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Modelling and simulation of chemical looping combustion process in a double loop circulating fluidized bed reactor

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HIGHLIGHTS

- First attempt of CFD study for CLC in a novel double looping fluidized bed.
- A reactive model has been developed and implemented in an in-house code.
- The two reactors coupled through the time-dependent boundary conditions.
- The predicted results show a good agreement with the measured data.
- The effects of operation conditions on reactive performance are investigated.

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ABSTRACT

A reactive CFD model has been developed and implemented numerically in an in-house code for a coupled double loop circulation fluidized bed reactor. In the current work it is utilized for the chemical looping combustion (CLC) process but the model can easily be modified for exploring some other chemical looping processes. The air reactor and the fuel reactor are operated in fast fluidization regime and simulated separately in a simultaneous mode. The connections between the two reactors are realized through time-dependent inlet-outlet boundary conditions. The model predictions are validated by comparison with experimental data reported in the literatures. Good agreement is observed between the experiments and simulations. Using this model, fluid dynamics and chemical process performance of the double loop reactor is investigated. The results show that the methane is rapidly consumed at a very short entrance section of the reactor and the axial distribution of the oxygen is more smooth. Higher reactant residence time and fuel reactor temperature increase the conversion of methane and oxygen. The methane conversion could reach 95% during the current study.

1. Introduction

The fact that greenhouse gas emission from the energy sector is linked to climate change has prompted research in a considerable number of technologies to address this issue. Chemical looping combustion (CLC) is one of the possible technologies which provides a novel route for inherent CO_2 capture with lower energy demand and cost penalty [1].

The typical configuration for CLC system consists of two interconnected fluidized bed reactors, comprising a fuel reactor (FR) operated as a bubbling bed and an air reactor (AR) operated in the fast fluidization regime. A metal oxide, known as oxygen carrier (OC), is used to supply the oxygen needed for fuel conversion and circulates between the two reactor units. The gaseous fuel is introduced to the FR and reacts with oxygen, provided by the OC, to give CO_2 and steam (1). In a subsequent step, this oxygen carrier is reoxidized to its initial state with air (2) in the AR. In this way, the mixing of fuel and air is avoided and CO_2 will inherently not be diluted with nitrogen which would otherwise require high energy cost. A large number of studies considering different areas of CLC have been summarized by several review papers [2–4].

$$(2n+m)Me_xO_y + C_nH_{2m} \rightarrow (2n+m)Me_xO_{y-1} + mH_2O + nCO_2 \quad (1)$$

$$MeO_{y-1} + \frac{1}{2}O_2 \rightarrow Me_xO_y \quad (2)$$

The development of Computational Fluid Dynamic (CFD) model for CLC process has been the focus of many researches since the

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Nomenclature

C_1, C_2, C_b, C_μ	turbulence model parameter, –
d_s	particle diameter, m
D_{ji}	binary diffusion coefficient, m^2/s
$D_{k,j}$	diffusion coefficient for component j in phase k, m^2/s
e	coefficient of restitution, –
E	activation energy, J/mol
$\vec{F}_D$	Drag force, $kg/m^2 s^2$
$\vec{g}$	gravity acceleration, m/s^2
g_0	radial distribution function, –
h	heat transfer coefficient, kW/(m^2 K)
H_i^R	reaction enthalpy for reaction i, kJ/mol
$\bar{\bar{I}}$	unit tensor, –
k	reaction rate coefficient, m/s
k_g	gas turbulent kinetic energy, m^2/s^2
$\vec{M}_k$	interfacial momentum transfer of phase k, $kg/m^2 s^2$
M	mole mass, kg/kmol
p_k	pressure of phase k, Pa
Pr	Prandtl number, –
Q	Heat transfer, J/m^3 s
R	gas constant, J/K mol
Re	Reynolds number, –
Re_p	particle Reynolds number, –
S_0	surface area of the reaction, 1/s
S_t	turbulent kinetic energy production, $kg/m^2 s^2$
t	time, s
T	temperature, K
$\vec{v}_k$	velocity of phase k, m/s
X	conversion, –
Y_j	mass fraction of j, –
z	axial coordinate, m
α_k	volume fraction of phase k, –
β	interfacial drag coefficient, –
γ_s	collisional energy dissipation, kg/m^3 s
ε_g	turbulent energy dissipation rate, m^2/s^3
κ_s	conductivity of granular temperature, kW/m K
λ_k	thermal conductivity of phase k, kW/m K
ν_j	stoichiometric coefficient, –
μ_k	viscosity of phase k, Pa · s
$\bar{\bar{\tau}}_k$	stress tensor of phase k, Pa
ω	mass fraction, –
Γ	interfacial mass transfer rate, kg/m^3 m
Θ	granular temperature, m^2/s^2
$\bar{\bar{\tau}}_t$	turbulent stress tensor, Pa
AR/FR	air reactor or fuel reactor, –
B	bulk, –
i	reaction number, –
k	gas(g) or solid(s) phase, –
mf	minimum fluidization, –
t	turbulent, –
w	wall, –
0	initial, –
$dilute$	dilute, –
e	effective, –
m	molecular, –
max	maximum, –

mathematical modelling and simulation of the reactor is essential for its design, optimization and upscaling. Most of CLC simulation studies available on the literature focused on modelling the typical configuration which composes of a high velocity riser as the AR and a low velocity bubbling fluidized bed as the FR [5–14], However several studies [5–8] found that the bubbles formed and the reacting gas bypassing in the bubbling bed could result low gas conversion. Up to date, only a few attempts [15–17] were made for other reactor design possibilities.

SINTEF Energy Research and the Norwegian University of Science and Technology have designed a double loop circulating fluidized bed (DLCFB) reactor for CLC process. In the DLCFB system, the air reactor as well as the fuel reactor are operated in the fast fluidization regime for a better gas-solid contact and flexible operation. In order to understand the physical phenomena, explore the chemical process performance of the CLC process in this novel DLCFB system, it is beneficial to develop a simulation tool which further can be used to optimize the operating conditions, on scale-up and design of industrial scale reactors.

This study makes a first attempt on CFD modelling and simulations for the CLC process in the novel DLCFB reactor as defined above. A reactive multiphase CFD model for an interconnected DLCFB reactor has been developed and implemented using an in–house Fortran code. Methane is used as the gaseous fuel and NiO is chosen as OC. The main objective of this paper is to validate the model and investigate the CLC performance in the DLCFB reactor system with different operating conditions.

2. Experimental setup

The concept for the CLC reactor system developed by SINTEF Energy Research and Norwegian University of Science and Technology is schematically represented in Fig. 1(a). The air reactor as well as the fuel reactor are operated as a circulating fluidized bed (CFB) and the system is therefore called a double loop circulating fluidized bed reactor system (DLCFB). The fast fluidization regime in the FR has the objective of raising the fuel conversion with a better utilization of the upper part of the rector. The continuous solid exchange between the reactor units was realized by means of two divided loop-seals. The loop-seals are fluidized through three bubble caps (central, external and internal) so that the solids entrained by one reactor can be lead into the other reactor or re-circulated back into the original one. There is also a bottom extraction/lift used to balancing the hold up of the two units.

Both reactors are of 6 m height while the diameter of the AR and FR is 0.23 m and 0.154 m respectively. The fluidizing gas is fed from bottom of the reactors. The solid outflow from one reactor will inject into the bottom of the other reactor through the cyclones and external loop-seals. Differential pressure transducers were placed along the reactor bodies to measure the local pressure distribution.

3. Computational model

3.1. Fluid dynamics model

A two-fluid reactive model based on the kinetic theory of granular flow (KTGF) implemented in an in-house code is used to describe the hydrodynamics and the reactions in the fluidized reactors. In the two-fluid model, each phase is described by a set of governing equations and closures. For the gas phase, the transport equations can be derived by adopting suitable averaging process for local instantaneous equations [18], while the transport equations for solid phase originate from the ensemble average of a single-particle quantity over the Boltzmann integral-differential equation [19]. Detailed descriptions of the model can be found in