Inside the Reactor: Kinetic Model of Methanol-to-Gasoline based on Spatially Resolved Profiles

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The conversion of e-methanol, produced via water electrolysis coupled with carbon capture technologies, into gasoline-range hydrocarbons and other valuable products through the Methanol-to-Gasoline (MtG) process represents a promising alternative to conventional fossil fuels. A new technology demonstrated by TU Bergakademie Freiberg and distributed by Chemieanlagenbau Chemnitz enables the direct catalytic conversion of methanol into gasoline in a single fixed-bed isothermal reactor, eliminating the intermediate dimethyl ether reactor, which was originally developed by Mobil using two adiabatic fixed-bed reactors in series. The aim of this work is to develop an MtG kinetic model in a single reactor that incorporates spatially resolved concentration and temperature profiles obtained using a Compact Profile Reactor (CPR).

The CPR consists of a stainless-steel tube (ID 4 mm, L_{bed} 600 mm) loaded with 445.0 mg of H-ZSM-5 catalyst (200–400 µm). A stainless-steel sampling capillary equipped with orifices and fixed in position runs through the center of the reactor. A K-type thermocouple is inserted inside the capillary, with its tip aligned with the sampling orifices, allowing measurement of local gas temperature. To obtain highly resolved axial profiles, the reactor is moved relative to the stationary capillary, enabling sampling at 10, 30 and 50 mm, with outlet measurements collected at 60 mm. The catalytic experiments were conducted at 5.5 bar and at three temperatures (350 °C, 375 °C and 400 °C), with liquid hourly space velocities (LHSV) between 1 and 10 h^{-1} under steady-state conditions after 6 h of reaction time.

The spatially resolved concentration and temperature profiles provide detailed insight into reaction progression. For example, at 350 °C and an LHSV of 1 h^{-1}, methanol is rapidly converted in the initial reactor section, accompanied by the formation of light olefins and a distinct temperature maximum near the inlet. The local hot spot is associated with the highly exothermic methanol dehydration occurring at high methanol concentrations. Further downstream, olefin fractions decrease while paraffinic species increase, reflecting progressive methylation and hydrogen transfer reactions consistent with MtG reaction mechanism. Simultaneously, the temperature gradually stabilizes as the reaction rate declines and heat becomes more uniformly distributed along the catalyst bed.

The kinetic model is based on coupled mass balance equations with Langmuir–Hinshelwood–Hougen–Watson type rate expressions and Arrhenius temperature dependence. The resulting system of ordinary differential kinetic equations was solved with fourth order Runge-Kutta method in Matlab. Kinetic and adsorption parameters were estimated by nonlinear least-squares regression, minimizing the squared deviation between experimental and predicted concentration profiles.

The MtG reaction is highly complex, involving multiple parallel reactions and consecutive pathways. The CPR provides detailed concentration and temperature profiles, enabling a more accurate description of the reaction and offers quantitative insight into how operating parameters influence product composition.