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Macroscopic fuel reactor modelling of a 5 kW_{th} interconnected fluidized bed for in-situ gasification chemical looping combustion of coal

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HIGHLIGHTS

- A model is developed for the combustion of coal in a novel 5 kw fluidized bed system.
- The fluid dynamics and mass transfer in the fuel reactor with a riser are simulated.
- The model predicts the effects of different operation conditions on the performance.
- The sensitivity analysis for the efficiency of combustion and carbon capture is done.

ARTICLE INFO

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ABSTRACT

A macroscopic model is developed to simulate the fluid dynamics with the transfer of heat and mass in the fuel reactor and the riser of a novel 5 kW_{th} interconnected fluidized bed system for chemical looping combustion of coal. The fuel reactor and the riser are divided into a bottom bed consisting of bubble and emulsion phases, a freeboard with splash and transport phases, a transition zone with different cross-section areas and a riser providing the driving force to recirculate solids between the fuel and air reactors. The developed model is validated by the experimental cases with different operation conditions such as thermal power, temperature and coal feeding rate. Subsequently, the effects of reactor temperature, solids inventory, oxygen carrier to coal ratio and compositions of the fluidizing agent on the reactor performance are analyzed in details by the help of the validated model. The sensitivity analysis shows that the reactor temperature is the most relevant parameter affecting the combustion efficiency and CO_2 capture efficiency. Furthermore, increasing the oxygen carrier to coal ratio increases the combustion efficiency but decreases the CO_2 capture efficiency, while increasing the volume fraction of CO_2 in the fluidizing agent has the opposite effect on the performance of this experimental unit.

1. Introduction

Chemical looping combustion (CLC) technology has been considered as a very promising CO_2 capture technology from fossil fuel combustion [1,2]. The oxygen carrier transfers the oxidizer from the air reactor to the fuel reactor, so that the fuel no longer mix with the air directly in the fuel reactor. Since gas emissions mainly consist of CO_2 and H_2O, the nearly pure CO_2 can be captured with less energy consumption in comparison with the conventional CO_2 capture technologies.

The plenty of oxygen carriers are required as the bed material to supply the oxidizer and to be heat carrier circulating between the fuel reactor and the air reactor. The interconnected fluidized bed reactor system has been the most popular reactor for CLC, because this reactor configuration can intensify the contact between gas and particles and circulate the bed inventory between two reactors. Lyngfelt et al. proposed the design criterion of an interconnected fluidized bed reactor system for CLC [3] and operated a continuous 10 kW_{th} CLC reactor using gaseous fuel [4]. Their works demonstrated the feasibility of this reactor for the CLC technology. Designing and using different interconnected fluidized bed reactor systems, several research groups successfully applied CLC to solid fuels [5–14]. The performance of these reactors, such as fuel conversion, the distribution of carbonaceous gases, the residence time of solid materials, are mainly determined by the behavior in the fuel reactor [15,16]. The operation conditions of the fuel reactor also have great influence on the risk of agglomeration/ sintring and attrition/fragmentation that impair the reactivity of oxygen carriers and pose a negative effect on the fuel conversion

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Nomenclature

A_0	gas distributor area per nozzle
A_c	section area of the fuel reactor (m^2)
Ar	Archimedes number
C_{bottom}	solid concentration in the bottom bed
$C_{freeboard}$	solid concentration in the freeboard bed
$C_{c\text{-}a}$	solid concentration in the core-annulus zone
C_{spl}	solid concentration in the splash phase
C_{tran}	solid concentration in the transition zone
C_{carbon}	carbon concentration in the fuel
$C_{b,i}$	concentration of gas compositions in bubble phase
$C_{e,i}$	concentration of gas compositions in emulsion phase
$C_{g,i}$	concentration of gas for reduction of oxygen carriers
D_B	diameter of bubbles (m)
d_i	stoichiometric coefficient for gas combustion
d_p	diameter of bed material (m)
E	activation energy
F_b	flow of gas compositions in the bubble phase (mol/s)
F_{char}	flow of carbon exiting from the fuel reactor (mol/s)
F_{coal}	rate of coal feeding (kg/s)
F_e	flow of gas compositions in the emulsion phase (mol/s)
F_{exc}	flow of gas from the emulsion to bubble phase(mol/s)
F_d	drag force
F_{dil}	flow of gas compositions in the dilute phase (mol/s)
F_p	friction between particles and wall
F_{OC}	solid circulation rate (kg/s)
F_w	friction between gas and wall
$F_{w,j}$	solid flow by the wall-layer (kg/s)
F_{WGS}	flow of gas composition from WGS reaction (mol/s)
H_{bot}	height of bottom bed zone (m)
H_r	height of reactor (m)
k_{be}	coefficient of mass transfer between emulsion and bubble phase
k_g	mass transfer coefficient
K	chemical parameters for the reaction rate
Mw	molecular mass (kg/kmol)
P	pressure (Pa or Bar)
r_g	grain radius (μm)
R	mass transfer resulted from chemical reaction (kg/m^3 s)
R_{OC}	oxygen transport capacity of the oxygen carriers
S_{area}	section area (m^2)
t_r	mean reaction time (s)
t_{mr}	mean residence time (s)
u_g	gas velocity (m/s)
U_g	superficial gas velocity (m/s)
U_{mf}	minimal fluidization velocity (m/s)
U_B	velocity of bubble phase (m/s)
$U_{g,int}$	velocity of interstitial gas velocity (m/s)
U_t	terminal velocity of particles (m/s)
u_g	real velocity of gas (m/s)
V	volume of each cell (m^3)
x	mass fraction
X	mass fraction
X_{OC}	conversion rate of oxygen carriers
$\overline{X_{OC}}$	mean conversion rate of oxygen carriers
$\overline{X_{OC,in}}$	mean conversion rate of oxygen carriers at the inlet of the fuel reactor
$\overline{X_{OC,out}}$	mean conversion rate of oxygen carriers at the outlet of the fuel reactor
X_{char}	char conversion rate
y_i	molar fraction of gas i

Greek symbols

δ_B	volume fraction of bubble phase
ρ_s	average density of solids (kg/m^3)
$\rho_{m,i}$	molar density of the reacting material (mol/m^3)
ε_s	volume fraction of solids in each cell
ε_g	volume fraction of gas in each cell
ε_B	average bed porosity
τ_i	time for complete solid conversion for the reaction
Ω_{OD}	oxygen demand
η_{comb}	combustion efficiency
η_{CC}	CO_2 capture efficiency

Subscript

mf	minimum fluidization condition
sta	saturation condition
OC	oxygen carrier
int	interstitial gas
WGS	water gas shift reaction

[17,18]. Therefore, it is significant to seek optimized reactor design and operation conditions for the fuel reactor.

Along with the experimental research, the computational fluid dynamics (CFD) [19–21] and the macroscopic model [22–24] provide other essential tools to investigate the fluid dynamics and chemical kinetics in the fuel reactor. Using CFD model, Mahalatkar et al. not only predicted the emission of the fuel reactor but also captured the reasonable conversion rate of solid fuels and oxygen carriers at different reactor temperatures [25]. Emden et al. used the two-fluid model to research the influence of different reactor configuration and operation including buffer position, solid circulation rate and air reactor length on the reduction degree of oxygen carrier in the fuel reactor [20]. Parker carried out the three-dimensional simulation by using the computational particles instead of the real oxygen carrier particles in the circulating fluidized bed [26]. The simulated solid circulation rate and efficiency had good agreement with the experimental measurements.

However, the computational cost of CFD methods is rather high on account of the large amount and the long reaction time of oxygen carriers, especially for the parametric study [24–26]. The macroscopic model maintaining the effect of fluid dynamics based on empirical/semi-empirical expressions, by contrast, can make out the relationship between operation parameters and performance at much lower cost [27]. Pallares and Johnsson reviewed the utilization of macroscopic model in the large-scale circulating fluidized bed [27]. This literature showed that the macroscopic model provided satisfying results of fluid dynamics like the axial volume fraction along the bed, particle size segregation and superficial solids net flow with much lower computation time. Considering the chemical reaction model of oxygen carriers derived from experiments [28], Abad et al. developed a macroscopic model to simulate the CLC of gaseous fuel and solid fuel in the fuel reactor separately [15,29,30]. This developed model was also used to investigate the influence of different parameters on the performance of $1MW_{th}$ chemical-looping combustion of coal, and the optimal temperature and solid inventory were suggested for attaining the maximum carbon separation efficiency [31]. Focusing on developing the model for fuel reactor, Peltola et al. modeled the methane combustion in the dual fluidized bed system and provided a nice method to improve the performance of an pre-commercial scale CLC system [23,32]. Furthermore, the macroscopic model of fuel reactor was used to study the chemical looping with oxygen uncoupling process [33] and the biomass combustion [24].

It has been validated that macroscopic model of the fuel reactor is