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Simulation of hydrodynamic and mass transfer performances in monolith channel

Zhigang Lei*, Yanyan Guo, Chengna Dai, Linghua Zi, Biaohua Chen

State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Box 266, Beijing 100029, China

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ABSTRACT

In this work, the gas-liquid two-phase flow patterns and characteristics in Taylor flow regime in monolith channel were simulated by means of volume of fluid (VOF) method taking benzene and propylene as model system. Four types of flow patterns (i.e., bubbly flow, Taylor flow, Taylor-annular flow, and annular flow) were first identified in the range of gas velocity from 0.01 to 3.0 m s^{-1} and liquid velocity from 0.01 to 0.05 m s^{-1}. Then, the effect of contact angle and superficial velocity on hydrodynamic performance was investigated, confirming that the angle 0° is more appropriate. The hydrodynamic performance was intensified in the region of thin liquid film between gas bubble and the wall as well as the interface between gas bubble caps and liquid slug. Finally, the mass transfer performance of two-phase flow in monolith channel was investigated using one Taylor unit cell model. It was found that the mass transfer coefficients for monolith catalyst in Taylor flow regime is at least one order of magnitude higher than those for both structured catalytic packings and traditional pellet catalyst, exhibiting the advantage of monolith catalyst for process intensification.

1. Introduction

Gas-liquid-solid three-phase catalytic reactions are widely used in petrochemical, fine chemical, biological and environmental engineering, and other fields. The reactors mainly consist of stirred tank slurry bed reactor, bubble reactor, fixed-bed reactor, etc., in which pellet catalyst is widely used [1,2]. In recent years, monolith structured multiphase reactor, as a new type of "process intensification" reactor, has a broad application prospect in the multiphase catalytic processes such as hydrogenation reaction and other industrial processes, due to their unique advantages such as large surface area, small pressure drop, high percent conversion, enhanced multiphase flow mass transfer, low axial mixing, and ease to scaling-up compared to traditional pellet catalysts [3–5]. Moreover, monolith catalysts can avoid the filtering problem of slurry catalyst in reactor. Therefore, many researchers are paying more attention to studying monolith catalysts for process intensification. For example, Vergunst et al. [3] studied the catalytic performance of monolith catalyst in phenyl acetylene hydrogenation reaction, and found that phenyl acetylene conversion is not obviously influenced by catalyst loading. Metkar et al. [6] studied the performances of Fe- and Cu- monolith catalysts in nitrogen selective catalytic reaction. It was found that at low temperatures (≤350 °C) Cu-monolith catalysts exhibit higher catalytic activity, but at high temperatures (≥ 400 °C) Fe-monolith catalysts show better catalytic activity.

On the other hand, as an important chemical intermediate product, more cumene is demanded year by year. In industrial production, cumene is mainly obtained by benzene and propylene under alkylation reaction. Kaeding and Holland [7] studied the synthesis of cumene over HZSM-5 molecular sieve catalyst for the alkylation of benzene with propylene. Their experimental results showed that the selectivity of cumene ranges from 88 to 94%, and the main by-product di-isopropylbenzene is about 4–6%. Sasidharan et al. [8] investigated the catalytic performance of NCL-1 zeolite on the alkylation of benzene with isopropanol to produce cumene. Their experimental results showed that NCL-1 catalyst has a high activity and selectivity, and cumene selectivity is about 65–90%. However, one of the main problem using pellet catalysts for the alkylation of benzene with propylene is high pressure drop. Besides, when the zeolite pellet catalysts are deactivated, only the external surface is deactivated but the interior is still effective, indicating that utilization efficiency of pellet catalysts is low. Moreover, in our previous work [9], it was confirmed that monolith catalyst exhibits the lower pressure drop, higher cumene selectivity and higher effectiveness factor; and regular triangle or rectangle channel is

* Corresponding author.
E-mail address: leizhg@mail.buct.edu.cn (Z. Lei).

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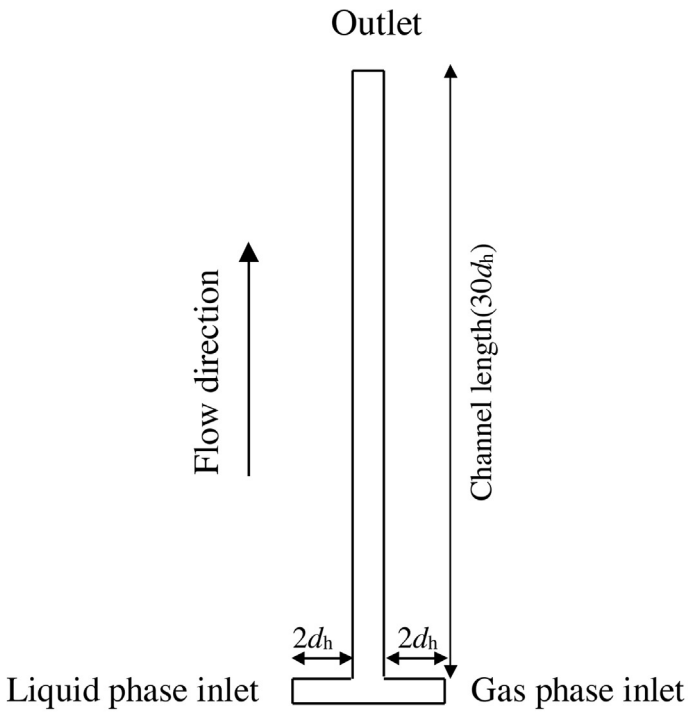
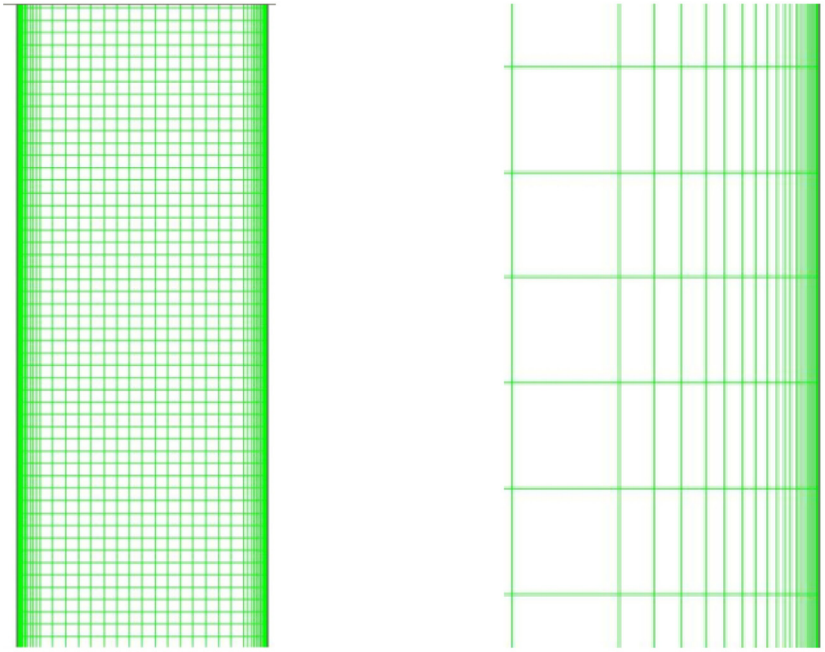


(a)



(b) (c)

Fig. 1. Schematic overview of computational domain (a), grid detail (b), and close-up view of grid near the wall (c).

optimum when considering pressure drop and cumene selectivity together. Therefore, monolith catalyst is proposed in this work as the replacement of pellet catalyst for the alkylation of benzene with propylene.

However, no systematic and critical research on gas-liquid-solid three-phase hydrodynamics and mass transfer for the alkylation of benzene with propylene in monolith catalyst has been done by far. This reaction system is concerned because the main reaction is fast

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