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Fixed bed catalytic reactor modeling for TAME synthesis

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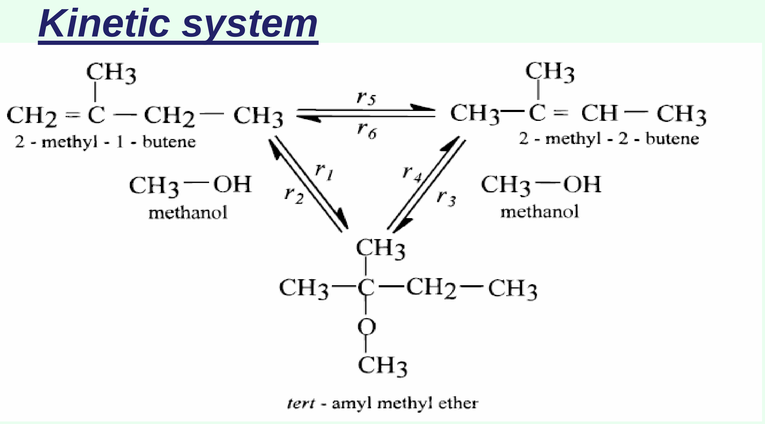
Introduction

This study develops a model in *gPROMS*® ModelBuilder simulating the behavior of a fixed bed catalytic reactor for TAME synthesis. Data obtained from the model is processed using *gRMS*® and Microsoft Excel®. All physical properties data for the components are imported from *Multiflash*® database. TAME synthesis process is widely used in the petrochemical sector. It is carried out in tubular reactors in the presence of cationic resin catalyst (e.g. Amberlyst 35 wet) as a fixed bed. The model developed is based on MESH equations (considering time, radial and axial coordinates), and LHHW kinetic model expressed in activities. UNIQUAC thermodynamic model is used. The results of model simulation are presented as temperature and composition profiles. Some data from laboratory pilot plant experiments are used to be compared with simulation results as a measure of model validation.

Kinetic system



TAME reaction system

Rate equations for TAME synthesis

$$r_1 = L^2 \frac{k_1 K_{1B} K_M \left(a_{1B} a_M - \frac{a_T}{K_{eq1}}\right)}{(1 + K_{1B} a_{1B} + K_{2B} a_{2B} + K_M a_M + K_T a_T)^2}$$

$$r_3 = L^2 \frac{k_2 K_{2B} K_M \left(a_{2B} a_M - \frac{a_T}{K_{eq2}}\right)}{(1 + K_{1B} a_{1B} + K_{2B} a_{2B} + K_M a_M + K_T a_T)^2}$$

The kinetic model [1-3] follows the Langmuir-Hinshelwood-Hougen-Watson mechanism with one or two active centres.

$$r_5 = L \frac{k_3 K_{1B} \left(a_{1B} - \frac{a_{2B}}{K_{eq3}}\right)}{1 + K_{1B} a_{1B} + K_{2B} a_{2B} + K_M a_M + K_T a_T}$$

Mathematical Model

Component Balance

$$\frac{\partial C_i}{\partial t} = -v \frac{\partial C_i}{\partial z} + \varepsilon D_z \frac{\partial^2 C_i}{\partial z^2} + \varepsilon D_r \left(\frac{\partial^2 C_i}{\partial r^2} + \frac{1}{r}\frac{\partial C_i}{\partial r}\right) + \rho_b \sum_{j=REAC} \nu_{i,j} r_j \qquad z \in (0, L), r \in (0, R), i \in COMP$$

Energy Balance

$$\rho_f C_{pf} \frac{\partial T}{\partial t} = -\rho_f C_{pf} v \frac{\partial T}{\partial z} + k_z \frac{\partial^2 T}{\partial z^2} + k_r \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right) + \rho_b \sum_{j=REAC} r_j \left(-\Delta H_j\right)$$

Cooler energy balance

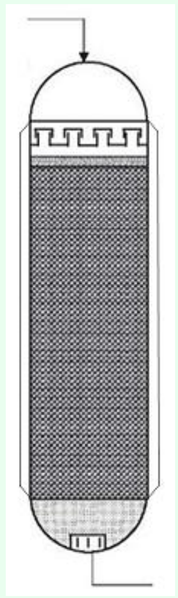
$$\rho_c V_c C_{pc} \frac{\partial T_c}{\partial t} = F_c C_{pc} \left(T_c^{in} - T_c\right) + Q$$

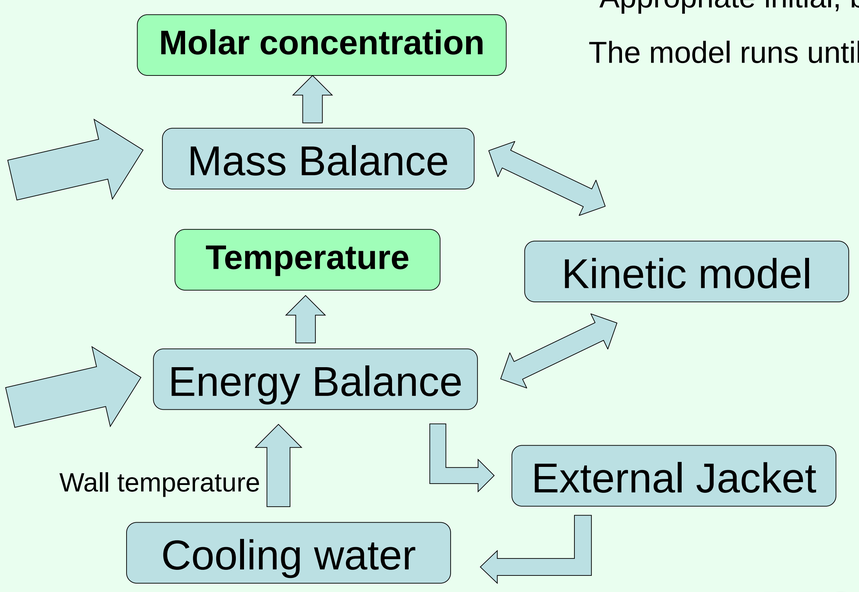
Appropriate initial, boundary conditions and connectivity equations are added.

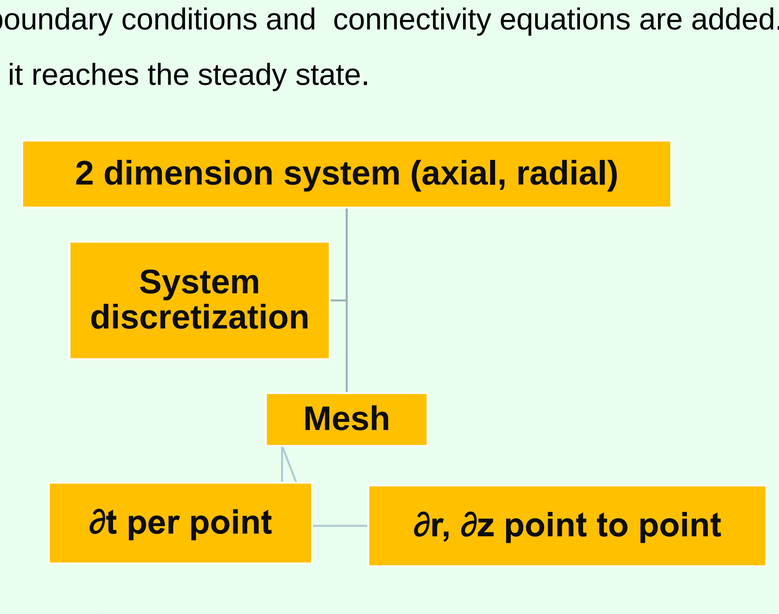
The model runs until it reaches the steady state.

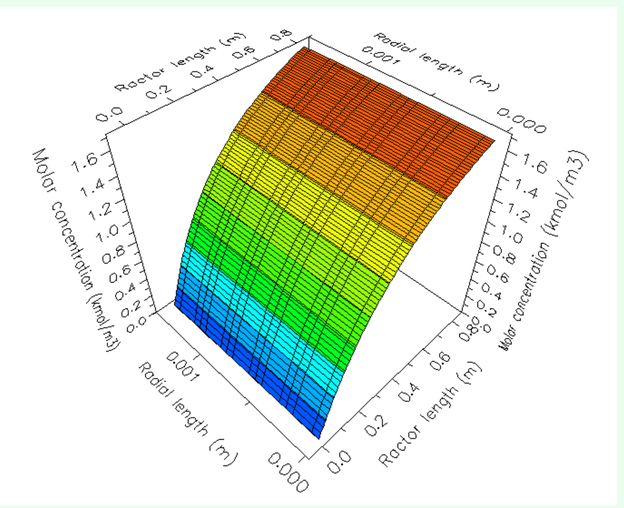
Temperature varies along the reactor due to the exothermic reactions. A jacket with water as coolant is installed. The model considers the same temperature at the wall at both sides.

Model implementation



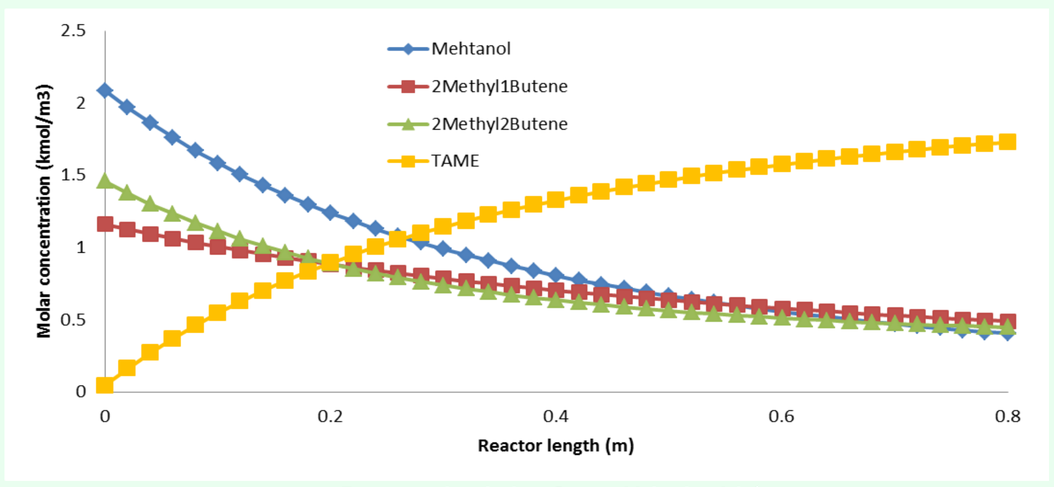




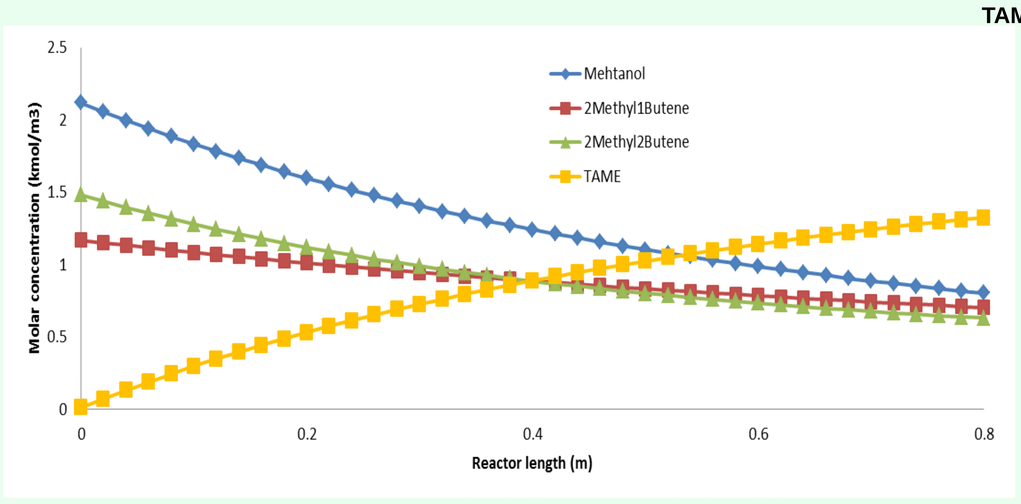


TAME profile through the reactor

RESULTS



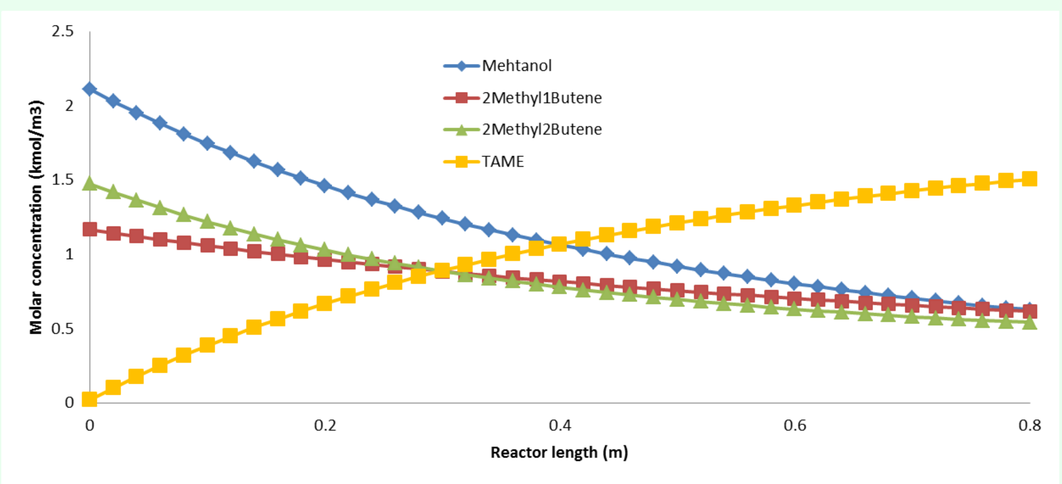
Reactor simulation Space Velocity 1 h^{-1}



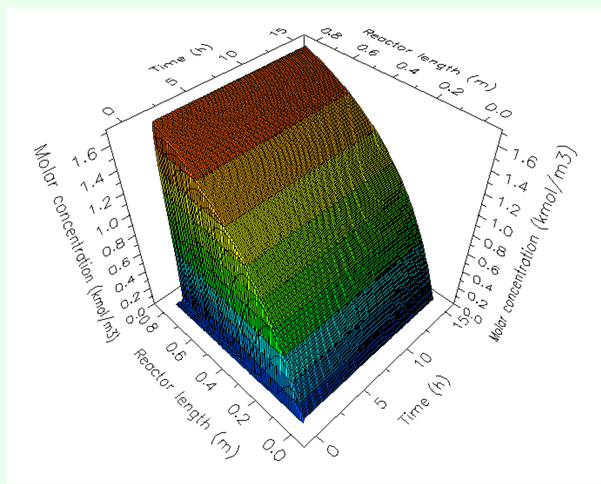
Reactor simulation Space Velocity 2 h^{-1}

Conversion comparison		
S.V. (h^{-1})	Model	Pilot plant
1	64.05%	63.23%
1.5	53.66%	51.10%
2	41.60%	37.33%

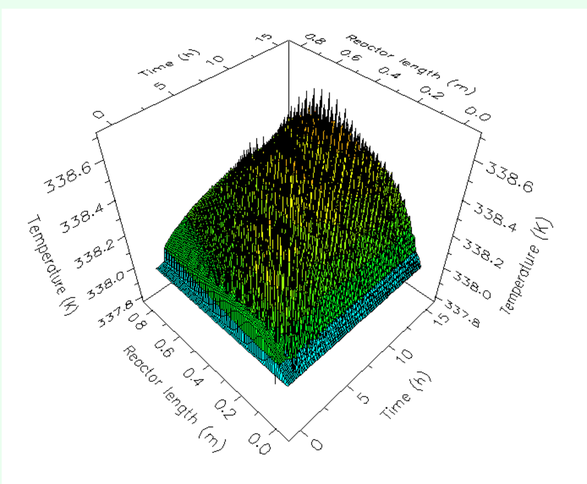
Conversion results show a good response from the model to reality..



Reactor simulation Space Velocity 1.5 h^{-1}



TAME production



Temperature profile

Conclusions

The model developed in this project proves the possibility to obtain fidelity data at an industrial level. External data base *Multiflash*® for temperature dependent physical properties is proven to be very useful allowing the model to account for properties dependence on temperature. The model answered reasonably to the parameter modification and the comparison with data obtained from pilot plant shows good agreement. A larger parameterization study of the model should be made in future, to improve the model applicability.

References

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