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CFD Analysis of Bubble Hydrodynamics in a Steam Reactor for Hydrogen Production Chemical Looping Reforming System

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Abstract: **-- Three reactor chemical looping reforming system is used for hydrogen production by capturing the harmful gases like CO2, NOx and SOx using a metal oxide as an oxygen carrier and steam. We investigate the bubble hydrodynamics and flow physics by the use of Ansys FLUENT which is based on finite volume approach. The numerical model of the steam reactor is also developed to understand chemical kinetics between gas-solid phases based on kinetic theory of granular flow. A Eulerian multiphase model has been used to describe the continuum principle of two-fluid models for both gas and solid phase. In the present work, steam and iron oxide is used as fuel and oxygen carrier respectively. The numerical results are validated with the experimental and numerical results available in open literature. The simulation is found to capture the bubble hydrodynamics in terms of bubble generation, rise, growth and rapture in the unsteady and steady-states in a better manner. Numerical simulations are carried out to capture the bubble hydrodynamics and the relationship between the molar fraction of products and gas phase and bubble formation. Solid volume fraction contour is used to understand the better flow physics and chemical kinetics.**

Keywords: CFD simulation, chemical looping reforming, CO2 capture, hydrogen production, steam reactor, Eulerian multiphase model.

I. INTRODUCTION

The major drawback of the conventional combustion system is emission of harmful gases like CO2, NOx and SOx, which are responsible for greenhouse effect and also leads to global warming. Many researchers have focused towards an alternative combustion system that is more effective than the conventional combustion system as well as energy efficient and generation of new fuel that has eco-friendly nature [3]. We can consider the hydrogen as a fuel of the future because it emits only water vapor after combustion and it has high energy yield than other fuels like natural gas, gasoline etc. Chemical looping reforming is an innovative approach, which captures the 100% carbon dioxide and produces hydrogen in very cost effective manner. Hydrogen production from natural gas, gasoline, electrolysis produces 8 to 9 tons of CO2 per one of hydrogen [7]. Fig. 1 shows the Air, fuel and steam reactors are the three essential parts of the three reactors chemical looping reforming system. A processed oxygen carrier is fed into the air reactor, where it reacts with the air from the atmosphere fed from the bottom of the reactor. Completely oxidized oxygen carrier is come out at the outlet of the air reactor. Then the oxygen carrier is fed in to the fuel reactor will react with the fuel. Carbon dioxide and the water vapor are the outlet products of the fuel reactor. 100% CO2 will be captured after condensing the water vapor. Now, reduced oxygen carrier from the fuel reactor will supply in to the steam reactor for the production of the hydrogen. In the steam reactor reduced oxygen carrier will convert in to the partially oxidized oxygen carrier by reacting with the water vapor fed from the bottom distributor plate of the steam reactor. CFD approach is now becoming more popular to model a fluidized bed reactor containing two different phases like gas and solid phase [1,2].Many researchers had investigated chemical looping reforming by numerically and experimentally but quite a few researchers had studied the unsteady flow physics and bubble hydrodynamics in the fluidized bed reactor[4-10]. The unsteady aspect of the chemical reaction kinetics and flow physics is important to find the conversion of the chemical reaction in the fluidized bed reactor. Aim of the present study is to understand the unsteady bubble formation at the beginning part of the chemical, which is more important to understand the later quasi-steady phase.
Iron oxide as oxygen carrier and steam as fuel for steam reactor was used to study the bubble hydrodynamics in the present numerical simulation of CLR process.

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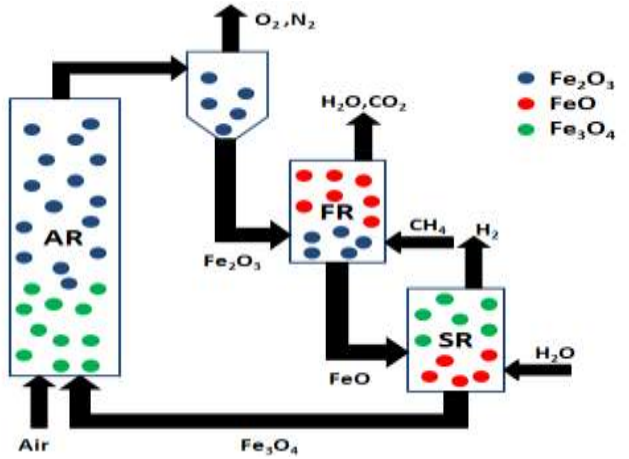

Figure.1. Schematic of three reactor chemical looping reforming process.

CLR system with three inter connected reactors in which Fe3O4 is oxidized into Fe2O3 in the air reactor(AR), Fe2O3 will reduced to FeO in the fuel reactor(FR) and FeO will oxidized to Fe3O4 in the steam reactor(SR). Eq. (1), (2) and (3) describes low temperature (750K-1150K) exothermic reaction in air reactor, high temperature (850K-1650K) endothermic reaction in the fuel reactor and low temperature (750K-1250K) exothermic reaction in steam reactor respectively.

$$8Fe_3O_4 + 2O_2 \rightarrow 12Fe_2O_3 \text{ (AR)} \quad (1)$$

$$12Fe_2O_3 + CH_4 \rightarrow 8FeO + CO_2 + 2H_2O \text{ (FR)} \quad (2)$$

$$8FeO + 8/3H_2O(g) \rightarrow 8/3Fe_3O_4 + 8/3H_2 \text{ (SR)} \quad (3)$$

II. NUMERICAL CONSIDERATIONS:

The conversion principles of mass, momentum, energy and species transport are very useful to understand highly complex fluid dynamics and chemical reaction between gas and solid phase in the chemical looping reforming. Fig. 2 shows the 2D geometry and quadrilateral cells of the steam reactor. The width and height of the reactor are 0.25 m and 1 m respectively. The grid independence test has been performed by the gelderbloom [11] considering same geometry clearly illustrates that numerical cell size greater than 10 times of the oxygen carrier particle size would capture real flow physics in the fluidized bed reactor. Based on that study, we divided our two dimensional steam reactor geometry in to the 2500 quadrilateral cell. The heat transfer coefficient between the gaseous phase and solidus phase used for the present simulation were reported by Gunn [12]. For solid particles the collision coefficient was 0.85.

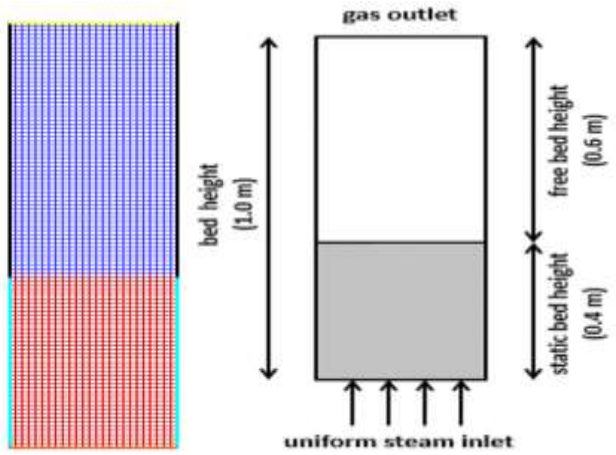

Figure. 2. Schematic and grid of the steam reactor.

Unsteady multiphase flow has been solved using finite volume approach based phase coupled technique in ansys FLUENT by taking 2nd order upwind scheme. The convergence criteria 10-5 has been taken for given unsteady chemical kinetics for scaled residuals component and time step of 10-3 s. Velocity inlet for the bottom of the steam reactor and pressure outlet for the outlet of the steam reactor. No slip condition was used for the side walls of the steam reactor for gas-solid phase. QUICK scheme has been used for the convective terms in the flow physics inside the steam reactor. The model parameters used for the base case in the present study are similar to those used by Deng et al. [1].

III. RESULTS AND DISCUSSIONS

To study the bubble hydrodynamics of chemical reaction in steam reactor here gas and solid phase were numerically simulated by multiphase CFD model. The C-language base user define code has been taken for proper chemical reaction between gas and solid phase. The chemical reaction between gas-solid phases was take place at 1050 K. The 100 wt. % H2O as fuel in the steam reactor is fed with uniform inlet velocity from the bottom distributor plate. The iron oxide as oxygen carrier with fluidization velocity is kept in static bed region. Chemical reaction between reduced oxygen carrier and oxygen present in the steam gives H2 as gaseous product. Due to variation in reactor temperature, uneven formation of active sites leads us to study the unsteady bubble hydrodynamics in the reactor. Fig. 3 shows results of numerical simulation in form of molar fraction of hydrogen and water vapor carried out considering similar model geometry and computational grid as deng et al [1] by taking hydrogen as fuel and calcium sulphate as oxygen carrier.

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Fig. 3 shows variation in molar fraction of gaseous phase along the center line of the reactor (x = 12.5 cm) and at a height of (y = 30 cm) from the inlet in dense bed region and at the outlet. We made two major changes in the deng et al model are pressure outlet boundary condition at outlet of the reactor against outflow condition and second order discretization scheme instead of first order scheme, which results in to a minor changes in the results. Fig. 3(a) shows sudden decrease in the molar fraction of gaseous reactant hydrogen from unity to oscillate around 0.6 in initial period of up to 1.0 s. Conflicting trend has been seen with molar fraction of gaseous product water vapor increasing from zero and oscillates around 0.32. After 1.0 s reaction reached to the quasi-steady state and molar fraction of H2 and H2O are 0.67 and 0.35 respectively. At the outlet quasi-steady state achieved after 4.0 s with 0.67 and 0.35 molar fraction of gaseous reactant H2 and product H2O respectively. Good agreement between the present results with deng et al [1] allowing us to further carry out the simulation by considering steam as fuel and iron oxide as oxygen carrier to study the bubble hydrodynamics.

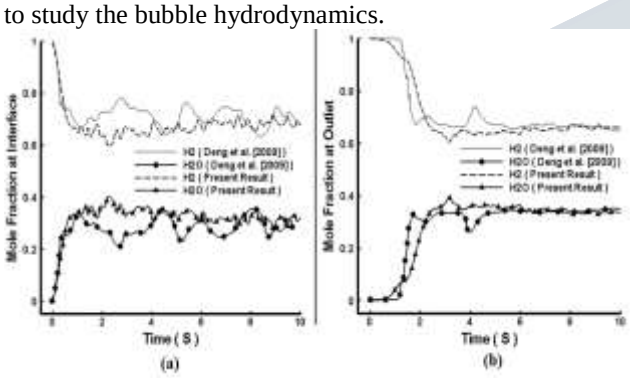

Figure. 3. Molar fraction in gas phase along the centerline of the reactor(x = 12.5 cm) and (a) at height of 30 cm of inlet and at (b) outlet

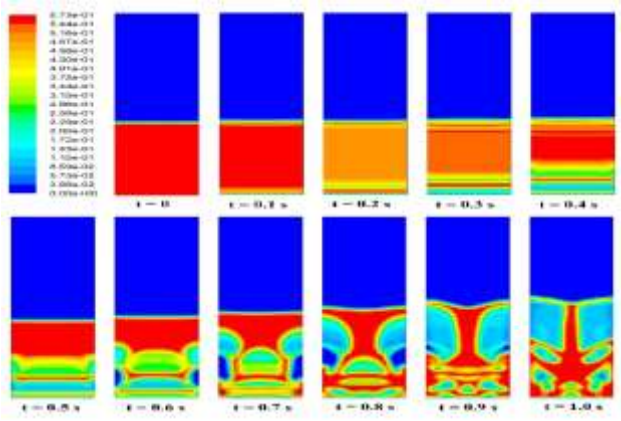

Figure. 4. Solid volume fraction contour from 0 to 1 s.

Fig. 4. Shows solid volume fraction contour of chemical reaction between steam and iron oxide from 0 s to 2 s for better understanding of unsteady bubble hydrodynamics inside the steam reactor. Steam was fed with uniform velocity from bottom distributor plate and iron oxide initially patched in static bed region by giving lower velocity than steam. The momentum transfers between steam to iron oxide and suitable reaction temperature allows igniting the reaction in steam reactor. Fig. 4 shows the bubble hydrodynamics in steam reactor is divided in to the generation, rise, growth and rapture phase. As the reaction stimulates, smaller bubbles are created near the distributor plate in the dense bed region for small period of the time. Larger bubbles creates low pressure zone behind them where small bubbles are trail behind them. These pressure gradient increase the speed of the smaller bubble towards the larger bubble and merge with larger bubble. Continue formation of the larger bubble creates two vertical columnar structure from the bottom distributer plate in the narrow flow passage inside steam reactor. Due to the gravity and density gradient of gas-solid particles; solid particles are pushed upwards by the rising slug and after short span of time solid particles are pushed downward along the center and the wall of the steam reactor. The cross section of the reactor was rectangular, similar that used by Clift and Grace [13]. Solid particles are moves upward by rising slug and moved back down along the wall of reactor forming core annulus structure is similar to that reported by Clift and Grace [13] using rectangular cross section reactor (similar to the present study).

Fig. 5 shows the development of solid volume fraction profile after 1.0 s. It elaborates better understanding of the unsteady and quasi-steady bubble dynamics and chemical kinetics in the steam reactor. The reaction rate is different inside the reactor due to the difference in gas velocities inside the bubble and slug and fluidization velocity of solid particles. The unsteady nature of the reaction is observed within the 1.5 s after that reaction progress towards the quasi-steady state. The global inter-mixing of gas and solid phase inside the reactor with the continuous bubble formation, rise, growth and burst is achieved by the continuous supply of the fed steam through bottom of the steam reactor. The unsteady bubble hydrodynamics inside the reactor is clearly noticeable up to 1.5 s. Gas and solid particles achieved quasi steady state after the core annulus structure was burst by global intimate mixing between both phases.

Fig. 5 shows the numerical simulation of the steam reactor in form of the solid volume fraction contour, which justifies the unsteady flow physics and chemical reaction of the three reactor chemical looping reforming process.

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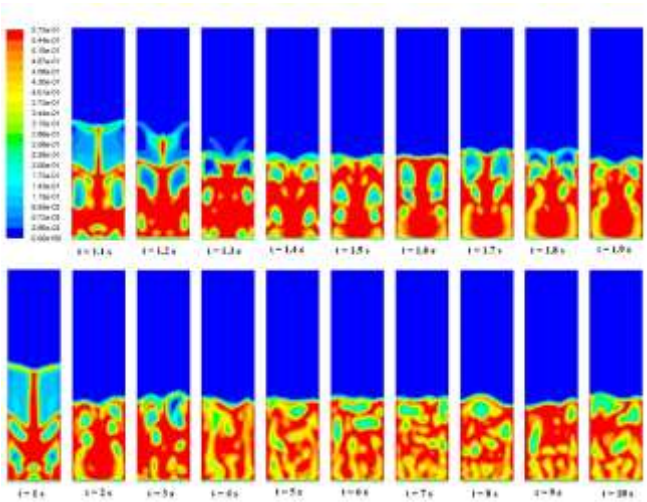

Figure. 5. Unsteady and quasi-steady development of solid volume fraction contour

IV. CONCLUSION

Steam reactor of three reactor chemical looping reforming system was numerically simulated using iron oxide as oxygen carrier and steam as fuel using Ansys FLUNT. This numerical model gives better understanding of temporal development of bubble hydrodynamics, unsteady state and quasi steady state inside the steam reactor. In the present simulation, It is noticeable that unsteady bubble hydrodynamics lies in 0-2 s. After that due gradient in density between gas and solid phase columnar bubble structure will collapse and chemical process inside the steam reactor achieves quasi-steady state.

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