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Three-dimensional CFD simulation of an MgO-based sorbent regeneration reactor in a carbon capture process

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ABSTRACT

Carbon dioxide is the primary greenhouse gas emitted through human activities; therefore, efficient reduction of CO_2 is regarded as one of the key environmental challenges of the current century. Different processes have been introduced in the literature for CO_2 capture; among these, solid sorbent processes have shown potential advantages such as easy regeneration and high capacity. In order to achieve steady CO_2 capture using solid sorbents, a circulating fluidized bed (CFB) is used that consists mainly of a carbonator reactor (where the CO_2 is adsorbed by solid sorbents) and a regenerator (where carbonated sorbents release CO_2 and a concentrated CO_2-steam mixture is produced). Different solid sorbents have been developed to be utilized in carbon capture units such as MgO-based sorbents and CaO-based sorbents. In this study, an MgO-based solid sorbent was used due to its capability to capture CO_2 at high temperature (300–550 °C), which is in the vicinity of the operating conditions of advanced power plants (e.g., integrated gasification combined cycles [IGCC]). The use of MgO-based sorbents results in a lower energy penalty in the carbonation/regeneration cycle of MgO-based sorbents. In this study, three-dimensional computational fluid dynamics (CFD) simulations of the regeneration unit of the carbon capture process using MgO-based solid sorbents were investigated and the performance of the fluidized bed regenerator unit (operating at different conditions) was studied.

1. Introduction

Energy consumption in the United States is predicted to rely mainly on fossil fuels (coal up to 19% and natural gas up to 28%) in 2040, while renewables are predicted to comprise up to 11% of total U.S. energy consumption (the rest are oil and other liquids [32%], liquid biofuels [1%], and nuclear [9%]) in 2040 (EIA, 2013). Furthermore, coal is expected to make up 35% of the electricity generation sector fuel source in 2040 [1], and it is projected that coal-powered power plants will continue to have the highest fraction of electricity generation in the United States despite their role in the production of CO_2 as a greenhouse gas [2].

Carbon capture and sequestration (CCS) is expected to result in a 19% reduction in CO_2 emission in the world by 2050 according to the Energy Information Association [1]. Cost-effective CCS results in the use of coal as one of the major fuel sources for electricity generation while still reducing carbon emissions (without affecting the economic growth). Advanced power generation technologies, such as integrated gasification combined cycles (IGCC), are expected to be among the leading contenders for power generation conversion because of their higher efficiencies, flexible products, and potential environmental advantages (such as more efficient CO_2 capture) compared to conventional coal combustion (pulverized coal) processes.

As of today, available commercial technologies for CO_2 capture include: MDEA, UOP Honeywell's Selexol™, and Linde's Rectisol. These liquid-solvent-based processes, which are widely used in industry, have some shortcomings including degradation of solvents by impurities, high heat of regeneration, and low operating temperature which is associated with a high energy penalty. Compared to the liquid solvent processes mentioned above, solid sorbents have a lower energy penalty because of the higher operating temperature [3–5], which translates into a reduced energy penalty for CO_2 sorption and regeneration processes. Among them, the MgO-based solid sorbents showed high capacity and reactivity toward CO_2 capture as well as high operating temperature and pressure that make them suitable for use in CCS units in advanced power generation plants. In other words, since the MgO-$MgCO_3$ equilibrium curve is close to the operating condition of advanced power plants [6], there would be lower energy penalties in the carbonation/regeneration cycle of MgO-based solid sorbents. Thus, in this paper, an MgO-based sorbent for CO_2 capture was used. In order to avoid efficiency losses in IGCC power plants, it is desirable to remove CO_2 in the temperature ranges between 300 °C and 500 °C, which makes regenerable MgO-based sorbents a very good candidate for this process.

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List of symbols

C	Concentration of CO_2 [=] $kmol/m^3$
D_e	Effective diffusion coefficient [=] m^2/s
d_p	Particle diameter [=] m
e_{pp}	Particle-particle restitution coefficient
$g_{0,pp}$	Radial distribution function
$\vec{g}$	Gravity acceleration vector [=] m/s^2
H_d	Heterogeneity coefficient
I_{2D}	Second invariant of solid deviatoric stress tensor [=] 1/s
I	Identity matrix
k_d	Regeneration reaction rate constant [=] $kmol/(m^2 \cdot s)$
k_{θ_p}	Granular conductivity [=] $kg/(m \cdot s)$
$\dot{m}_g$	Mass transported from the solid phase to the gas phase due to reaction [=] $kg/(m^3 \cdot s)$
$N_{MgCO_3}{}^0$	Initial concentration of $MgCO_3$ [=] $kmol/m^3$
P	Pressure [=] kPa
r	Radius [=] m
Re	Reynolds number
R_g	Universal gas constant, 8.314 [=] $kJ/(kmol \cdot K)$
t	Time [=] s
T	Temperature [=] K
$\vec{v}$	Mean velocity vector [=] m/s
x	$MgCO_3$ conversion

Greek letters

$\alpha_{p,max}$	Maximum packing limit
$\alpha_{p,min}$	Minimum frictional limit for solid volume fraction
α	Volume fraction
$\overline{\beta}$	Drag coefficient [=] $kg/(m^3 \cdot s)$
τ	Stress tensor [=] kPa
μ	Viscosity [=] $kg/(m \cdot s)$
λ	Bulk viscosity [=] $kg/(m \cdot s)$
η	$1/2(1 + e_{pp})$
θ_p	Granular temperature [=] m^2/s^2
γ_p	Granular temperature dissipation rate [=] m^2/s^3
φ	Angle of internal friction [=] degrees
ρ	Density [=] kg/m^3
δ	Dirac delta function

Subscripts

b	Bulk
c	Non-reactive core
col.	Collisional
e	Equilibrium
fric	Frictional
g	Gas
i	Interface
kin	Kinetic
p	Particle
t	Terminal

One of the challenges in utilization of novel technologies, such as CO_2 capture using solid sorbents, is the fact that the most promising technologies for CO_2 capture are still under development at the lab or bench scales. To successfully scale up these processes, a tool such as computational fluid dynamics (CFD) is needed to fill the gap between lab/bench-scale and industrial-scale systems. CFD has been proven to be a cost-effective tool for conducting virtual experiments, troubleshooting, simulations, prototype testing, and parametric studies [7–11]. Analysis using CFD complements and reduces physical testing and it can result in significant time and cost savings. A three-dimensional (3D) computational fluid dynamics (CFD) approach was used in this paper as an excellent tool to design fluidized bed systems for continuous CO_2 removal using solid sorbents.

2. Multiphase CFD equations for gas-solid flow systems

The continuity and momentum equations for each phase are derived from the general Reynolds Transport Theorem, which also is called the two-fluid model (TFM).

The closure for the interaction forces is sought based on the flow characteristics [9,10].

According to the TFM governing equations, conservation of mass or continuity equations for gas and solid phases are, respectively:

$$\frac{\partial(\alpha_g \rho_g)}{\partial t} + \nabla \cdot \left(\alpha_g \rho_g \overrightarrow{v_g}\right) = \dot{m}_g \tag{1}$$

$$\frac{\partial(\alpha_p \rho_p)}{\partial t} + \nabla \cdot \left(\alpha_p \rho_p \overrightarrow{v_p}\right) = -\dot{m}_g \tag{2}$$

$$\alpha_g + \alpha_p = 1 \tag{3}$$

The momentum equations for the gas and particulate phases are based on the Navier-Stokes equation and have been modified to include the drag force between phases. Conservation of momentum for gas and solid may be expressed as [10]:

$$\begin{aligned}\frac{\partial}{\partial t}\left(\alpha_g \rho_g \vec{v}_g\right) + \nabla \cdot \left(\alpha_g \rho_g \vec{v}_g \vec{v}_g\right) = &-\alpha_g \nabla P + \nabla \cdot \overline{\overline{\tau}}_g \\ &+ \alpha_g \rho_g \vec{g} - \overline{\beta}\left(\vec{v}_g - \vec{v}_s\right)\end{aligned} \tag{4}$$

$$\begin{aligned}\frac{\partial}{\partial t}\left(\alpha_p \rho_p \vec{v}_p\right) + \nabla \cdot \left(\alpha_p \rho_p \vec{v}_p \vec{v}_p\right) = &-\alpha_p \nabla P - \nabla P_p + \nabla \cdot \overline{\overline{\tau}}_p \\ &+ \alpha_p \rho_p \vec{g} + \overline{\beta}\left(\vec{v}_g - \vec{v}_p\right)\end{aligned} \tag{5}$$

The stresses experienced by the particles due to translation and collisions are referred to as solid-phase kinetic and collisional stresses. Kinetic and collisional stresses depend on the magnitude of particle velocity fluctuations (granular temperature). In this study, the gas phase turbulence was neglected because of a low Reynolds number. The transport equation for granular temperature is derived based on the kinetic theory of granular flow (KTGF) [10,12]:

$$\begin{aligned}\frac{3}{2}\left(\frac{\partial}{\partial t}(\rho_p \alpha_p \theta_p) + \nabla \cdot \left(\rho_p \alpha_p \vec{v}_p \theta_p\right)\right) = \left(-P_p \overline{\overline{I}} + \overline{\overline{\tau}}_p\right) \\ : \nabla \vec{v}_p + \nabla \cdot \left(k_{\theta_p} \nabla \theta_p\right) - \gamma_p\end{aligned} \tag{6}$$

The continuum approach generally relies on closure relations for the particles viscosity that most often are derived from the granular kinetic theory in the kinetic-collisional regime and from soil mechanics in the dense-frictional regime [10,13–15,37]. In this study, the solid viscosity was assumed to be the summation of the kinetic, collisional, and frictional viscosity in the entire range of solid volume fractions as suggested by Nikolopoulos [16]. The closing relations for gas and solid stress tensors, solid pressure, granular conductivity, and granular energy dissipation and gas-solid drag coefficient are presented in Table 1 [10].

The parameter H_d in Eqs. (13) and (14) represents the heterogeneity factor and is defined as drag force calculated by EMMS (Energy Minimization Multi-Scale) divided by drag force calculated by the homogeneous model of Wen and Yu [17]. An EMMS approach was used in this study for calculating the drag force between the gas and solid phases [16,18–20].

The available drag model in the literature can be categorized as homogeneous and non-homogeneous drag models. Homogeneous models