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Computational fluid dynamics simulation for chemical looping combustion of coal in a dual circulation fluidized bed

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ABSTRACT

A dual circulation fluidized bed system is widely accepted for chemical looping combustion (CLC) for enriching CO_2 from the utilization of fossil fuels. Due to the limitations of the measurement, the details of multiphase reactive flows in the interconnected fluidized bed reactors are difficult to obtain. Computational Fluid Dynamics (CFD) simulation provides a promising method to understand the hydrodynamics, chemical reaction, and heat and mass transfers in CLC reactors, which are very important for the rational design, optimal operation, and scaling-up of the CLC system. In this work, a 5 kW_{th} coal-fired CLC dual circulation fluidized bed system, which was developed by our research group, was first simulated for understanding gas leakage, flow pattern and combustion efficiency. The simulation results achieved good agreement with the experimental measurements, which validates the simulation model. Subsequently, to improve the combustion efficiency, a new operation condition was simulated by increasing the reactor temperature and decreasing the coal feeding. An improvement in the combustion efficiency was attained, and the simulation results for the new operation condition were also validated by the experimental measurements in the same CLC combustor. All of the above processes demonstrated the validity and usefulness of the simulation results to improve the CLC reactor operation.

1. Introduction

Chemical looping combustion (CLC), which has the characteristic of CO_2 inherent separation, is a novel fossil fuel utilization technology [1,2]. Lattice oxygen atoms in the oxygen carrier instead of oxygen molecules in air are used to oxidize the fossil fuel indirectly. In this process, the utilization of chemical energy is cascaded, thereby achieving higher energy conversion efficiency. A typical CLC reactor is composed of an air reactor (AR) and a fuel reactor (FR). The fossil fuel is oxidized via an oxygen carrier with high oxygen potential (usually metal oxide, Me_xO_y) in the FR, and the resulting products are CO_2, H_2O and an oxygen carrier with low oxygen potential (Me_xO_{y-1}). High-purity CO_2 can be easily obtained from the flue gas through a simple condensation process. The high oxygen potential OC is regenerated in the AR as the low oxygen potential OC is re-oxidized by air. Circulation is formed as the high oxygen potential OC is further transferred into the FR.

Due to the complex multiphase reactive flows present in CLC reactors (usually dual-circulation fluidized beds [3–6], also a small amount of fixed bed [7]), a comprehensive understanding to the multiphase reactive flows is important for the rational design, optimal operation and scaling-up of the CLC reactors. As an effective tool, numerical simulation has been used by many researchers. Based on the description of the fluid dynamics of the reactor, two categories of models can be identified [8]: macroscopic fluid dynamics models (MFD) [9–13] and computational fluid dynamics models (CFD). Based on the description to the particle phase dynamics, the CFD models can also be divided into three categories: the two-fluid model, the CFD-DEM (discrete element method) model [14,15], and the CPFD (computational particle fluid dynamics) model [16,17]. In CFD simulation based on the Navier–Stokes equation for describing the fluid flow, less artificial factors existed. Generally speaking, the CFD simulation result is more credible than that of MFD simulation. Among the CFD simulations, the two-fluid CFD model is widely adopted in the literature because it can provide almost all of the details of multiphase reactive flows within an acceptable computational cost. In the present work, we mainly focused on the CLC–CFD simulation using the two-fluid model.

Generally the CFD simulation in this aspect can be distinguished between CLC of gaseous fuels and one using solid fuels. Since the CLC of gaseous fuels is relatively simple on the experimental investigation end as well as on the numerical simulation end, both CFD model (reaction kinetic model for gas–solid heterogeneous reaction and multi-scale hydrodynamics model for particle cluster) development and thermo-chemical performance understanding have been widely investigated for the CLC of gaseous fuels.

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Nomenclature

C_i	concentration of gas i (mol/m^3)
C_d	drag coefficient
d_s	granular diameter (m)
$D_{i,m}$	diffusion coefficient for species i in the mixtures (m^2/s)
e	coefficient of restitution
E	activation energy (kJ/mol)
G_0	radial distribution function
$\mathbf{g}$	acceleration due to gravity (m/s^2)
h	heat transfer coefficient (W/m^2 K)
H	specific enthalpy (J/kg)
J_i	diffusion flux of species i (kg/m^2 s)
k	chemical reaction rate constant (mol^{1-n}/m^{3n-2} s^{-1})
k_0	pre-exponential factor of the rate constant
n	reactor order
Nu	Nusselt number
p	pressure (Pa)
P_s	solid pressure (mol/m^3)
Pr	Prandlt number
Q	heat transfer between phases (W/m^2)
r	reaction rate (mol/m^2 s)
R	constant of the ideal gases (J/mol K)
Re	Reynolds number
S	net rate of production of species i (kg/m^{3}s)
Sc	Schmidt number
T	temperature (K)
$\mathbf{u}$	velocity vector (m/s)
Y_i	mass fraction of species i

Greek letters

α	volume fraction
β	interphase momentum exchange coefficient (kg/m^3 s)
ε	dissipation rate of turbulent kinetic energy (m^{-2} s^{-3})
Θ_s	granular temperature
κ	turbulent kinetic energy (m^2/s^2)
λ	thermal conductivity (W/m^2 K)
μ	viscosity (kg/m s)
ξ_s	particle phase bulk viscosity (kg/m s)
ρ	density (kg/m^3)
$\boldsymbol{\tau}$	stress-strain tensor (Pa)

Subscripts

g	gas phase
gs	from particle phase to gas phase
i	specie index
s	particle phase
sg	from gas phase to particle phase
AR	air reactor
FR	fuel reactor
LStran	fluidization stream of loop seal
LSrev	reverting stream of loop seal
t	turbulent index

The accurate CFD prediction of CLC is first dependent of a reasonable gas–solid heterogeneous reaction kinetics model. Deng et al. [18,19], for the first time, developed the reaction kinetic models for calcium sulfate ($CaSO_4$, as an oxygen carrier) and hydrogen, and from CFD simulations, they concluded that a high reactor temperature enhances the conversion of hydrogen. Similar simulations were conducted by Jung and Gamwo [20] for the reaction between NiO and methane, Wang et al. [21] for the reaction between NiO and methane, and Wang et al. [22] for the reduction reaction between CuO/Al_2O_3 oxygen carrier and coal gas containing CO, H_2, H_2O and CO_2. Kruggel-Emden et al. [23] investigated the validity of the heterogeneous reaction kinetics models by conducting a CFD simulation in the FR; the results revealed that the empirical polynomial based models proposed by Kruggel-Emden et al. [24] provide an accurate representation to the reaction rate.

On the other hand, describing the heterogeneous particle cluster formed in the circulated fluidized bed reactors is another challenging task for CLC–CFD simulation. Wang et al. proposed a series of models, e.g., CSD drag coefficient model [25], multi-scale chemical reaction model [26] and multi-scale heat transfer model [27], to capture more accurately the local non-uniform characteristics in a dual circulating fluidized bed. The usual parameters of the pressure profile, solid volume fraction distribution and gas compositions at the outlet were investigated. The results indicated that these non-uniform based models can substantially improve the accuracy of simulation result. Recently, a three-dimensional interconnected fluidized bed CFD simulation was conducted by Guan et al. [28]. In this simulation, the effect of the drag models on the computational results was investigated, and the pressure profile and solid volume fraction distribution were studied in detail. The results indicated that the Gidaspow and Syamlal-O'Brien drag models both produced accurate predictions to the reactor. Using CFD simulations, Chen et al. [29] proposed a parameter to correlate the occurrence of bubbles and the dynamic properties; based on the CFD simulation and the proposed parameter, the velocity, volume fraction, formed bubble and the species distributions in the FR were investigated.

Generally speaking, the reliability of CFD simulation for multiphase CLC processes has been demonstrated. As an example, Mahalatkar et al. [30] simulated the FR experiments by Son and Kim [31], Mattisson et al. [32], Leion et al. [33] and Abad et al. [34]; the simulation results agreed well with the experiments. Based on these achievements, CFD simulation as an effective tool was widely utilized to investigate the thermo-chemical performances of CLC combustors and influencing factors involved in CLC. Harichandan and Shamim [35] conducted a FR CFD simulation using $CaSO_4$ as the oxygen carrier and H_2 as the fuel to investigate the effects of bed height, bed width, free board height and particle diameter on the fuel conversion rate; the results demonstrated a significant increase in the conversion rate with higher dense bed height, lower bed width, higher freeboard height and smaller oxygen carrier particle. Using the commercial CFD software Fluent, Kruggel-Emden et al. [36] simulated a CLC system that is comprised of an interconnected AR and FR. The spherical shrinking core model and the linear shrinking core model for the reaction kinetics were evaluated and compared; the effects of different kinetic models, oxygen carrier mass flows and reactor bed heights on the methane conversion and bed temperature were investigated. Recently, Wang et al. [37] conducted a multiphase CFD simulation for chemical looping reforming (CLR) in dual circulation fluidized beds; the effects of bed temperature, superficial gas velocity and H_2O/CH_4 ratio on the gas conversion efficiency were investigated.

Note that great achievements in the CLC of gaseous fuels have laid the foundation for the CFD simulation of CLC with solid fuels. Among the CFD simulations using solid fuels, Mahalatkar et al. [38,39], for the first time, utilized FLUENT to simulate the quartz tube reactor that was used in the coal CLC experiments of Leion et al. [40]. With different bed temperatures and different steam inlet concentrations, the CO_2 and CO concentrations in the outlet were found to agree well with the experimental measurements. Wang et al. [41] conducted a simulation of a continuous coal feeding CFB fuel reactor. The results of the outlet gas concentrations were in agreement with the experimental measurements;