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Modeling and validation of a pilot-scale aqueous mineral carbonation reactor for carbon capture using computational fluid dynamics

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HIGHLIGHTS

- The CFD model for a pilot-scale aqueous mineral carbonation reactor is developed.
- Computational cost is reduced by using the CFD-lumped correlation model.
- The proposed CFD model is validated by experimental data from the pilot-plant.
- The errors of the CFD model for the CO_2 removal efficiencies are less than 8%.

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ABSTRACT

In anticipation of the successful establishment of carbon capture, utilization, and storage (CCUS) technology, a pilot-scale aqueous mineral carbonation plant, that removes CO_2 through a reaction with a $Ca(OH)_2$ solution, was built in Incheon, South Korea. Using computational fluid dynamics (CFD), two reactors with a diameter of 2.2 m and a height of 6.0 m were modeled and validated for reactor scale-up and optimization. Because a direct simulation of bubble breakage, coalescence, and interphase mass transfer results in enormous computational costs for modeling the pilot-scale multiphase reactor, a CFD-lumped correlation model was introduced to simulate a large reactor; this resulted in acceptable computational costs and maintained the simulation accuracy. In order to ensure the acceptability of the CFD model, two-step verification was conducted. The CFD model results were compared with the experimental data and published empirical correlations with regard to the gas holdup, interfacial area, and mass transfer coefficient. Subsequently, the CO_2 removal efficiencies of the CFD model were compared with the pilot-plant data. The errors of the CFD model for three hydrodynamic parameters and the CO_2 removal efficiencies were in the range of 1–8%. The validated CFD model will be used for designing a four times larger mineral carbonation reactor, that will be built in 2017.

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1. Introduction

As global warming has become a worldwide issue, carbon capture, utilization, and storage (CCUS) technologies are attracting increasing attention because these methods can remove CO_2, the major contributor to global warming. Carbon capture and storage, algae cultivation, carbon dioxide concrete curing, polymer production, and mineral carbonation are some representative CCUS technologies. Carbon capture and storage is the most promising technology and has been the focus of many research studies. However, this technology has several limitations, including the high cost of CO_2 separation, which has reached the minimum value reported so far but is still not profitable, high transportation costs, and lack of suitable locations for storing the captured CO_2 (Li et al., 2016; Metz, 2005; Nakaten et al., 2014). Among other technologies, mineral carbonation is commercially available and cost-effective owing to a direct reaction of CO_2 in the flue gas with the $Ca(OH)_2$ solution from the waste mineral system and without the need for complex separation units (Gerdemann et al., 2007; Huijgen et al., 2006; Oelkers et al., 2008; Xie et al., 2012). In addition, carbonate minerals are very stable for long-term storage (Metz et al., 2005). For this reason, Calera Inc., California, USA, has constructed a pilot-plant to utilize 10 MW of flue gas for producing more than one million tons of building materials (Kolstad and Young, 2010). Skyonic Corporation, Texas, USA, operates a demonstration facility aimed at capturing 75 000 ton of CO_2 per year from flue gas and for producing 14.3 million ton of sodium bicarbonate at a cement

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Nomenclature

a	interfacial area, m^2/m^3
D	column diameter, m
d_b	bubble diameter, m
g	gravitational acceleration, m/s^2
k	turbulent kinetic energy, m^2/s^2
n	bubble number density
R	ideal gas constant
t	time, s
T	Temperature, K
u	velocity vector, m/s
U_g	superficial gas velocity, m/s
v_p	average bubble velocity weighted by the bubble number, m/s
v_i	interfacial velocity, m/s
z	axial position along the flow direction (z-direction)

Greek letters

ε	energy dissipation, m^2/s^3
α	phase volume fraction
μ	molecular dynamic viscosity, Pa s
μ_t	turbulence dynamic viscosity, Pa s
ν_m	solution kinematic viscosity, m^2/s
ρ	density, kg/m^3
σ	surface tension, N/m
ϕ	solid weight fraction in solution
c_w	solid concentration by weight percent.
ψ	factor depending on the shape of the bubbles

Abbreviations

CCUS	carbon capture, utilization, and storage
CFD	computational fluid dynamics
E-E	Eulerian-Eulerian
MRF	multiple reference frame
PBM	population balance model

Subscripts

g	gas
l	liquid
s	solid
m	mixture of liquid and solid

plant in Capitol Aggregates (Jones et al., 2010). DW E&C Incheon, South Korea, built a pilot-scale aqueous mineral carbonation plant with two reactors of 2.2 m in diameter and 6.0 m in height that can capture 10 ton of CO_2 per day. For designing a carbonation reactor, computational fluid dynamics (CFD) has been used to model the three-dimensional (3D) hydrodynamics. Strasser and Wonders (2008) employed CFD to investigate a commercial-scale slurry bubble column reactor. Using CFD, Park et al. (2016) designed and optimized a carbonation reactor for solid suspension. Molaei Chalchooghi (2013) used CFD to obtain the bed void fraction and dense region height to simulate a carbonation reactor.

In order to maximize the net CO_2 absorption amount in an aqueous mineral carbonation reactor, it is important to reduce the reactor's power consumption as much as possible because other sources of CO_2 may be released during the power generation (Huijgen et al., 2006). As the reactor size increases, the power consumption in a reactor with impellers increases dramatically and is proportional to five squares of impeller diameter. Consequently, a bubble column reactor is the most suitable mineral carbonation reactor for capturing more than a million tons of CO_2 per year. However, most studies on bubble column reactors have been conducted at a laboratory-scale. Akita and Yoshida (1974) and Hikita et al. (1980) suggested empirical correlations for the gas holdup, interfacial area, and mass transfer coefficient but their studies were conducted at a small scale with a column diameter of less than 30 cm. Because it is difficult to measure complex hydrodynamics in bubble columns, experimental results for large bubble columns have been rarely reported (Shi et al., 2017). Only Kataoka et al. (1979) and Koide et al. (1979) have investigated the use of industrial-scale bubble column reactors with a diameter of more than 2.0 m; however, these studies only compared experimental results conducted in industrial-scale and laboratory-scale without presenting generic tendency for gas holdup, interfacial area, mass transfer coefficient, i.e., no available correlation for large bubble column. In addition, studies on bubble column reactors using CFD have been biased by laboratory-scale conditions. Yang and Xiao (2017) and Bordel et al. (2006) used CFD to study complex bubble size distributions in bubble columns with a diameter smaller than 15 cm. In order to simulate the complexity of the hydrodynamics, a population balance model (PBM) that accounted for bubble breakage, coalescence, and growth or shrinkage due to mass transfer was employed (Kotoulas and Kiparissides, 2006; Wang et al., 2006). Due to the very large computational time required for PBM model, studies for large-scale bubble column reactors have not been published (Bhole et al., 2008; Chen et al., 2004).

In this study, CFD modeling was conducted for a pilot-scale reactor in Incheon and a CFD-lumped correlation model was used to reduce the computational costs. Where bubble breakage and coalescence were considered by lumped correlation, Hibiki and Ishii (2002) correlation, which was derived from the one-dimensional bubble number density and interfacial area transport equations. Meanwhile, hydrodynamics and interphase mass transfer were considered by CFD. To determine the suitability of the CFD-lumped correlation model, a two-step verification process was conducted. First, for the gas holdup, interfacial area, and mass transfer coefficient, a validation was performed because these parameters are important for representing the hydrodynamics of a reactor and calculating the amount of mass-transferred CO_2. A CFD model qualification was performed by comparing the results with experimental data and well-known, published empirical correlations. Second, using the validated hydrodynamic parameters, the amount of mass-transferred CO_2 was determined with the CFD model and the CO_2 removal efficiencies were derived. Finally, a comparison of the CO_2 removal efficiencies from the CFD model and from actual pilot-plant data completed the validation.

2. Experimental setup

The pilot-scale reactor has a diameter of 2.2 m and a height of 6 m. The high-performance gas distributor has nine nozzles. The two types of nozzles are shown in Fig. 1. The three nozzles in the upper part are type A nozzles and the six nozzle in the lower part are type B nozzles. Although the type A nozzle is longer than the type B nozzle, the nozzles are nearly the same because only the lower part of the nozzle (420 mm in length) has holes that blow out gas. The diameter of the evenly distributed holes is 5 mm. Tiny impeller with a diameter of 15 cm is located at a height of 1.2 m on the side wall; it prevents sedimentation and operates at a speed of 150 rpm. The reactor and gas distributor are shown in Fig. 2.

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