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Multi-scale simulation of chemical looping combustion in dual circulating fluidized bed

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HIGHLIGHTS

- A modified multi-scale gas–solid flow-reaction coupled model is developed.
- Multi-scale characteristic of chemical looping combustion system is investigated.
- Predicted results show a good agreement with experimental data.

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ABSTRACT

Chemical looping combustion (CLC) in an interconnected fluidized bed has attracted more and more attention owing to its novel technology with inherent separation of CO_2. In recent years, some models have been developed to investigate the gas-particle flow and reactive characteristics during the CLC process. However, multi-scale structures in reactors make it complex to perform a simulation. In the current work, a multi-scale gas–solid flow-reaction coupled model is developed and applied to the simulation of the CLC process in a dual circulating fluidized bed (DCFB) system with consideration of the impact of multi-scale structures on chemical reactions, mass and heat transfer. By comparisons of gas pressure and gas components with experimental data, the present model shows a better prediction. The influence of clusters on the gas compositions and temperature field is analyzed.

1. Introduction

With the global warming, carbon dioxide (CO_2) emissions have attracted more and more attention. Chemical looping combustion is a promising CO_2 capture technology, which isolates the fuel source from the oxygen source by oxygen carriers and achieves inherent separation of CO_2 [1,2]. In the last two decades, diligent research efforts have been devoted to develop the CLC system [3–5]. Cuadrat et al. [6] investigated a coal fuelled CLC reactor using ilmenite as oxygen carriers. It was found that the optimization of the CLC with coal can result in energy production with high CO_2 capture. García-Labiano et al. [7] exploited an energy potential of acid through the combustion of H_2S using the CLC system. It was concluded that the H_2S concentration of 20 vol.% was high enough to turn CLC into an auto-thermal process. Haonsen et al. [8] studied the CLC performance in a rotating bed reactor and discussed the effects of process parameters by means of experiments. Miller et al. [9] emphasized that the Mg-promoted hematite enhanced oxygen transfer capacity of hematite and showed better performance for methane CLC. Zhang et al. [10] performed a comparison between fluidized bed and fixed bed for a pressurized coal-fuelled CLC process. It was demonstrated that the fluidized bed mode had the superiority for a long-term stable operation.

Computational fluid dynamics (CFD) provides an effective insight into the hydrodynamics of the complicated multiphase flow and has been applied to the simulation of the CLC process [11–13]. Peng et al. [14] employed a CFD–DEM model to evaluate some factors that influenced the solid circulation rate (SCR) in chemical looping systems. The results indicated that the flow regime in the air reactor was the main mechanism to determine the fluctuation frequency and amplitude of SCR. Guan et al. [15] incorporated the kinetic theory of granular flow into a three-dimensional CFD model to predict the hydrodynamics characteristic in the interconnected fluidized bed for the CLC process. It was found that the drag model had a significant impact on the prediction of the gas–solid flow and the solids flow patterns in the fuel reactor (FR) depended strongly on the operating parameters in the air reactor (AR).

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Nomenclature

a	acceleration (m s^{-2})
d_c	cluster diameter (m)
d_s	particle diameter (m)
c_p	specific heat capacity (J kg^{-1} K^{-1})
f	volume fraction of dense phase
F	force acting on each particle or cluster (N)
g	gravity (m s^{-2})
h	local heat transfer coefficient (J m^{-2} s^{-1} K^{-1})
h_{dc}	inter-phase heat transfer coefficient (J m^{-2} s^{-1} K^{-1})
K_{dc}	inter-phase mass exchange coefficient (m s^{-1})
M	Molar weight (g mol^{-1})
n	reaction order
N_{df}	energy dissipation (W kg^{-1})
r	reaction rate (kmol m^{-3} s^{-1})
S	mass source (kg m^{-3} s^{-1})
T	temperature (K)
u	velocity (m s^{-1})
U	superficial velocity (m s^{-1})
X_i	mass fraction of gas species
X_{ox}	reduction or oxidization degree of oxygen carriers

Greek letters

α	specific surface area (m^{-1})
β	drag coefficient (kg m^{-3} s^{-1})
ε	volume fraction
λ	thermal conductivity (W m^{-1} K^{-1})
μ	viscosity (Pa s)
ρ	density (kg m^{-3})

Subscripts

c	cluster
den	dense phase
dil	dilute phase
int	interface
g	gas phase
s	particle phase

The dual circulating fluidized bed (DCFB) system including two interconnected circulating fluidized beds has the potential for the CLC process owing to its low particle attrition rate and excellent gas–solids contact, as shown in Fig. 1. Meanwhile, the staged fluidization of the air reactor controls the global circulation rate of the system [16]. Penthor et al. [17] presented the CLC performance in the DCFB system using a copper based oxygen carrier and revealed that the solids inventory and circulation were critical parameters for the fuel conversion. The impact of internal installation on the particles residence time was evaluated [18]. The results revealed that the effect of internal loop was enhanced when fluidization velocities were increased in reactors. Wang et al. [19,20] investigated the flow and reactive characteristic for the CLC process in the DCFB system by means of CFD modeling, where a cluster structure-dependent (CSD) drag model was used to consider the cluster impact. From the simulated results, we can find that there was an improvement of the predictions in some extent. However, the cluster effects on reactions and inter-phase heat transfer were neglected. Lu et al. [21] pointed out that an isolated particle had significantly higher mass and heat transfer rates than the particle in the cluster by an investigation of the gas-cluster mass and heat transfer. An increase of the cluster porosity can promote the gas-cluster mass and heat transfer rates. Hence, it is necessary to take into account the cluster impact on mass and heat transfer during the CLC process.

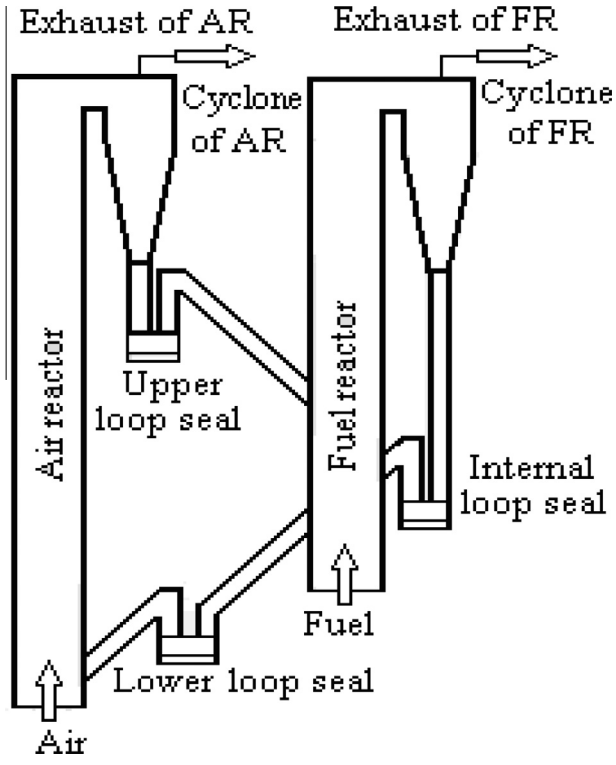

Fig. 1. Sketch of a DCFB reactor system.

In recent studies, Hou et al. [22,23] established the relationship between mass transfer and flow structures for fast fluidized beds and developed a multi-scale mass transfer (MSMT) model based on energy-minimization multi-scale (EMMS) method. In this model, the cluster impact on mass transfer was considered. The simulated results of the ozone decomposition process showed a better agreement with experimental data. The MSMT model was further validated for the catalytic oxidation of carbon monoxide in a circulating fluidized bed [24]. The results also demonstrated that the clusters played an important role in the gas–solid mass transfer. To describe the effect of clusters on chemical reaction, mass and heat transfer simultaneously, a multi-scale chemical reaction model coupling heat transfer was developed in our previous work [25], where the temperature discrepancy between cluster phase and dispersed phase was incorporated and the cluster structure-dependent (CSD) drag model was adopted to provide local structural parameters. By simulating the regeneration reaction of oxygen carriers in riser reactors, the multi-scale chemical reaction model promoted the accuracy of predicted results.

This work focuses on the investigation of the multi-scale flow and reactive characteristics for the whole CLC process by means of CFD modeling. For the simulation of the DCFB system consisting of two circulating fluidized beds, employing a multi-scale model coupled with chemical reaction and heat transfer is more rational to reflect the influence of the temporal-spatial multi-scale structures on the chemical looping system, which is not available in recent literatures. The advantage of this approach lies in the more