Modelling Heat and Mass Transfer in Microreactor for Methanol to Hydrocarbons

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Introduction

Methanol-to-Hydrocarbons (MTH) is a process to convert Methanol into higher hydrocarbons. Synthesis of methanol from methane is a developed technology. Therefore, MTH is an important alternative route to produce liquid transportation fuels from natural gas rather than crude oil. Product composition depends on the catalyst used and process conditions; either light olefins (MTO) or gasoline range hydrocarbons could be produced (MTG).

Typically, SAPO-34 is used in the MTO and ZSM-5 is used in the MTG process.

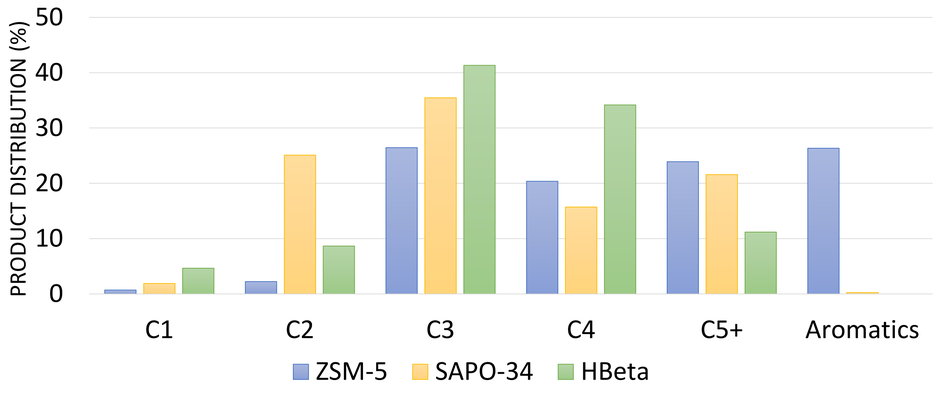

Figure 1. Product distribution by catalyst

Today, increasing availability of natural gas, i.e. shale gas, biogas, brings back the interest in methane transformation into higher value-added products.

The reaction kinetics and deactivation [1].

$$r_1 = k_1 * X_A * a$$
$$r_2 = k_2 * X_C^2 * a$$
$$r_3 = k_3 * X_A * X_D * a$$
$$r_4 = k_4 * X_C * X_D * a$$

$$-\frac{da}{dt} = (k_{dA} * X_A + k_{dC} * X_C + k_{dD} * X_D) * a$$

Where,

$$X_i = \frac{C_i * M_{Wi}}{\sum C_{i0} * M_{Wi}}$$

C_i - Concentration of *i*
C_{i0} - Initial concentration of *i*
M_{wi} - Molecular weight of *i*

And A, C and D are hypothetical compounds with a mean molecular weight of hydrocarbons.

Where,

A: $CH_4O + C_2H_6O$
C: $C_2H_4 + C_3H_6$
D: $C_4H_8 + C_5H_{10} + C_6H_{12}$

k_1	0.733 x 10^{13} exp(-33358/RT)
k_2	0.127 x 10^{8} exp(-17633/RT)
k_3	0.204 x 10^{12} exp(-27987/RT)
k_4	0.634 x 10^{6} exp(-15855/RT)
k_{dA}	0.461 x 10^{9} exp(-26700/RT)
k_{dC}	0.139 x 10^{10} exp(-31600/RT)
k_{dG}	0.129 x 10^{13} exp(-38100/RT)

Table 1. Kinetic constants [1]

Objective: evaluate mass and heat transfer of MTH reaction over ZSM-5 catalyst in a packed bed microreactor using COMSOL Multiphysics®.

Computational Methods

The physics used in the model were **Transport of Diluted Species**, **Heat Transfer in Porous Media** and **Free and Porous Media Flow**, in order to reproduce the mass, heat and momentum balances, respectively.

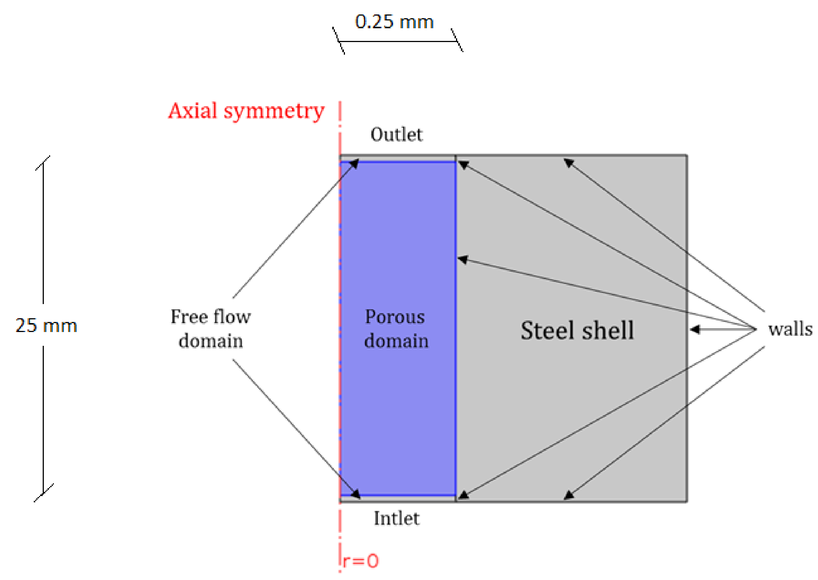

Figure 2. Tubular reactor geometry and boundary conditions.

Materials used as approximations:

- Nitrogen: inlet gas;
- Alumina: catalyst;
- High-strength alloy steel: steel shell.

The mesh had 167,000 domain elements. Quadrilateral elements and sophistication near the wall were applied.

Results

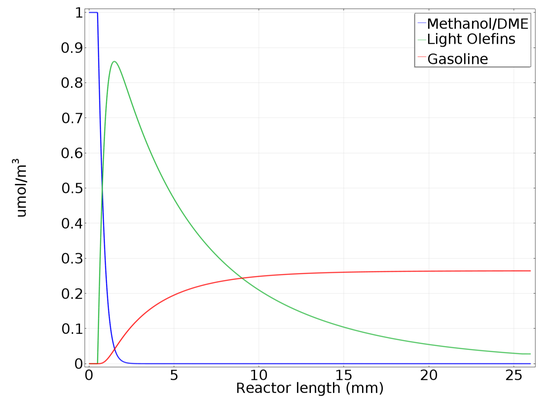

Figure 3. Product distribution along the microreactor for 10h of reaction and 1 µmol/m³ of Methanol in a 30% solution.

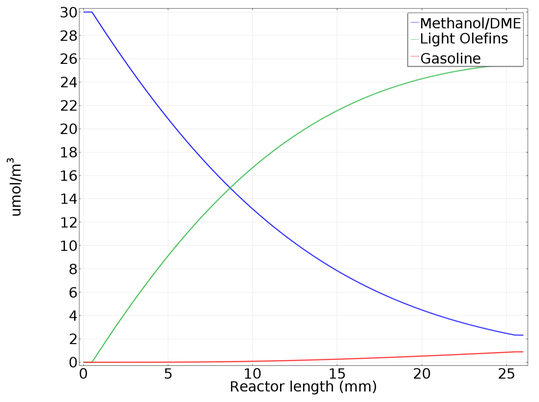

Figure 4. Product distribution along the microreactor for 10h of reaction and 30 µmol/m³ of Methanol in a 30% solution.

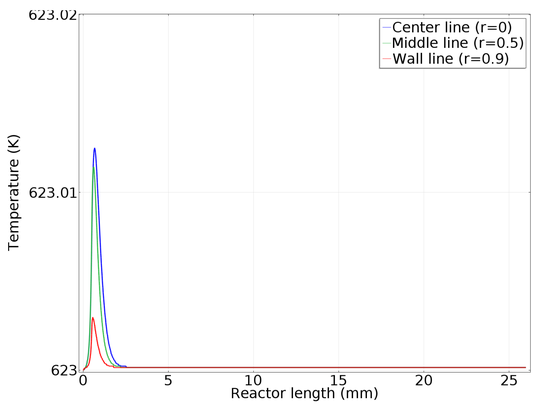

Figure 5. Temperature distribution along the microreactor for 10h of reaction and 1µmol/m³ of Methanol in a 30% solution.

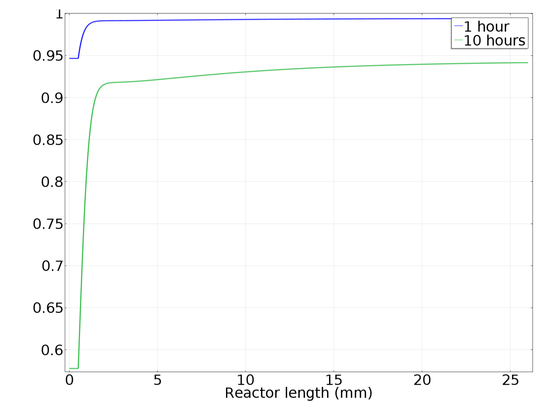

Figure 6. Activity distribution along the microreactor for 1 µmol/m³ of Methanol in a 30% solution.

Conclusions

- The model provided satisfactory concentrations of Methanol to produce Gasoline or Light Olefins with the microreactor provided.
- Temperature is uniform along the reaction;
- This model can be used as a framework for scale up processes.

References

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.

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Excerpt from the Proceedings of the 2015 COMSOL Conference in Curitiba