Multi-Scale Modelling of Catalytic Microreactors

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Introduction

Microreactors are important alternative to conventional reactors in chemistry, chemical, pharmaceutical and semiconductor industries due to their operation characteristics such as increased mass and heat transfer, uniform flow, safety, high throughput through array configurations, smaller plant size and lower cost of production (Ehrfeld et al., 2000; Hessel et. al., 2004).
Catalytic continuous microreactors can be designed as packed-bed configuration or alternatively as a catalytic wall concept. Models for such reactors need to be able to describe both the gas-phase and the surface phenomena at different length- and time-scales. Surface reactions are traditionally modelled by a mean field (MF) model, which cannot always accurately capture complex surface dynamics. This might results in lack of understanding of the interactions underpinning the system and consequently leads to an inaccurate microreactor design.
The aim of this work is thus to develop a multi-scale framework of continuous microreactors with platinum (Pt) catalytic walls, which uses a macroscopic computational fluid dynamics (CFD) approach for the bulk phase, coupled with a microscopic kinetic Monte Carlo (kMC) method to describe the surface dynamics. The well-known system of CO oxidation (Raimondeau and Vlachos, 2002) and NO reduction (Fink et al., 1994) is used as a test case and comparison with conventional MF predictions are used to validate the multi-scale microreactor model.

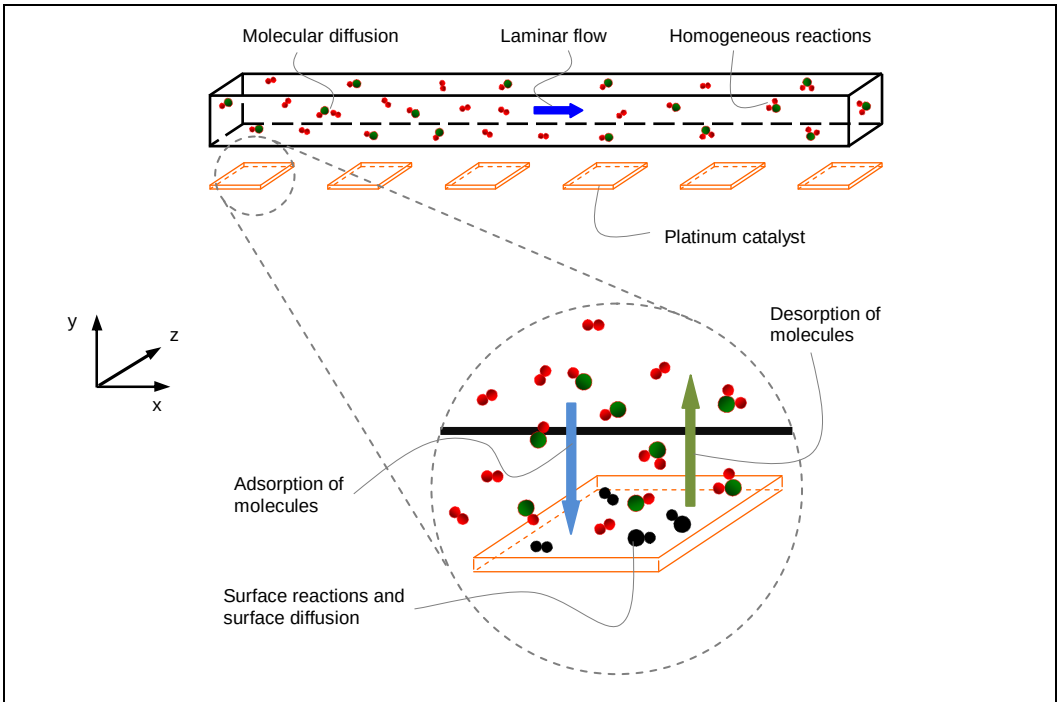

Figure 1: A multi-scale microreactor model.

Use of COMSOL Multiphysics

The multi-scale microreactor model consists of a coupled macroscopic gas-phase micro channel and a number of microscopic surface lattices representing a catalytic surface. The gas-phase is based on a convection-diffusion equation, modelled by using COMSOL Multiphysics and COMSOL MATLAB features, while the catalytic surface reactions use a kinetic Monte Carlo (kMC) approach, including effects of adsorption, desorption, surface reactions and surface diffusion. A number of kMC lattices depending on the discretisation of the computational domain are used to effectively represent the reactive surface.
The correctness of the multi-scale microreactor model will be validated with continuum MF model, simulated by the COMSOL Multiphysics software package.

Conclusion

The proposed multi-scale microreactor framework can provide accurate predictions of the complex system behaviour and has a potential for better understanding the surface reaction mechanism. Moreover, the results could significantly contribute to the improvement of the microreactor and surface catalyst design.

Reference

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