Beds (CMFB) reactor was proposed. First, the pressure drop and adsorbent attrition of the CMFB reactor were calculated by Eulerian-Lagrangian Computational Particle-Fluid Dynamics (CPFD) modelling with Barracuda software and compared with traditional Fluidized Bed (FB) reactor. Second, a CMFB experimental platform was designed based on the CPFD model. At last, the pressure drop, adsorbent attrition and performance for CO₂ capture were systematically investigated in the CMFB experimental platform. The results showed that much lower pressure drop and lower adsorbent attrition were achieved by CMFB reactor than by FB reactor due to large inlet area and reduced feed velocity. The CMFB reactor can gain long-term energy-saving effects in HVAC. Furthermore, the breakthrough time increased by about 35% and the saturation time reduced by about 17% in CMFB reactor for CO₂ capture than that in FB reactor.

Keywords: CO₂; adsorption; HVAC; fluidized bed;

<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_d</td>
<td>Drag coefficient</td>
</tr>
<tr>
<td>D_p</td>
<td>Interphase drag coefficient (1/s)</td>
</tr>
<tr>
<td>F</td>
<td>Rate of momentum exchange per volume between the gas and particle phases (N/m³s)</td>
</tr>
<tr>
<td>f</td>
<td>Probability distribution function</td>
</tr>
<tr>
<td>g</td>
<td>Gravitational acceleration (m/s²)</td>
</tr>
<tr>
<td>I_p</td>
<td>Magnitude of the impact value (kgᵃ·mᵇ/ₐᵇ)</td>
</tr>
<tr>
<td>m_p</td>
<td>Particle mass (kg/m³)</td>
</tr>
<tr>
<td>n_p</td>
<td>Number of particles in a numerical particle</td>
</tr>
<tr>
<td>N_p</td>
<td>Number of numerical particles</td>
</tr>
<tr>
<td>p</td>
<td>Gas pressure (Pa)</td>
</tr>
</tbody>
</table>

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1. Introduction

Efficient and cost-effective CO₂ capture is of great importance in various applications pertaining to environment, cryogenic air separation and personal confined spaces such as submarines, aerospace shuttles and some buildings [1,2]. In recent years, a lot of attentions have been devoted to design the CO₂ capture reactor system using solid adsorbents which can be combined into the central air conditioning in buildings [3-5].

The adsorption reactor, as one of the key equipments of CO₂ capture system, is used for contacting CO₂-laden gas streams with solid adsorbents. Therefore, the study of efficient and cost-effective adsorption reactor is very important for CO₂ capture in Heating, Ventilation and Air Conditioning (HVAC). At present, many kinds of reactors have been applied in the field of CO₂ capture using solid adsorbents, such as fixed bed, moving bed and fluidized bed reactors [6-9]. Fixed and moving beds have poor heat transfer and great diffusional resistance [10]; fluidized beds have the advantages of excellent gas-solid contact, minimum diffusional
resistance and superior mass and heat transfer characteristics. Fluidized beds are likely to be superior to the fixed and moving beds [11].

Fluidized beds have been applied widely in a variety of industrial processes at conventional scales ranging from decimeters to meters [12,13]. In recent years, there is a growing interest in the miniaturization of fluidized beds, because micro-scale fluidized beds have the advantage of high heat and mass transfer efficiency, reduced pressure drop, good mixing of reactant and catalyst, improved safety, and other specific required characteristics [14,15]. Applications of micro fluidized bed have been reported, such as the Macro-scale Photocatalytic Fluidized Bed Reactor (MPFBR) [16], the Micro Fluidized Bed Reaction Analyzer (MFBRA) [17], the Micro Membrane Fluidized Bed Reactor (MMFBR) [14] and other micro-structured fluidized beds [18,19].

Potic et al. [20] first introduced the concept of micro fluidized beds as referring to beds with inner diameters of a few millimeters. Liu et al. [21] investigated the fluidization characteristics of gas-solid micro fluidized beds. The minimum fluidization velocity in gas-solid micro fluidized beds were studied by Guo et al. [22]. Recently, Wang and Fan [23] carried out a series of gas-solid fluidization experiments using fluid catalytic cracking (FCC) particles in micro-channels. Doroodchi et al. [19] examined the hydrodynamics of three liquid-solid micro fluidized beds. In addition to the experimental studies, computational particle fluid dynamics (CPFD) has been extensively used to improve understanding of fluidized beds and micro fluidized beds in terms of minimum fluidization velocity and bed expansion characteristics [24-26]. Wang et al. [14] found that a micro-structured fluidized bed reactor can be operated in turbulent fluidization regime with much lower gas flow rates compared with bigger scale fluidized bed reactors by numerical simulations. Snider et al. [27] presented application of the hybrid Euler-Lagrange method for modeling the gasification process in large industrial fluidized bed reactors. Lim et al. [28] carried out CPFD simulations in bubbling fluidized beds, and they found that bed pressure drops are similar to those obtained from experimental data.

At present, nearly all the previous studies were about the fluidization characteristics of single micro fluidized bed containing very small amounts of bed materials, but multiple micro fluidized beds used together in one reactor for scale-up application was rarely involved. A suitable CO₂ capture reactor which can meet the designed constraints of low pressure drop,
high adsorption performance and low adsorbent attrition under high air flow is urgently needed to develop in HVAC.

In this study, a novel CMFB reactor was proposed to meet the requirements of HVAC. The pressure drop and particle attrition in the CMFB and FB reactors were simulated by CPFD model. The performance of the CMFB and FB reactors in terms of pressure drop, CO\textsubscript{2} adsorption and adsorbent attrition were investigated experimentally. The CPFD simulation data are compared with the experimental results in the CMFB reactor, and compared with that in the FB reactor.

2. CPFD mathematical model

2.1. Governing equations

The CPFD methodology takes an Eulerian-Lagrangian approach to describe the gas-solid flow in three dimensions. The gas phase is described as continua by averaged Navier-Stokes equations and the solid phase is modeled as discrete particle. The gas phase is strongly coupled with the discrete particles phase in mass, momentum and energy conservation equations. The particle momentum description follows the multi-phase particle-in-cell (MP-PIC) numerical method, which provides a Lagrangian description of particle motion coupled with the gas by ordinary differential equations [29]. As there is no reaction and interphase mass transfer, no gas phase energy equations are needed. For the gas phase, the volume averaged gas mass and momentum equations are

\[
\frac{\partial \theta_g \rho_g}{\partial t} + \nabla \cdot (\theta_g \rho_g \mathbf{u}_g) = 0 \tag{1}
\]

\[
\frac{\partial (\theta_g \rho_g \mathbf{u}_g)}{\partial t} + \nabla \cdot (\theta_g \rho_g \mathbf{u}_g \mathbf{u}_g) = -\nabla p + \nabla \cdot (\theta_g \tau_g) + \theta_g \rho_g g - F \tag{2}
\]

where \( \mathbf{u}_g, \rho_g, \theta_g, p, \tau_g, \) and \( g \) are the gas velocity, the gas density, the gas volume fraction, the gas pressure, the gas stress tensor and the gravitational acceleration, respectively. \( F \) is the rate of momentum exchange per volume between the gas and particle phases.

\[
F = \int f \int m_p \left( D_p (\mathbf{u}_g - \mathbf{u}_p) - \frac{1}{\rho_p} \nabla p \right) dm_p d\mathbf{u}_p \tag{3}
\]

where \( f, m_p, D_p, \mathbf{u}_p \) and \( \rho_p \) are the particle distribution function, the particle mass, the
interphase drag coefficient, the particle velocity and the particle density, respectively.

For the particle phase, the particles are modeled using the Lagrangian method with the numerical particles each containing \( n_p \) particles with identical properties located at position \( (x_p, y_p, z_p) \). The particle acceleration is

\[
\frac{d\mathbf{u}_p}{dt} = D_p \left( \mathbf{u}_g - \mathbf{u}_p \right) - \frac{1}{\rho_p} \nabla p + g - \frac{1}{\theta_p \rho_p} \nabla \tau_p
\]  

(4)

where \( \theta_p \) and \( \tau_p \) are the volume fraction of particles and the particle normal stress.

The particle movement is given by

\[
\frac{dx_p}{dt} = \mathbf{u}_p
\]  

(5)

2.2. Interphase drag model

The interphase drag model used here is [29]

\[
D_p = C_d \frac{3 \rho_g}{8 \rho_p} \left| \mathbf{u}_g - \mathbf{u}_p \right| r_p
\]  

(6)

where

\[
C_d = \begin{cases} 
\frac{24}{\text{Re}} \left( 1 + 0.15 \text{Re}^{-0.687} \right) \theta_g^{2.65} & \text{Re} < 1000 \\
0.44 \theta_g^{2.65} & \text{Re} \geq 1000
\end{cases}
\]  

(7)

\[
\text{Re} = \frac{2 \rho_g \left| \mathbf{u}_g - \mathbf{u}_p \right|}{\mu_g} \left( \frac{3V_p}{4\pi} \right)^{1/3}
\]  

(8)

(9)

where \( \mu_g \) and \( V_p \) is the gas viscosity and the particle volume.

2.3. Particle stress model

In the CPFD scheme, the particle-particle collisions are modeled by the particle normal stress [29], which is given by

\[
\tau_p = \frac{P \theta_p^\beta}{\max \left( \left( \theta_p - \theta_{cp} \right), \epsilon (1 - \theta_p) \right)}
\]  

(10)

where \( P \) is a positive constant and \( \theta_{cp} \) is the particle volume fraction at close packing. \( \beta \) and \( \epsilon \) are dimensionless constants. \( \beta \) is recommended to be 2 - 5.

2.4. Attrition model
In CPFD model, the particle attrition caused by single particle-wall collision is calculated by the following expression:

\[ I_p = w(\alpha_p) \cdot m_p^a \cdot u_p^b \]  \hspace{1cm} (11)

where \(w(\alpha_p)\) is the weighting factor which is a function of the impact angle \(\alpha_p\). Exponents \(a\) and \(b\) are constants. In this study, \(w(\alpha_p)\) is left default, the mass exponent \(a\) and particle velocity exponent \(b\) are left to be 1 and 2 [30].

2.5. Numerical solution

The flow diagram of the different modules that constitute the CPFD model and the variables that are exchanged between the modules are displayed in Fig. 1. In the CPFD approach, the particle properties are mapped from the Eulerian grid to the particle locations. The particle properties are also then mapped from the particles to the grid to get grid-based properties. Each grid cell contains numbers of numerical particles. The particle volume fraction at cell \(\xi\) from mapping particle volume to the grid is

\[ \theta_{p\xi} = \frac{1}{V_\xi} \sum_{1}^{N_p} n_{p} v_{p\xi} s_{p\xi} \]  \hspace{1cm} (12)

where \(V_\xi, N_p, n_p\) and \(s_{p\xi}\) are the volume of cell \(\xi\), the total number of numerical particles in the cell, the number of real particles in a numerical particle and the interpolation operator, respectively. The sum of the gas and particle volume fractions must equal unity, \(\theta_p + \theta_g = 1\), which is used to solve gas continuity and momentum equations in the next time step.

The mass and momentum equations are approximated and solved by finite volumes with staggered scalar and momentum nodes. The numerical particle velocity at the following time step is updated from integration of Eq. (4).

\[ \mathbf{u}_p^{n+1} = \mathbf{u}_p^n + \Delta t \left( D_p \mathbf{u}_{p\xi}^{n+1} - \frac{1}{\rho_p} \nabla p_{p}^{n+1} - \frac{1}{\rho_p \theta_p} \nabla \tau_{p}^{n+1} + g \right) \]  \hspace{1cm} (13)

where \(\mathbf{u}_{p\xi}^{n+1}\), \(\nabla p_{p}^{n+1}\) and \(\nabla \tau_{p}^{n+1}\) are the interpolated gas velocity, the interpolated pressure gradient and the interpolated particle stress gradient at the particle location, respectively.

The new particle location at the next time step is

\[ \mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \mathbf{u}_p^{n+1} \Delta t \]  \hspace{1cm} (14)

The gas momentum equation implicitly couples the gas and the particles by the
interphase momentum transfer. The interphase momentum transfer at momentum cell $\xi$ is

$$ F_p^{n+1} = \frac{1}{V_\xi} \sum_{p=1}^{N_p} S_{p} \left[ D_p \left( u_p^{n+1} - u_{\xi}^{n+1} \right) - \frac{1}{\rho_p} \nabla p_p^{n+1} \right] n_p m_p \quad (15) $$

The summation is over all numerical particles $N_p$ in the cell.

**BEGIN:** Set up initial condition

Apply gas-particle interaction (drag model)
Eq. (6) (7) (8) (9)
In: $u_p^1 \theta_p^1 p^1 x_p^1$, out: $u_p^{n+1} D_p^n$

Apply particle-particle interaction and move particles
Eq. (4) (5) (10) (13) (14)
In: $u_{\xi}^{n+1} \theta_{\xi}^n p_{\xi}^n x_{\xi}^n$, out: $u_p^{n+1} x_p^n$
Interphase momentum transfer: Eq. (15)
In: $u_{\xi}^{n+1} u_p^{n+1} D_p^n$, out: $F_p^{n+1}$
Apply particle attrition model: Eq. (11)
In: $u_p^{n+1}$, out: $I_p^{n+1}$

$t = t + \Delta t$, $n \Rightarrow n + 1 \ (t = n \cdot \Delta t)$

Determine volume fraction: Eq. (12)
In: $x_p^1$, out: $\theta_p^1 \theta_p^n$

Solve Navier-Stokes equations (gas phase)
Eq. (1) (2) (3)
In: $u_p^1 \theta_p^1 p_{\xi}^{n-1} \theta_{\xi}^n \theta_p^n D_p^{n-1}$, out: $u_p^n p^n$

$t < t_{end}$ yes

no

**End**

3. **CMFB and FB reactors models**

The three-dimensional CMFB and FB reactors were modeled with Barracuda’s CPFD software. The schematic diagram of the CMFB reactor model is depicted in Fig. 2. The CMFB reactor contains 100 micro fluidized beds. For every micro fluidized bed, the length and width were 10 mm, the height was 42 mm, the thickness of the bed wall was 0.75 mm and the distributor was made of a mesh with size of 0.1 mm. The particles used in the simulations were set as FCC particles which is the most similar material to the adsorbent used in the
experiments in terms of physical characteristics in the material library of Barracudas software. The diameters and particle density of FCC particles were 300-500 μm and 1133 kg/m³, respectively. The initial bed heights consisted of 120 g FCC particles of the CMFB and FB were 25 mm and 154 mm, and the bulk density was the same 680 kg/m³. The particle close pack volume fraction was set as 0.6. Air was used as the fluidizing gas and the superficial velocities were ranging from 0 m/s to 1.59 m/s. Gas and particle properties and simulation conditions are listed in Table 1.

![Geometry of the CMFB reactor and initial conditions.](image)

**Table 1**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas</td>
<td>Ambient air (compressible)</td>
</tr>
<tr>
<td>Gas density (kg/m³)</td>
<td>1.225</td>
</tr>
<tr>
<td>Superficial gas velocity (m/s)</td>
<td>0 - 1.59 (0 L/min - 30 L/min)</td>
</tr>
<tr>
<td>Particle</td>
<td>FCC particles</td>
</tr>
<tr>
<td>Particle density (kg/m³)</td>
<td>1133</td>
</tr>
<tr>
<td>Bulk density (kg/m³)</td>
<td>680</td>
</tr>
<tr>
<td>Particle diameter (μm)</td>
<td>300 - 500</td>
</tr>
<tr>
<td>Bed mass (g)</td>
<td>120</td>
</tr>
<tr>
<td>Initial bed height (mm)</td>
<td>25 (CMFB); 154 (FB)</td>
</tr>
<tr>
<td>Close pack volume fraction</td>
<td>0.6</td>
</tr>
</tbody>
</table>

The inlet boundary for the gas phase was at the bottom of the reactor where room temperature and atmospheric pressure were set. A constant atmospheric pressure boundary condition was employed at the top of the beds where the gas left through. The positions of the boundary conditions are also depicted in Fig. 2. The particle normal-to-wall momentum retention coefficient was 0.3, the tangent-to-wall retention coefficient was 0.99 and the diffuse
bounce was 0, respectively. $P_s$, $\beta$ and $\varepsilon$ represent the constants for the particle normal stress model which were set at $P_s = 10$ Pa, $\beta = 3$ and $\varepsilon = 10^8$ as recommended by Snider et al [29]. The simulations were performed until 30 s total simulation time and the last 25 s were taken for averaging. The input parameters for the CPFD simulations are presented in Table 2.

**Table 2**

<table>
<thead>
<tr>
<th>Simulation parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Particle-to-wall interaction</strong></td>
<td></td>
</tr>
<tr>
<td>Normal retention coefficient, $e_n$</td>
<td>0.3</td>
</tr>
<tr>
<td>Tangential retention coefficient, $e_t$</td>
<td>0.99</td>
</tr>
<tr>
<td>Diffuse bounce, $D_f$</td>
<td>0</td>
</tr>
<tr>
<td><strong>Particle normal stress model</strong></td>
<td></td>
</tr>
<tr>
<td>Pressure constant of the solid-phase stress model, $P_s$</td>
<td>10 Pa</td>
</tr>
<tr>
<td>Dimensionless constant of the solid-phase stress model, $\beta$</td>
<td>3</td>
</tr>
<tr>
<td>Dimensionless constant of the solid-phase stress model, $\varepsilon$</td>
<td>$10^8$</td>
</tr>
<tr>
<td>Maximum momentum redirection from collision</td>
<td>40%</td>
</tr>
<tr>
<td><strong>Time settings</strong></td>
<td></td>
</tr>
<tr>
<td>Time step, $\Delta t$</td>
<td>0.001 s</td>
</tr>
<tr>
<td>Total time, $t$</td>
<td>30 s</td>
</tr>
<tr>
<td>Beginning time for average</td>
<td>5 s</td>
</tr>
</tbody>
</table>

**4. Experiment**

**4.1. Experimental apparatus**

The CMFB and FB reactors experimental platform were designed and built in accordance with the optimized geometry and operating conditions by the CPFD simulations described above. The schematic of the CMFB reactor is shown in Fig. 3 (a). The CMFB reactor consists of an enclosed cuboid housing section which was 130 mm, 130 mm, 250 mm in length, width and height respectively, and a CMFB section which was built by connecting 100 micro fluidized beds depicted in Fig. 2. The distributors were made of wire meshes with mesh size of 0.1 mm. At the bottoms of the reactors, two gas streams i.e. carbon dioxide and nitrogen with individual valves and mass flow controller were regulated to serve as the fluidizing gas or stripping gas. A series of temperature and pressure sensors are installed at different heights of the reactor walls for monitoring the fluidization behavior. CO$_2$ concentrations at the inlets and outlets of the reactors were continuously monitored by a mass
To demonstrate the performance of the CMFB reactor, the FB reactor was used as the comparison reactor which was 350 mm in height and 38.5 mm in internal diameter shown schematically in Fig. 3 (b). The distributor was made of porous metal with averaged pore size of 0.1 mm and 3 mm thickness.

According to OSHA Standards promulgated by Occupational Safety and Health Administration of America, the CO$_2$ concentration limit exposed to the air in workplaces is 0.5%. The 0.5% CO$_2$/N$_2$ gas mixture was used as the fluidizing gas which was prepared from pure CO$_2$ (99.99%) balanced with pure N$_2$ (99.995%) controlled by a mass flow controller, and pure N$_2$ was used as the purging gas for adsorbent regeneration. The adsorbent used in this study was synthesized by impregnating a mass ratio of 50% polyethyleneimine (PEI) into a macroporous resin support which had a pore volumes of 0.15 cm$^3$/g. The PEI-resin adsorbents had the particle density and diameters of 1133 kg/m$^3$ and 300-500 μm, and exhibits excellent adsorption capacity of 93.5 mg/g for 0.5% CO$_2$/N$_2$ gas mixture [9].
4.2. Experimental process design

The pressure drop measurements were performed for the empty beds, $\Delta P_e$, and the beds containing particles, $\Delta P_b$. The pressure drop due to bed of particles, $\Delta P$, was then calculated by:

$$\Delta P = \Delta P_b - \Delta P_e.$$

The average pressure drop over a period of 15 s (when the pressure drop was stable) was defined as the pressure drop at a given superficial gas velocity. During the experiment, the 0.5% CO$_2$/N$_2$ gas mixture was increased from 0 L/min to 30 L/min.

Before the adsorption experiment, the adsorbents was pretreated at 100 °C under flowing N$_2$ of 20 L/min for 60 min to remove the moisture and adsorbed CO$_2$ as much as possible. It was then cooled to the desired temperature and exposed to the 0.5% CO$_2$/N$_2$ gas mixture. The dynamic adsorption capacity ($q$) of the adsorbents is calculated using Eq. (16) [31]:

$$q = \frac{M C_i}{W} \int_0^\infty \left(1 - \frac{C_o}{C_i}\right) dt$$

(16)

where $M$, $W$ and $t$ are the total molar flow, the mass of adsorbents and the time, respectively. $C_i$ and $C_o$ are the CO$_2$ concentrations of the inlet and outlet gas. The saturation adsorption capacity is calculated at the saturation time when $C_o$ is equal to $C_i$, while the breakthrough adsorption capacity is calculated at the breakthrough time when $C_o$ is 5% of $C_i$. The regeneration experiments were conducted by rapidly heating the beds to 100 °C in pure N$_2$ with a flow rate of 20 L/min, and then the CO$_2$ adsorbed by the adsorbents could be desorbed.

The adsorbent attrition was determined by the ratio between the loss mass and the initial mass of the adsorbents after 10 consecutive cycles of CO$_2$ adsorption/desorption experiments under the flow rate of 30 L/min in the CMFB and FB reactors. The particle size distribution of the fresh and attrite adsorbents was obtained from standard sieve analysis.

The experimental conditions of the pressure drop, the performance for CO$_2$ capture and the adsorbent attrition measurements are summarized in Table 3.

### Table 3

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Bed particles</th>
<th>Fluidizing gas</th>
<th>Superficial fluidizing velocity (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure drop</td>
<td>0.5% CO$_2$/N$_2$</td>
<td>0 - 1.59 (0 - 30 L/min)</td>
<td></td>
</tr>
<tr>
<td>CO$_2$ adsorption</td>
<td>PEI-resin adsorbents</td>
<td>0.5% CO$_2$/N$_2$</td>
<td>1.06 (20 L/min)</td>
</tr>
<tr>
<td>Adsorbent regeneration</td>
<td>Pure N$_2$</td>
<td>1.06 (20 L/min)</td>
<td></td>
</tr>
<tr>
<td>Adsorbent attrition</td>
<td>0.5% CO$_2$/N$_2$</td>
<td>1.59 (30 L/min)</td>
<td></td>
</tr>
</tbody>
</table>
5. Results and Discussion

5.1. Pressure drop in CMFB and FB reactors

A proper identification of fluidization regimes is usually the first and key step towards the rational use of fluidized beds. The simulation snapshots of the cell vector magnitude and cell pressure drop of the bed containing particles, and the cell pressure drop of the empty bed in the CMFB reactor at $U = 1.59 \text{ m/s } (30 \text{ L/min})$ are shown in Fig. 5. It can be seen in the Fig. 5 (a) that the cell vector magnitudes distribute almost uniformly and equivalently after a special baffle was introduced in the CMFB reactor. The cell vector magnitudes in the distributor regions are much higher than the around regions. Fig. 5 (b) shows that the cell pressure drop of the empty bed at $U = 1.59 \text{ m/s}$ is only 4 Pa, which indicates that the cell pressure drop caused by the baffle can be ignored. Fig. 5 (c) indicates that the cell pressure at the bottom is always greater than the top one, and reduces gradually from the bottom to the top regions of every micro fluidized bed. Since the difference in dynamic pressure drop is proportional to the difference in bulk density, the data satisfy the elementary stability criterion according to which the bulk density must be a decreasing function of height.

Fig. 5. Snapshots of the cell vector magnitude (a) and cell pressure drop (c) of the bed containing particles, and the cell pressure drop of the empty bed (b) in the CMFB reactor at $U = 1.59 \text{ m/s}$.

The pressure drops in the CMFB and FB reactors varied with velocities were determined experimentally. Fig. 6 shows the typical pressure drop diagrams that indicate the linear increase with gas flow rates when the CMFB and FB are static and the subsequent levelling tendency irrespective of further increase in gas flow rates when the CMFB and FB have already been fluidized. In the same figure are plotted the pressure drops in the CMFB and FB reactors calculated from the simulation values. The transition points correspond to the minimum fluidization condition for the CMFB and FB with the flow rates being around 8.5 L/min and 2.0 L/min in the experiment and 10 L/min and 2.5 L/min in the simulation,
respectively. It can be seen that the pressure drop in the fluidized CMFB is 175 Pa which is much lower than 1250 Pa in the fluidized FB in the experiment, and 165 Pa which is much lower than 1100 Pa in the fluidized FB in the simulation. The pressure drops obtained from the simulation and experiment in the CMFB reactor achieve reductions of 86% and 85% as compared with that in the FB reactor, respectively.

The pressure drop predicted by the CPFD model is greater than the one observed in the experiment both in the CMFB and FB reactors. The main probable reason for this is that the bed materials used in the experiment has a higher porosity which leads to larger gas-solid contact area compared with the bed materials used in the simulation. The pressure drops obtained from the simulation and experiment show a similar tendency and the reductions achieved from the simulation and experiment are almost equal. Compared with the FB reactor, a lower pressure drop can be achieved by the CMFB reactor due to the relatively large inlet area and the reduced feed velocity.

![Fig. 6. Comparison of the simulation and experimental data of the pressure drops between the CMFB and FB reactors at different flow rates.](image)

The pressure drops in the CMFB and FB reactors obtained by CPFD simulations and experiments in this study are compared with those in different fluidized beds reported in a few literatures, given in Table 4. Guo et al. [22] and Liu et al. [21] reported low pressure drops of around 240 Pa and 600 Pa in the MFBs using several milligrams particles at a very low flow rate respectively. A low pressure drop of around 620 Pa in a MFB at a relatively high flow rate was published by Dang et al. [15]. The MFBs reported in above literatures have low pressure drop, but can only be used at millimeter or centimeter scale. Zhang et al. [8] evaluated CO₂
capture from ambient air in a laboratory-scale bubbling fluidized bed using 1.0 kg adsorbents, and obtained a high pressure drop of around 2500 Pa at a low flow rate. Lim et al. [28] carried out CPFD simulations in a bubbling fluidized bed containing large amounts of particles at a high flow rate, and achieved a very high pressure drop of 9450 Pa. A very high pressure drop of 7500 Pa in a large-scale fluidized bed column was also published by Chen et al. [25]. Comparing with all the reference data listed in Table 4, the pressure drop in the proposed CMFB in this study is the lowest. The CMFB reactor has lower pressure drop which can reduce the resistance overcome by the gas supply apparatus and then save energy consumption for gas supply. The CMFB reactor can gain long-term energy-saving effects in removing CO₂ from indoor air cyclically in HVAC.

Further research on the systematic and long-term energy consumption for CO₂ capture from indoor air using the CMFB reactor in HVAC is still needed which should include the evaluation of the capital costs for equipment and adsorbent, and the energy consumption for CO₂ adsorption and adsorbent regeneration.

### Table 4

<table>
<thead>
<tr>
<th>Bed type, Particles,</th>
<th>M&lt;sub&gt;bed&lt;/sub&gt;&lt;sup&gt;c&lt;/sup&gt; (kg)</th>
<th>H&lt;sub&gt;d&lt;/sub&gt;&lt;sup&gt;d&lt;/sup&gt; (mm)</th>
<th>Gas&lt;sub&gt;e&lt;/sub&gt;, V&lt;sub&gt;gas&lt;/sub&gt;&lt;sup&gt;e&lt;/sup&gt; (L/min)</th>
<th>ΔP&lt;sub&gt;CPFD&lt;/sub&gt;&lt;sup&gt;f&lt;/sup&gt; (Pa)</th>
<th>ΔP&lt;sub&gt;expt&lt;/sub&gt;&lt;sup&gt;g&lt;/sup&gt; (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMFB (present work)</td>
<td>MFB&lt;sup&gt;h&lt;/sup&gt; (100), FCC (CPFD), 8.5*8.5</td>
<td>0.12</td>
<td>air(CPFD)</td>
<td>165</td>
<td>175</td>
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<tr>
<td>FB (present work)</td>
<td>FB, 38.5 300-500</td>
<td>0.003</td>
<td>N₂, 0.6</td>
<td>240</td>
<td></td>
</tr>
<tr>
<td>Guo et al. [22]</td>
<td>MFB, 10.5 FCC, 83</td>
<td>0.007</td>
<td>air, 1.4</td>
<td>600</td>
<td></td>
</tr>
<tr>
<td>Liu et al. [21]</td>
<td>MFB, 12 silica sand, 460.6</td>
<td>0.04</td>
<td>air, 31</td>
<td>620</td>
<td></td>
</tr>
<tr>
<td>Dang et al. [15]</td>
<td>FB, 10*40 glass beads, 400-600</td>
<td>0.04</td>
<td>air, 8</td>
<td>2500</td>
<td></td>
</tr>
<tr>
<td>Zhang et al. [8]</td>
<td>FB, 67 PEI-silica, 250</td>
<td>1</td>
<td>air, 8</td>
<td>2500</td>
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<tr>
<td>Lim et al. [28]</td>
<td>FB, 300 MG-Si, 150</td>
<td>75</td>
<td>air, 720</td>
<td>9450</td>
<td></td>
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<tr>
<td>Chen et al. [25]</td>
<td>FB, 300*1000 Geldart B, 140</td>
<td>245</td>
<td>air, 54000</td>
<td>7500</td>
<td></td>
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</tbody>
</table>

<sup>a</sup>bed diameter; <sup>b</sup>particle mean diameter; <sup>c</sup>bed mass; <sup>d</sup>static bed height; <sup>e</sup>gas volume flow rate; <sup>f</sup>pressure drop obtained by CPFD simulation; <sup>g</sup>pressure drop obtained by experiment; <sup>h</sup>micro fluidized bed.

5.2. Adsorbent attrition in the CMFB and FB reactors
The simulation snapshots of particles trauma, an attrition index which determine the particle attrition in the CPFD models are shown in Fig. 7. It can be seen that the particle trauma in the CMFB and FB are ranging from 0 to $1.4 \times 10^{-6}$ and 0 to $8.6 \times 10^{-6}$ respectively. The mean particle trauma in the CMFB is $2.4 \times 10^{-7}$ which is much lower than $1.5 \times 10^{-6}$ in the FB, as also listed in Table 5.

In the experiment, the change of the cumulative particle size distribution of the fresh and attrite PEI-resin adsorbents in the CMFB and FB are shown in Fig. 8. It is clear that the distribution band of attrite particle size in the FB shifts to the lower size limit much more than that in the CMFB. The fragmentation of particles by attrition in the FB is much active than that in the CMFB. The adsorbent attrition calculated from the adsorbents mass remainings which are 117.5 g in the CMFB and 107.1 g in the FB is listed in Table 5, and it can be seen that the adsorbent attrition is just 2.1% in the CMFB, which is much lower than 10.7% in the FB reactor. The FB reactor significantly increases adsorbent attrition and, thereby, the cost of adsorbent replacement.
Fig. 8. Cumulative particle size distribution change in the CMFB and FB reactors.

Table 5

<table>
<thead>
<tr>
<th>Reactors</th>
<th>Modelling adsorbent attrition (%)</th>
<th>Experimental adsorbent attrition (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMFB reactor</td>
<td>2.4×10^{-7}</td>
<td>2.1</td>
</tr>
<tr>
<td>FB reactor</td>
<td>1.5×10^{-6}</td>
<td>10.7</td>
</tr>
</tbody>
</table>

5.3. Performance for CO₂ capture in the CMFB and FB reactors

During adsorption and desorption tests, a flow rate of 20 L/min was chosen in order to achieve fairly vibrant bubbling fluidization to facilitate sufficient gas-solid contact, mass transfer and heat transfer.

5.3.1. CO₂ adsorption performance

To demonstrate the superior performance of the CMFB reactor over the FB reactor, the breakthrough adsorption curve and saturated adsorption capacity of the PEI–resin adsorbent for 0.5% CO₂/N₂ gas mixture at the same flow rate were investigated in the CMFB and FB reactors respectively. As shown in Fig. 9, the CMFB reactor achieves a breakthrough time of about 0.84 h which is 35% larger than the 0.62 h in the FB reactor. The saturation adsorption time and capacities of about 2.73 h and 89.4 mg/g are achieved by the CMFB reactor, which is 17% shorter and 1.4% larger than about 3.31 h and 88.2 mg/g achieved by the FB reactor. These results suggest that the adsorbents can get more opportunities to contact with the gas, which increases the adsorbent utilization, accelerates overall kinetics and leads to a better adsorption performance for CO₂ capture in the CMFB reactor compared with that in the FB reactor.
reactor.

Fig. 9. Breakthrough adsorption curve and saturated adsorption capacity (inset) of the adsorbents in the CMFB and FB reactors.

5.3.2. Adsorbent regeneration

During the desorption experiments, the CO$_2$ concentrations of the outlet gases as a function of regeneration time are presented in Fig. 10. Nearly all of the CO$_2$ has been desorbed during 43 min in the CMFB reactor which is 17% less than the regeneration time of 52 min in the FB reactor. It can be seen that a rapid desorption provided by the CMFB reactor, indicating better gas-solid contact and superior heat-transfer characteristics than the FB reactor.

Fig. 10. Profiles of CO$_2$ concentration during desorption in the CMFB and FB reactors.

6. Conclusions

In this paper, a novel CMFB reactor was proposed for CO$_2$ capture in HVAC. The
performance of the CMFB reactor was systematically studied with the CPFD model and experiment and compared with the FB reactor in terms of pressure drop, adsorbent attrition and performance for CO₂ capture. The main conclusions can be summarized as follows.

(1) The CMFB reactor is able to achieve a large inlet area and a relatively low inlet velocity, thus yielding a low pressure drop. The pressure drop reductions of 86% in the experiment and 85% in the simulation are achieved as compared with that in the FB reactor. The CMFB reactor can gain long-term energy-saving effects in HVAC.

(2) After ten cycles of CO₂ adsorption/desorption experiments, lower adsorbent attrition of 2.1% is achieved in the CMFB reactor, than 10.7% in the FB reactor due to the reduced feed velocity.

(3) The CMFB reactor achieves a breakthrough time 35% larger and a saturation adsorption time 17% shorter than that of the FB reactor. It demonstrates a better adsorbent utilization by the CMFB reactor due to a longer contact time caused by a lower velocity.

(4) The CMFB reactor provides a regeneration time 17% less than that in the FB reactor. It demonstrates a rapid desorption in the CMFB reactor due to a superior gas-solid contact.

This proposed CMFB reactor can be a competitive and promising adsorption reactor for CO₂ capture using solid adsorbents in HVAC applications.

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References


