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# Numerical and experimental study of a novel compact micro fluidized beds reactor for CO<sub>2</sub> capture in HVAC



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#### ABSTRACT

In order to reduce the pressure drop and increase the adsorption performance for the CO<sub>2</sub> 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 CO<sub>2</sub> 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 CO<sub>2</sub> capture than that in FB reactor.

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#### 1. Introduction

Efficient and cost-effective  $\mathrm{CO}_2$  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  $\mathrm{CO}_2$  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 CO<sub>2</sub> capture system, is used for contacting CO<sub>2</sub>-laden gas streams with solid adsorbents. Therefore, the study of efficient and cost-effective adsorption reactor is very important for CO<sub>2</sub> capture in Heating, Ventilation and Air Conditioning (HVAC). At present, many kinds of reactors have been applied in the field of CO<sub>2</sub> 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 microstructured 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

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#### Nomenclature

$C_d$ Dr	g coefficient
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 $D_{\rm p}$  Interphase drag coefficient (1/s)

*F* Rate of momentum exchange per volume between

the gas and particle phases (N/m<sup>3</sup>s)

f Probability distribution function

g Gravitational acceleration (m/s<sup>2</sup>)

 $I_p$  Magnitude of the impact value (kg<sup>a</sup> m<sup>b</sup>/s<sup>b</sup>)

 $m_{\rm p}$  Particle mass (kg/m<sup>3</sup>)

 $n_{\rm p}$  Number of particles in a numerical particle

 $N_{\rm p}$  Number of numerical particles

p Gas pressure (Pa)
 P<sub>S</sub> Positive constant (Pa)
 r<sub>p</sub> Particle radius (m)
 Re Reynolds number
 S Interpolation operator

t Time (s)

u<sub>g</sub> Gas velocity (m/s)
 u<sub>p</sub> Particle velocity (m/s)
 U Superficial gas velocity (m/s)

V Volume

W Weighting factor  $x_n$  Particle location (m)

#### Greek letters

 $\rho$  Density (kg/m<sup>3</sup>)  $\theta$  Volume fraction

 $\tau$  Viscous stress tensor (N<sup>2</sup>/m<sup>2</sup>)

μ Gas viscosity (Pas) ε Constant number Constant number

#### **Subscriptions**

cp Close pack g Gas p Particle

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 modelling 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 CO<sub>2</sub> 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,  $\rm CO_2$  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

$$\frac{\partial \theta_{g} \rho_{g}}{\partial t} + \nabla \cdot \left(\theta_{g} \rho_{g} \mathbf{u}_{g}\right) = 0 \tag{1}$$

$$\frac{\partial \left(\theta_{g} \rho_{g} \mathbf{u}_{g}\right)}{\partial t} + \nabla \cdot \left(\theta_{g} \rho_{g} \mathbf{u}_{g} \mathbf{u}_{g}\right) = -\nabla p + \nabla \cdot \left(\theta_{g} \tau_{g}\right) + \theta_{g} \rho_{g} \mathbf{g} - \mathbf{F} \quad (2)$$

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.  $\mathbf{F}$  is the rate of momentum exchange per volume between the gas and particle phases.

$$\mathbf{F} = \int \int f m_{\rm p} \left( D_{\rm p} \left( \mathbf{u}_{\rm g} - \mathbf{u}_{\rm p} \right) - \frac{1}{\rho_{\rm p}} \nabla p \right) dm_{\rm p} d\mathbf{u}_{\rm p} \tag{3}$$

where f,  $m_p$ ,  $D_p$ ,  $\boldsymbol{u}_p$  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  $n_{\rm p}$  particles with identical properties located at position  $\mathbf{x}_{\rm p}$  ( $x_{\rm p}, y_{\rm p}, z_{\rm p}$ ). The particle acceleration is

$$\frac{d\mathbf{u}_{p}}{dt} = D_{p} \left( \mathbf{u}_{g} - \mathbf{u}_{p} \right) - \frac{1}{\rho_{p}} \nabla p + g - \frac{1}{\theta_{p} \rho_{p}} \nabla \tau_{p} \tag{4}$$

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

The particle movement is given by

$$\frac{d\mathbf{x}_{\mathbf{p}}}{dt} = \mathbf{u}_{\mathbf{p}} \tag{5}$$

#### 2.2. Interphase drag model

The interphase drag model used here is [29]

$$D_{\rm p} = C_{\rm d} \frac{3}{8} \frac{\rho_{\rm g}}{\rho_{\rm p}} \frac{|\mathbf{u}_{\rm g} - \mathbf{u}_{\rm p}|}{r_{\rm p}} \tag{6}$$

where

$$C_{\rm d} = \frac{24}{R_0} \left( 1 + 0.15 Re^{0.687} \right) \theta_{\rm g}^{-2.65} \ Re < 1000 \tag{7}$$

$$C_{\rm d} = 0.44\theta_{\rm g}^{-2.65} \ Re \ge 1000 \tag{8}$$

$$Re = \frac{2\rho_{\rm g}|\mathbf{u}_{\rm g} - \mathbf{u}_{\rm p}|}{\mu_{\rm g}} \left(\frac{3V_{\rm p}}{4\pi}\right)^{1/3} \tag{9}$$

where  $\mu_{\rm g}$  and  $V_{\rm p}$  is the gas viscosity and the particle volume.

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