Modelling of Heat and Mass Transfer in Microreactor for MTG Reactions

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Abstract

The great oil crises in the 70s justified the financing of synfuels in the subsequent decade, as an alternative to oil. Methanol to Gasoline (MTG) played an important role inside this scenario. In MTG, Methanol flows through the acid sites of a shape selective catalyst, usually ZSM-5, to be converted into higher hydrocarbons, producing a high quality Gasoline with no sulphur content and high octane number. Today, the great availability of natural gas, since the shale revolution, brings back the interest in low hydrocarbon transformation into higher value-added products. The main goal of this work was to evaluate the mass and heat transfer of an MTG process in a packed bed microreactor using COMSOL Multiphysics®.

In the model, Methanol and inert gas are injected in a tube. Methanol reacts at the porous domain and Gasoline leaves by the outlet. Three physics interfaces were used: Transport of Diluted Species, Heat Transfer in Porous Media and Free and Porous Media Flow. The kinetic model used was proposed by Benito et al. (1996). The microreactor has a microchannel section, where a series of tubes are disposed. Just one tube was represented by a 2D axial symmetric geometry (Figure 1). All parameters were settled on all physics in agreement with the kinetic model. Nitrogen, Alumina and High-strength alloy steel materials were used to approximate the behaviour of the flowing gas, catalyst and steel shell, respectively. A mapped mesh, very fine at the wall, with 167,000 domain elements were used. Finally, the study selected was time-dependent.

The product profile along the reactor (Figure 2) suggests that maximum conversion is around 30%. For initial concentration of 1 µmol/m³, Methanol is rapidly consumed, which generates a peak of Light Olefins at 10% of reactor length. After that, Light Olefins are gradually consumed, forming Gasoline until the process reaches the maximum conversion at 100% of the reaction length. The temperature profile (Figure 3) can be considered homogeneous in the microreactor, with the maximum variation of only 0.015 K. Heat is dispersed before reaching the wall, hence there is no perturbation in the tubes next to it. The deactivation (Figure 4) is more effective at the very beginning of the reactor. After 10 hours of reaction, major part of the reactor presented catalyst activity over 0.9, while before 1 mm it fell to less than 0.6.

The model successfully provided the appropriate initial concentration required to achieve the maximum conversion to Gasoline. In addition, it proved that the process is suitable to changing the final product to Light Olefins, by varying the reactor length or rising the initial concentration to 30 µmol/m³. This flexibility provides a better adaptation to the market demands, which increases the economic attractiveness of the process. The temperature profile clarifies the unnecessity of a heat transfer jacket for the microreactor. For a laboratory scale, the activity fall is not a problem. However, to an industrial scale, further studies need to be carried out and this model can be used as a framework for scale-up processes.

Reference

Benito, P. L. et al., 1996. Concentration-Dependent Kinetic Model for Catalyst Deactivation in the MTG Process. Industrial and Engineering Chemistry Research, 35(1), pp. 81-89.

Figures used in the abstract

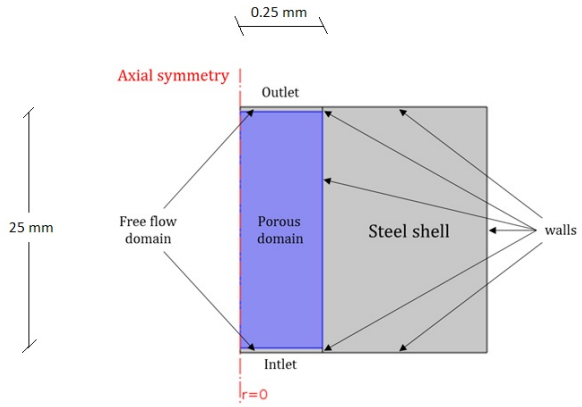

Figure 1: Tubular reactor geometry and boundary conditions.

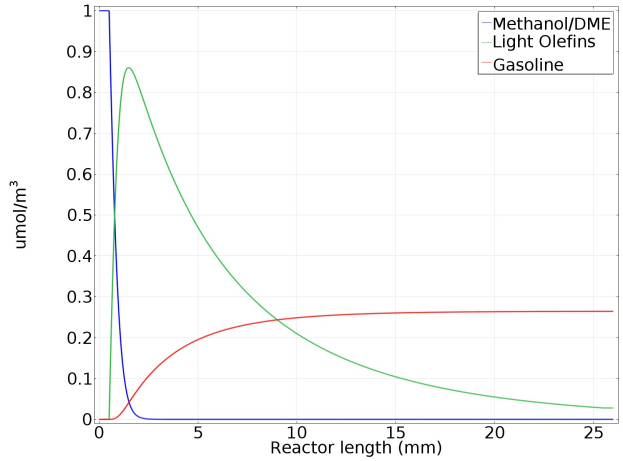

Figure 2: Product distribution along the microreactor for 10h of reaction.

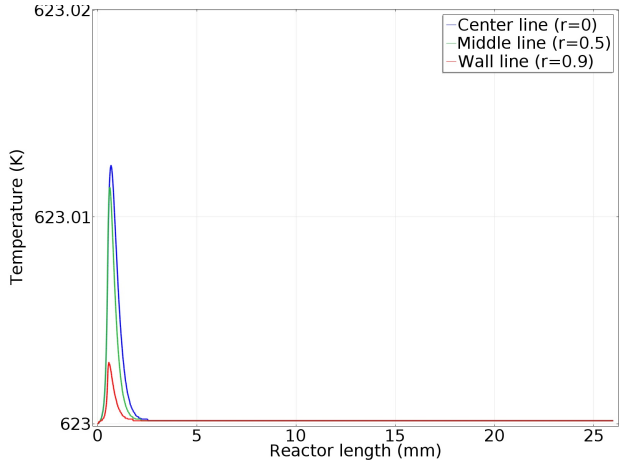

Figure 3: Temperature distribution along the microreactor for 10h of reaction.

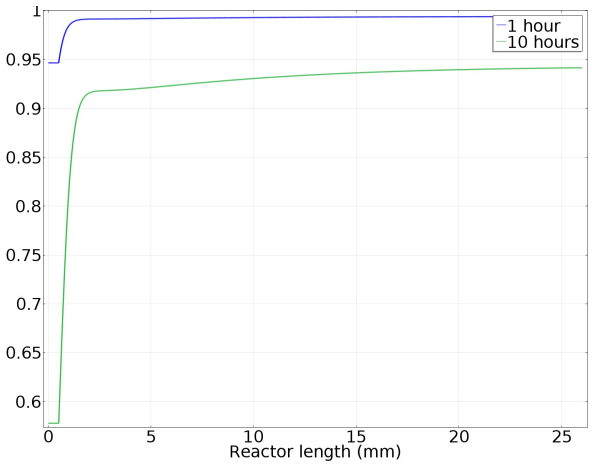

Figure 4: Deactivation along the microreactor.