Kinetics and reactor modeling of methanol synthesis from synthesis gas

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Abstract:

Methanol synthesis is a typical reaction in heterogeneous catalysis. The reaction is strongly exothermic and limited by chemical equilibrium. Hence, efficient heat transfer is a key issue for the reactor performance. In this work, we have studied a laboratory fixed-bed reactor packed with a $Cu/Zn/Al_2O_3$ catalyst in both adiabatic and isothermal tubular operational modes.

A methanol synthesis kinetic model was implemented in COMSOL Reaction Engineering Lab using the well known kinetic expression by Vanden Bussche and Froment [1]. Both 1D and 2D pseudo-homogeneous dispersion models were applied to describe the mass and heat transfer in the reactor.

Simulation of the reactor for the given operational conditions has been carried out to estimate reactor conversion and radial and axial temperature profiles. The effect of reactor shell temperature on the conversion has been studied and reported. Comparison of the results with similar work shows a good agreement.

Reference:

[1] K. M. Vanden Bussche and G.F. Froment, J. Catalysis, **161**, 1(1996)