STRUCTURED BEDS

I-14. Effect of Flow Maldistribution on Monolith Reactor Performance: A Modeling Approach

A. Motivation

In recent times, catalytic monolith reactors (MR) have been suggested as a possible alternative to conventional solid catalyzed gas-liquid reactors (Roy et al., 2004; Boger et al., 2004; Cybulski et al., 1998). Monolith reactors are claimed to have superior hydrodynamic and mass transfer characteristics compared to existing conventional multiphase reactors, such as trickle bed reactors (TBR) and slurry reactors.

A number of modeling work has been performed in the literature to predict the performance of monolith reactors (Edvinsson et al., 1994; Nijhuis et al., 2003). It was observed that monolith reactor outperforms the conventional reactors for most of the cases studied. Multiphase reactors are widely used in chemical process industries and a small improvement in productivity could translate into significant savings in operating cost. However, one important aspect which has got minimum attention in the modeling work is the lack of consideration for the distribution of gas and liquid phases at the entrance of the monolith reactor. Studies have shown that monolith reactors do suffer from gas and liquid phase non-uniform distribution (Heibal et al., 2001, Roy et al., 2003). Depending on the type of liquid distributors and gas and liquid superficial velocities used, the degree of phase non-uniformity varies (Roy et al., 2003). Non-uniformity of phases reduces the catalyst utilization and results in reduced productivity. In all modeling work done till now, uniform distribution has been assumed where every channel behaves similarly (single channel model). This is contrary to the real situation.

B. Research Objectives

In this work, the *single channel model* has been modified (or extended) and a *monolith scale model* has been proposed. In this model, the gas and liquid superficial velocities are calculated in each channel using liquid saturation data obtained from computed tomography studies. Subsequently the single channel model is employed in each channel. The overall reactor outlet concentration is then calculated using the mixing cup concentration of all the channel outlet concentrations. Hydrogenation of α-methyl styrene (AMS) is used as the test reaction to evaluate the model and to study the effect of flow maldistribution on monolith reactor performance.

C. Selected Results and Discussions

To demonstrate the impact of non-uniform distribution in a monolith bed on its performance, the developed modeling approach is implemented to simulate the performance of a monolith incorporated inside a loop having a recirculation tank. The monolith cross section is blocked by 25% and 50%, respectively, and only the remaining part is accessible to the gas and liquid flow uniformly. Figure 1 shows the conversion of AMS in the recirculation tank with time for three different cases. When all the channels are available uniformly for reaction (100% distribution), the conversion is the maximum. As the blockage increases, the conversion decreases.

Simulation was also done using the actual liquid saturation profile data as obtained using Computed Tomography. The liquid saturation profile data gives the liquid saturation in each monolith channels. Empirical correlations were proposed to calculate the gas and liquid superficial velocities in the channels from the corresponding liquid saturation values. Figure 2 shows the reactor conversion for a liquid velocity of 2.5 cm/s. CT scan shows a uniformity factor of about 60% (Roy et al, 2004 for the definition of uniformity factor) at this liquid velocity which indicates poor distribution. The simulation result clearly shows that the maldistribution could reduce the reactor outlet conversion up to ~30%.

D. Future Work

Sensitivity of this developed model will be investigate with respect to various operating parameters.

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E. Reference

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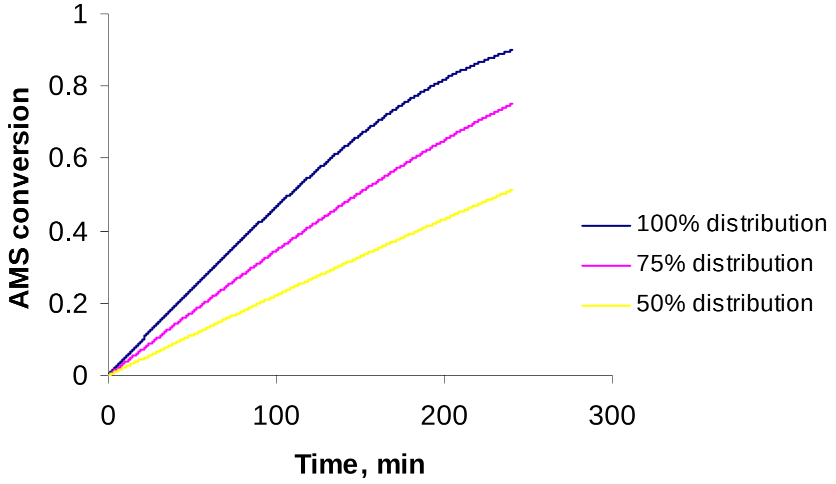

Figure 1: AMS conversion in the recirculation tank with time. P: 15 bar, V_L: 0.1 cm/s, V_G: 0.32 cm/s, recirculation tank capacity: 15 liters.

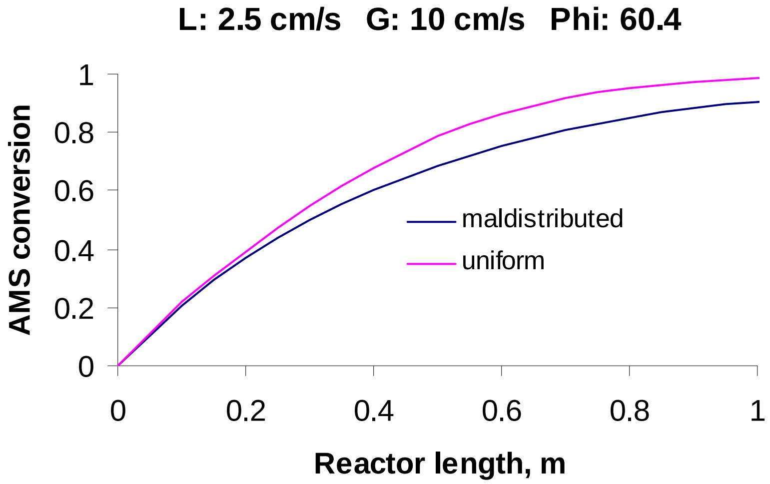

Figure 2: AMS conversion with reactor length. Pressure: 15 bar.