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Performance of fuel reactor in a chemical looping combustion system with different oxygen carriers

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ABSTRACT

The key purpose of the present research work is to numerically simulate the bubble hydrodynamics in the fuel reactor of a chemical looping combustion (CLC) framework. This analysis gives an insightful understanding of the generation, growth, rise, development and burst of bubbles inside the fuel reactor. In the present research work, natural gas (CH_4) has been utilized as the fuel though NiO and CuO have been utilized as the oxygen carrier particles individually. A commercial computational fluid dynamics (CFD) code has been utilized as a part of which the kinetic theory of granular flow has been considered and the kinetics of an oxygen carrier has been linked into the reactive fluid dynamic system through a user defined function (UDF). The transient bubble dynamics, solid volume fraction and the conversion rate of natural gas fuel are differentiated for the fuel reactor with NiO and CuO as the oxygen carrier particles.

1. Introduction

In the last couple of decades, the apprehension about the global climatic changes and their effect on the society has been one of the major thrust areas of research among each scientific group. The discharge of greenhouse gasses like CO_2, NO_x and SO_x are the major contributor to worldwide climatic changes with CO_2 being the pioneer in the list. It has been discussed by many scientists that a major part of CO_2 discharges from the combustion of fossil fuels and, in today's age, more than 33% of aggregate CO_2 are discharged from fuel combustion [1]. Chemical looping combustion (CLC) framework has been understood to be the best option arrangement that can possibly enhance the thermal efficiency of the plant with characteristic advantages of CO_2 partition with least energy losses [2]. In the novel process of CLC, there is no direct blending of the fuel and combustion air. There are two reactors namely air reactor and fuel reactor in the framework with CLC approach in which metal oxide particles are utilized for specific oxygen transport from the air reactor to the fuel reactor and then unadulterated CO_2 is acquired in the fuel reactor exhausts stream after condensation of water with no further gas partition processes. The CLC process has the instinctive characteristic of 100% carbon capture rates, an exceedingly concentrated stream of CO_2 set for sequestration, no NOx releases [3], and no expenses or energy penalties for gas partitions. The fuel reactor of a CLC framework is considered as a fluidized bed reactor (FBR) in which the gaseous and solid particles are dispersed in extremely complex manner and computational fluid dynamics (CFD) demonstrating can be utilized for better understanding of the unsteady and quasi-steady processes.

Fig. 1 represents the schematic of a CLC system with interconnected air reactor and fluidized bed fuel reactor in which reduction and oxidation processes takes place respectively. Hossain and Lasa [1] presented a review report on CLC for inherent CO_2 capture in which they have addressed the advances in CLC system in terms of selection of suitable oxygen carrier, design of reactors, power generations and economic impact on society.

Deng et al. [4] studied the behavior of bubble hydrodynamics in the fuel reactor of a hydrogen fuelled CLC system under steady operating conditions. Harichandan and Shamim [5] also simulated the same hydrogen fuelled system but explicitly discussed the quasi-steady characteristics of bubble hydrodynamics. Mohammad and Shamim [6] have investigated the unsteady behavior of hydrogen production process using a CLC system. Porrazzo et al. [7] performed the CFD analysis of a CLC system on micro scale and macro scale in which they mainly described the physics influencing the performance of the fuel reactor with respect to fuel combustion rate, cost estimation and overall thermal efficiency of the power plant. Harichandan and Shamim [8] studied the hydrodynamics of fuel reactor in a CLC system and the effect of fuel-oxygen carrier combination.

However, there have been limited numbers of investigations on the unsteady behavior of bubble formation, rise, growth and burst in the

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Nomenclature

V_q	volume of phase q
α_q	phasic volume fraction
$\hat{\rho}_q$	physical density of phase q
ρ_q	physical density of phase q
ρ_{rq}	phase reference density or the volume average density of the q^{th} phase
$\bar{\bar{\tau}}_q$	q^{th} phase stress–strain tensor
μ_q	Shear viscosity of phase q
λ_q	bulk viscosity of phase q
F_q	external body force
$F_{lift,q}$	lift force
$F_{wl,q}$	wall lubrication
$F_{vm,q}$	virtual mass force
$F_{td,q}$	turbulent dispersion force
R_{pq}	interaction force between phases
P	Pressure
Θ_g	particle temperature
u_p'	fluctuating velocity
β_{pgas}	The interphase momentum transfer

fuel reactor of a CLC system using CH_4 as the gaseous fuels. Though a hydrogen-fueled CLC system has been claimed to have better thermal efficiency (around 12% more) than a conventional thermal power plant [9] but, hydrogen-fueled CLC system produces pure steam in the fuel reactor without capturing any CO_2 in the process. The primary objective of the present study is to analyze the transient behavior of bubble hydrodynamics in the fuel reactor of a CLC system by considering natural gas as the fuel with Cu- and Ni-based metal oxide as oxygen carriers. In addition, the second objective of the present study is to investigate the conversion rate of natural gas fuel with respective oxygen carrier particles in the form of NiO and CuO.

The CLC process described in the present study has two chemical reactions in the fuel reactor at 1050 K as follows:

$$CH_4 + 4CuO \rightarrow CO_2 + 2H_2O + 4Cu \quad \begin{matrix}\text{Reduction reaction}\\ \Delta G = -590\ \text{kJ/mol}\\ \Delta H = -217\ \text{kJ/mol}\end{matrix} \tag{1}$$

$$CH_4 + 4NiO \rightarrow CO_2 + 2H_2O + 4Ni \quad \begin{matrix}\text{Reduction reaction}\\ \Delta G = -259\ \text{kJ/mol}\\ \Delta H = 134\ \text{kJ/mol}\end{matrix} \tag{2}$$

In both the cases, the natural gas fuel is reduced to CO_2, H_2O and metal (Cu or Ni) in the fuel reactor (bubbling fluidized bed) and metal (Cu or Ni) is transported to the air reactor (circulating fluidized bed) that got oxidized back to metal oxide (CuO or NiO). The flue gas from the air reactor contains nitrogen and any unreacted oxygen. The present study considers the simulations of the bubbling fluidized bed reactor only and the first order reaction rate with respect to the partial pressure of natural gas has been referred from Hossain and Lasa [1].

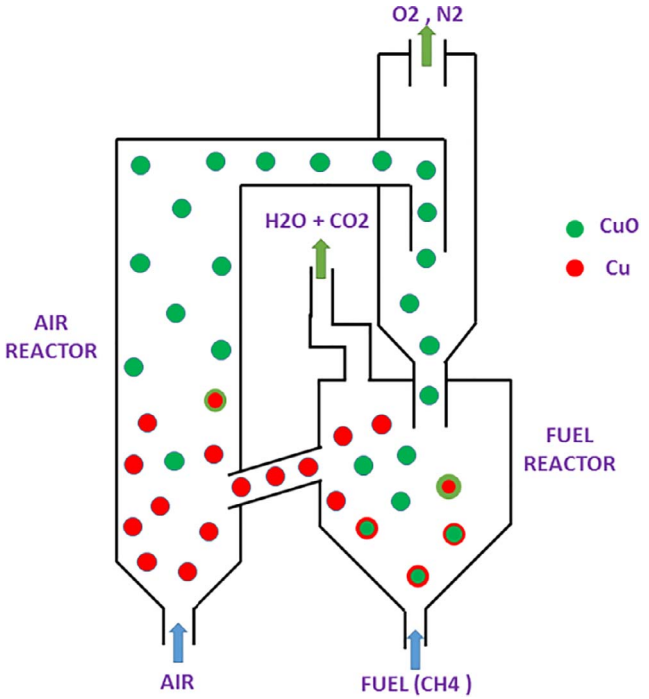

Fig. 1. Fluidized bed reactors in a CLC system.

2. Mathematical modeling

Eulerian approach has been considered in the present study for the analysis of two-stage flow having gas and solid flow regimes. Continuity, momentum and energy equations are resolved independently for the respective phases. The collision and fluctuation of the granular particles in the fluidized bed are investigated by considering the kinetic theory of granular flow. The computation of momentum exchange between phases has been customized by considering user-defined functions in ANSYS Fluent.

2.1. Hydrodynamic model

The governing equations considered for the unsteady two-phase flow are highlighted as follows:

2.1.1. Volume fraction equation

The volume of phase q, V_q, is defined as:

$$V_q = \int_V \alpha_q dV \tag{3}$$

where $\sum_{q=1}^{n} \alpha_q = 1$ and α_q is the phasic volume fraction.

The effective density of phase q is: $\hat{\rho}_q = \alpha_q \rho_q$, where ρ_q is the physical density of phase q.

2.1.2. Conservation equations

The conversion equations used for solving gas–solid flow regimes for the general case of an n-phase flow are listed as below:

2.1.2.1. Continuity equation. The volume fraction of each phase is calculated from a continuity equation:

$$\frac{1}{\rho_{rq}}\left(\frac{\partial}{\partial t}(\alpha_q \rho_q) + \nabla\cdot(\alpha_q \rho_q \hat{v}_q) = \sum_{p=1}^{n} (\dot{m}_{pq} - \dot{m}_{qp})\right) \tag{4}$$

where ρ_{rq} is the phase reference density, or the volume average density of the q^{th} phase in the solution domain.

2.1.2.2. Momentum equations. The conservation of momentum for phase (q) is given by:

$$\frac{\partial}{\partial t}(\alpha_q \rho_q \vec{v}_q) + \nabla\cdot(\alpha_q \rho_q \vec{v}_q \vec{v}_q) = -\alpha_q \nabla p + \nabla\cdot\bar{\bar{\tau}}_q + \alpha_q \rho_q g + \sum_{p=1}^{n} (\vec{R}_{pq} + \dot{m}_{pq}\vec{v}_{pq} - \dot{m}_{qp}\vec{v}_{qp}) + (\vec{F}_q + \vec{F}_{lift,q} + \vec{F}_{wl,q} + \vec{F}_{vm,q} + \vec{F}_{td,q}) \tag{5}$$

where $\bar{\bar{\tau}}_q$ is the q^{th} phase stress–strain tensor.