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CFD-PBE simulation of gas-phase hydrodynamics in a gas-liquid-solid combined loop reactor

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Abstract: The computational fluid dynamics (CFD)–population balance equations (PBE) coupled model is employed to investigate the hydrodynamics in a gas-slurry internal loop reactor with external slurry circulation. The predicted radial profiles of local gas holdup and bubble diameter are in good agreement with the corresponding experimental data. The spatio-temporal velocity profile of the gas phase reveals that the upward movement of gas is slowed down and the residence time of gas is prolonged by the downward momentum of the slurry. Introduction of the external slurry can greatly improve the uniformity of gas holdup distribution in the reactor, especially in the downcomer-tube action region. Moreover, the interaction between the downward slurry and upward gas can lead to small bubble size and high interfacial area as well as good mass and heat transfer. The above results suggest the function of external slurry circulation for the internal loop reactor and would be helpful for optimizing the design and scale up of reactors.

Key words: CFD-PBE simulation, external slurry circulation, gas-liquid-solid, hydrodynamics, population balance model

1 Introduction

As a modified three-phase fluidized-bed reactor, the loop reactor has been widely used in chemical processing and other related tasks due to its simple construction without moving parts, good mass and heat transfer behavior, efficient mixing with low energy consumption, straightforward operation with low cost and so on (Lo and Hwang, 2003; Vial et al, 2005; Giovannettone et al, 2009; Deng et al, 2010). The loop reactor is usually divided into external and internal loop reactors (Kilonzo and Margaritis, 2004; Wang et al, 2007). As shown in Fig.1a, the internal loop reactor is usually constructed by mounting a draft tube inside the fluidized bed. Liquid (or slurry) is brought up by gas sparged into the draft tube or the annulus region and falls down due to gravity, which results in overall liquid (or slurry) circulation in the reactor. The external loop reactor has an external downcomer attached to the fluidized bed. Gas is dispersed at the bottom of the riser and a global liquid (or slurry) circulation is induced due to the pressure difference between the riser and downcomer (Fig.1b).

Although liquid (or slurry) circulation in the both loop reactors can enhance mixing and improve heat and mass transfer between gas and liquid (or slurry) phases, the driving force arising from the pressure difference in an external loop reactor cannot be flexibly adjusted, and mass or heat transfer between gas and liquid (or slurry) in an internal loop reactor is slightly improved limitedly as gas flows co-currently with slurry. Therefore, several modified configurations of loop reactors were proposed to meet the requirement for slow chemical reactions, such as Fischer-Tropsch and methanol syntheses (Zhang and Zhao, 2006; Lu et al, 2009; Zhang et al, 2003, 2010b; Liu et al, 2008). Among these reactors, the combined gas-liquid (or -slurry) loop reactor proposed by Lu et al (2009) makes use of the advantages of the external and internal loop reactor. It includes a liquid (or slurry) spray section in the upper part, a sieve plates section in the middle part, and an internal loop section in the lower part. External liquid (or slurry) circulation is introduced by a downcomer tube (Fig.1c), which can enhance the driving force because of the pressure difference between the riser and the annular region and increase the interfacial area between the gas and liquid (or slurry) phases.

In this combined gas-liquid-solid three-phase loop reactor, gas-phase properties, such as gas holdup, bubble movement characteristics and bubble size distribution strongly affect heat and mass transfer and chemical reactions. Although gas-phase properties have been investigated experimentally in the traditional internal loop reactors or bubble columns by many researchers (Jin et al, 2005, 2007; Zhang et al, 2008), little research has been carried out on combined loop reactors. In order to efficiently design and scale up this kind of reactor for liquid fuel synthesis using fine catalyst particles, a thorough understanding is needed of the hydrodynamics resulting in

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