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Modeling and simulation of circulating fluidized bed reactors applied to a carbonation/calcination loop

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ABSTRACT

A fluid dynamic model for a gas-solid circulating fluidized bed (CFB) designed using two coupled riser reactors is developed and implemented numerically with code programmed in Matlab. The fluid dynamic model contains heat and species mass balances to calculate temperatures and compositions for a carbonation/calcination loop process.

Because of the high computational costs required to resolve the three-dimensional phenomena, a model representing a trade-off between computational time requirements and accuracy is developed. For dynamic processes with a solid flux between the two reactor units that depends on the fluid dynamics of both risers, a dynamic one-dimensional two-fluid model is sufficient.

A two-fluid model using the constant particle viscosity closure for the stress term is used for the solid phase, and an algebraic turbulence model is applied to the gas phase. The numerical model implementation is based on the finite volume method with a staggered grid scheme. The exchange of solids between the reactor units constituting the circulating fluidized bed (solid flux) is implemented through additional mass source/sink terms in the continuity equations of the two phases.

For model validation, a relevant experimental analysis provided in the literature is reproduced by the numerical simulations. The numerical analysis indicates that sufficient heat integration between the two reactor units is important for the performance of the circulating fluidized bed system.

The two-fluid model performs fairly well for this chemical process operated in a CFB designed as two coupled riser reactors. Further analysis and optimization of the solution algorithms and the reactor coupling strategy is warranted.

1. Introduction

Recently, extensive research has been dedicated to processes that reduce CO_2 emissions to the atmosphere via carbon capture and sequestration because CO_2 is a key greenhouse gas. The CO_2 capture processes can be divided into three categories, pre-combustion CO_2 capture, chemical looping processes and post-combustion CO_2 capture. One way of capturing CO_2 in both the pre-combustion and the post-combustion processes is via the addition of solid sorbent particles operating continuously in cycles of carbonation and decarbonation to keep sorption rates high enough to allow CO_2 separation.

The pre-combustion CO_2 capture processes convert hydrocarbons to synthesis gas, an H_2-rich gas containing some CO and CO_2, which can subsequently be burned, producing steam. CO_2 capture occurs while reforming the hydrocarbons, shifting the equilibrium towards production of H_2. Steam methane reforming (SMR) can be improved by adding solid particles that adsorb CO_2 from the gas phase and shift the equilibrium towards products. In the sorption enhanced steam methane reforming process (SE-SMR), higher H_2 yields are produced and the CO_2 is separated from the product stream (Wang, Chao, & Jakobsen, 2011). SE-SMR is thus a pre-combustion CO_2 capture process.

Related processes include chemical looping combustion (CLC) and chemical looping reforming (CLR). In these two processes, the circulating fluidized bed reactor (CFBR) consists of an air reactor (AR), where a metal is oxidized with the oxygen present in air, and a fuel reactor (FR), where the oxidized particles release oxygen, driving combustion in a controlled manner, without producing NO_x and avoiding the costly O_2 production unit. The primary difference between CLC and CLR is that in CLR, the process steam is fed into the fuel reactor, thus allowing partial oxidation, obtaining H_2 and CO in the outlet stream in addition to CO_2 and H_2O (Rydén, Lyngfelt, & Mattisson, 2006).

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Nomenclature

Latin letters

a_s	particle surface-to-volume ratio, 1/m
A	area, m^2
Cp_k	specific heat capacity of phase k, J/(kg K)
d_p	particle diameter, m
d	reactor unit diameter, m
D_h	hydraulic diameter, m
$D_{k,i}$	mass diffusivity coefficient for species i in phase k, m^2/s
f_k	friction coefficient for phase k, –
g	gravitational acceleration, m/s^2
G	solids stress modulus, Pa
h	interfacial heat transfer coefficient, $W/(m^2 K)$
h_{NC},h_R	heat transfer coefficient wall-air from natural convection and from radiation, $W/(m^2 K)$
h_{wall}	heat transfer coefficient between solids and the wall, $W/(m^2 K)$
ΔH	enthalpy of reaction, J/kmol
k_{air}	thermal conductivity of air, W/(m K)
L	reactor unit height, m
m	mass, kg
M	molecular weight, kg/kmol
p	gas pressure, Pa
r	carbonation net reaction rate, $kmol/(m^3 s)$
R	universal gas constant, J/(kmol K)
S	specific surface area, m^2/kg CaO
S_{sp}, S^0_{sp}	specific surface area of carbonated sample, m^2/kg
t	time, s
T_k	temperature of phase k, K
T_p,	temperature of the incoming solids, K
T_{wall}	temperature at the wall, K
T_k, T_k^{Re}	stress tensor for phase k, kg/(m s)
v_k	velocity of phase k, m/s
X	sorbent conversion, –
y_i	mole fraction of species i,–
z	axial coordinate, m

Greek letters

α_k	volume fraction of phase k, –
ε	porosity, –
α_{wall}, ε_{wall}	absorptivity and emissivity of the carbonator wall for radiative heat transfer, –
β	interfacial friction coefficient, $kg/(m^3 s)$
Γ	net mass source of solids, $kg/(m^3 s)$
η_{cap}	CO_2 capture efficiency, –
λ_k	thermal conductivity of phase k, W/(m K)
μ_k	viscosity of phase k, kg/(m s)
ν_g	gas phase kinematic viscosity, m^2/s
ν_i	stoichiometric coefficient for species i, –
ξ_i	diffusion volume of species i (Fuller, Schettler, & Giddings, 1966), –
ρ_k	density of phase k, kg/m^3
ρ_{app}	apparent absorbent density, kg/m^3
σ_k	viscous stress tensor for phase k, kg/(m s)
σ_{sb}	Stefan–Boltzmann constant, $W/(m^2 K^4)$
φ_p	sphericity,–
ω_i	mass fraction of species i, –

Subscripts/Superscripts/Abbreviations

1	carbonator
2	decarbonator/calciner
CFB	circulating fluidized bed
CFBR	circulating fluidized bed reactor
eff	effective
eq	equilibrium
i	species
in	inlet, incoming, inner
k	phase
m	molecular
g	gas
o	outer
out	outlet, outer
p	particle, solids
surr	surroundings
stat	static
t	turbulent

The goal of the post combustion CO_2 capture processes is to capture the CO_2 generated during combustion from the exit flue gases. Rodríguez, Alonso, and Abanades (2011) investigated the potential of a carbonation–decarbonation loop to separate the CO_2 from power plant flue gases.

Conventional models for fluidized bed reactors, such as the Kunii-Levenspiel model and the Van Deemter model, assume that the solids are in pseudo-steady state or stagnant (Jakobsen, 2008, pp. 894–915; Kunii & Levenspiel, 1991). The distribution profiles of the solids are thus predefined. Those models are not appropriate for CFB reactor simulations because the dynamics of the solid flux cannot be included. The solid fluxes and particle CO_2 contents change as the solids circulate through the reactor. Therefore, a complete set of the governing equations must be solved to include the dynamics of the solids.

In this study, the complete CFB model is developed and validated by comparing the simulated results with experimental data from the literature. To exploit the CFB model potential, a process operating in the fast fluidization regime is simulated, where the interfacial phenomena and the solid dynamics depend upon the axial evolution of the process within each reactor unit in addition to the coupling between reactor units. For other processes operating in the bubbling bed regime in a single unit fluidized bed or for CFB processes with a fixed solid flux and thus steady-state operation, simpler models can be employed. Such reactors may be fairly well represented using the Kunii-Levenspiel type of model with stationary solid patterns. In the Kunii-Levenspiel type of models, there are no momentum equations for computing the bed expansion; thus, the bed expansion is neglected.

2. Model description

In this section, the governing equations, the constitutive closure relations and the boundary and initial conditions used in the model are described.

Fluidized systems are classified according to the prevalent flow regime. From lower to higher inlet gas velocity, the different gas-solid flow regimes are bubbling bed, slugging, turbulent, fast fluidization and pneumatic conveying (Jakobsen, 2008, p. 869).

The two reactor units constituting a CFBR can be designed to operate in different fluidization regimes. In this way, the CFB reactor design can be tailored to a specific process to provide optimal residence times, mixing, temperatures, etc. In the present work, the CFBR consists of two interconnected reactor units, both operating in the fast fluidization regime, one for carbonation and one

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