(436a) Influence of Bubble Growth at the Catalytic Surface on Heat and Mass Transfer in Gas-Liquid-Solid Microreactors

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Renée M. Ripken, Jeffery A. Wood, Johannes G.E. Gardeniers and Séverine Le Gac

University of Twente, The Netherlands

Here, we studied the influence of gas bubble growth at the catalytic surface on the heat and mass transfer in a microreactor using a numerical simulation framework built in COMSOL Multiphysics 5.2. Although the gas bubbles are detrimental for the heat transfer, mass transfer is increased as a result of the surface heterogeneity.

Industrial catalytic systems are rarely monophasic, and the majority of the processes are heterogeneous; the catalyst is solid while the reactants and products are in the gas and/or liquid phase. During some catalytic reactions, such as the reforming of alcohols and sugars, the reactants are dissolved in the liquid and typical products such as H_2, CO and CO_2 are formed as gases. When the gaseous products nucleate and grow into bubbles on the catalytic surface, a multiphase system is formed where the interplay of different transport phenomena is relatively complex. To obtain insight in this matter, we have developed a theoretical model to study the heat and mass transfer at the microscale in such a multiphase system.

A 2D microreactor with a channel of 250 Î¼m deep etched into a silicon substrate, covered with a glass top-layer was considered as the model system. A 10 Î¼m thick TiO_2-layer is coated at the bottom of this channel that acts as the catalyst support layer. The system is heated from the silicon side and dissipates heat to air through the glass top-layer, while the rest of the system is thermally insulated. A no-slip boundary condition is assumed on the channel wall and catalytic surface, with the bubble treated as a perfect slip wall. We focus on the external mass transfer limitations, while, including reaction kinetics.

We evaluated the bubble deformation caused by shear force as a function of fluid flow and bubble size. Typically, growing bubbles that are smaller than the channel diameter deform because of the fluid flow, but also relax to their initial state due to the surface tension. This oscillatory behavior is much faster than the reaction kinetics; therefore, bubbles can be approximated as being static. When the bubble size reaches the channel diameter, it detaches from the catalytic surface.

By adjusting the size of the bubbles and the distance between them, higher fluid velocity near the catalytic surface can be achieved. Similarly, mass transfer of the reactants to and products from the catalytic layer is enhanced. However, the heat transfer is negatively affected; gas bubbles act as an insulating layer, increasing the thermal entrance length compared to a system without bubbles. For highly endothermic reactions, a longer residence time is required to reach similar conversion as for a system without bubbles on the surface.

In the future, these simulation results can be potentially useful towards enhancing microreactor performance by giving insight into the role of geometry and operating parameters on relevant transport phenomena and how these affect conversion, yield and selectivity for gas-liquid-solid microsystems in which bubbles are growing at the catalytic surface.

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