Modeling of Fuel Reactor in a Chemical Looping combustion Process by using CFD

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1. INTRODUCTION & OBJECTIVE

Chemical looping combustion (CLC) process is a budding technology for improving the thermal efficiency of a system with potential of 100% carbon capture and absolutely no NO_x formation. In the present research work, the bubble hydrodynamics inside the fuel reactor of a CH_4–fueled CLC system has been numerically investigated. ANSYS Fluent has been used to carryout numerical simulation in which the reaction kinetics is incorporated into the reactive system of the fuel reactor by a user defined function (UDF). In the present case, CuO is used as oxygen carrier materials in combustion processes. The bubble hydrodynamics in terms of development, growth, rise and burst are visualized and analyzed the solid-gas molar fraction inside the fuel reactor. The present results are validated with numerical and experimental results available in the open literature. Different operating temperatures are considered to analyze the effect of temperatures on the fuel conversion rate.

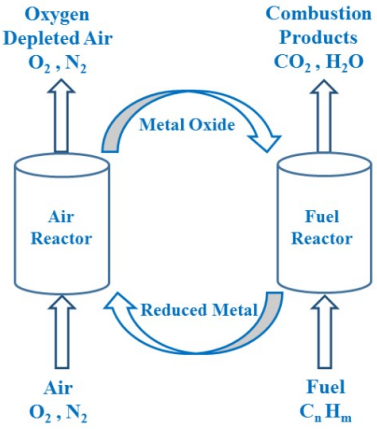

Figure 1. Schematic of a chemical looping combustion system.

Fig. 1 represents the schematic of a CLC system that has two inter-connected reactors: fuel reactor and air reactor carrying out reduction and oxidation of metal oxides respectively. The oxygen in the metal oxide gets reacted with the hydrocarbon fuel supplied to the fuel reactor. In the process, the metal oxide gets reduced and the reduced metal transferred to air reactor where it gets oxidized. In the air reactor, depleted oxygen and nitrogen are exited to atmosphere whereas in fuel reactor, carbon dioxide and water vapor at very high temperature are escaped to outside atmosphere. The water vapor can easily be condensed with CO_2 being captured up to 100 % and stored for future uses. In the process, no NO_x is formed leading to a clean combustion process fully addressing to the greenhouse gas concerns. The chemical reactions between fuel and oxygen carrier materials in the fuel reactor is highlighted as below:

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$$CH_4 + 4CuO \rightarrow CO_2 + 2H_2O + 4Cu \qquad \text{(with CuO as an oxygen carrier)} \qquad (1)$$

2. RESULTS & DISCUSSION

Bubble Development Phenomena in Fuel Reactor:

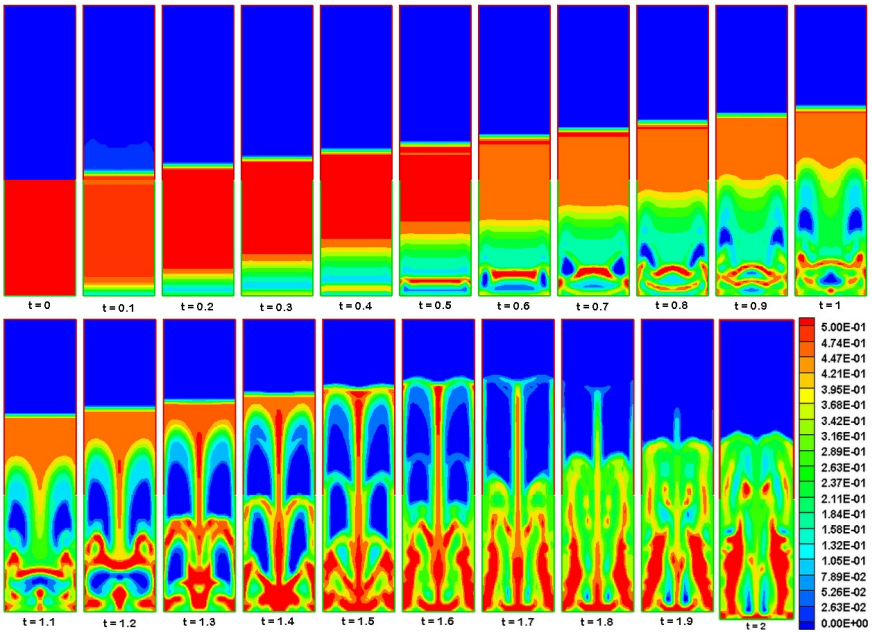

Figure 2. Unsteady development of bubbles in FR.

The continuous evolution of solid volume fraction profiles in fuel reactor for t = 0 to t = 2.0 s has been shown in figure 2. The results are qualitatively matched with the findings of Deng et al. [1] and Harichandan and Shamim. [2] However, the quantitative difference of the present results are due to the different set of fuel and metal oxide particles with higher order discretization scheme adopted in present simulations. Also, the boundary conditions at outlet considered for present simulation can be another reason for the quantitative difference as Deng et al. [1] have used outflow boundary condition for similar physical parameters. Fig. 2 gives an enhanced perceptive of the bubble dynamics and reacting state of affairs in fuel reactor in terms of formation, rise, growth, and development of bubbles in the unsteady and quasi-steady states between t = 0 - 2.0 s. At the onset of fuel supply, the reaction will start in the lower region of the reactor where metal oxide granules are concentrated and small gaseous bubbles will be originated from the distributor plate of the fuel reactor. These bubbles continue to grow with the advent of reaction by merging with adjacent bubbles. Actually, the relatively smaller bubbles which are germinated nearby the distributor attempt to rise up leading to the formation of two vertically offset columns of bubbles. The smaller bubbles trail behind the larger ones. The leading larger bubbles have low-pressure wake zones which pull the trailing smaller bubbles towards them and thus coalesce of leading larger bubbles and the accelerating smaller bubbles take place. Also, the rising larger bubbles moving at higher velocities coalesce with the adjacent smaller ones.

Thus, the narrow flow passage of the reactor observes a quick growth of bubble sizes that lead to the formation of slugs and the rising slugs push the solid particles in the dense bed region to

move upward. However, the heavier metal-oxide particles are driven down to the fuel reactor distributor end along the central core of the reactor due to density gradient of particles of different phases and gravity. This phenomenon is observed from 0.5 s to 1.5 s and at 1.5 s, a distinct core-annulus region has been formed. This physical phenomenon has also been ascertained by Clift and Grace [3] for almost similar kind of fuel reactor geometry and operating parameters.

Collumnar Structure Formation:

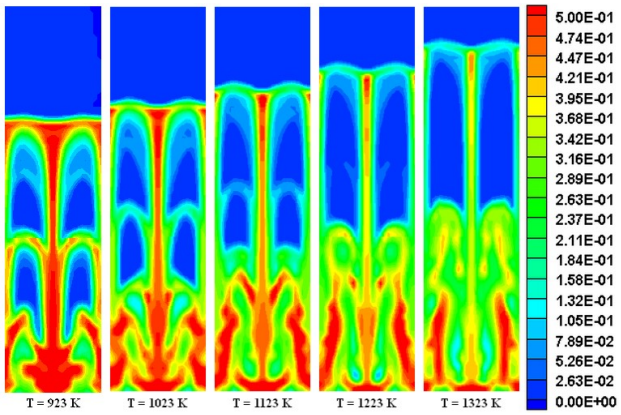

Figure 3. Columnar structure obtained at different temperature.

The columnar structure for different temperatures has been presented in Fig. 3. It is noticed that the columnar structure of gaseous and solidus mixture at the coral annulus of the reactant are obtained at a different instantaneous time corresponding to different temperature ranges. This columnar structure has been noticed to take less time for formation at a lower temperature than at higher temperature. It may be due to the fact that the reaction rate at lower temperatures is considerably less than its counter-part at high temperatures. In the present simulations, the columnar structures are obtained at t = 1.4 s, t = 1.5 s, t = 1.6 s, t = 1.7 s and t = 1.8 s for temperatures T = 923 K, T = 1023 K, T = 1123 K, T = 1223 K and T = 1323 K respectively as shown in Fig. 3.

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