Multi-Scale Modeling of a ZoneFlow^{TM} Structured Catalytic Reactor for Steam Methane Reforming

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The multi-scale modeling of ZoneFlow^{TM} structured catalytic reactors for steam methane reforming is addressed. Compared to packed bed, ZoneFlow^{TM} reactors aim at reducing pressure drop, improving heat transfer and increasing catalyst effectiveness. Aspects of the catalyst, kinetic modeling, intra-catalyst diffusion, reactor modeling and required scale-bridging strategies are discussed.

To measure the intrinsic reaction kinetics, a micro-packed bed reactor was designed and a range of operating conditions selected based on a set of theoretical criteria. These ensure plug flow, isothermal operation and negligible interfacial and intra-catalyst transport limitations. Isothermal operation required bed dilution and co-feeding of hydrogen to dampen the reaction rates. Non-linear regression is applied to estimate the rate parameters and discrimination between competing kinetic models follows from physicochemical and statistical testing. The Langmuir-Hinshelwood-Hougen-Watson approach is applied to derive rate expressions that incorporate the details of the reaction mechanism and facilitate use and integration in the reactor model.

For the simulation of a commercial reactor, the catalyst coating was described as pseudo-continuum for which the internal porosity and tortuosity were experimentally and theoretically determined. The complex flow pattern is described by means of a CFD model. To bridge the scales of turbulence, the RANS approach was adopted and closure models based on the turbulent viscosity, conductivity and diffusivity were introduced. A k-epsilon turbulence model was applied and validated with cold flow pressure drop tests in a wide range of flow rates. The reactor model further accounts for thermal conduction in the tube wall and in the reactor internals coated with catalyst and for radiative heat transfer. The latter is described by means of the Rosseland-WSGGM model. Detailed measurements of the heat transfer between the tube wall and the process gas in a wide gas flow rate range allowed further model validation. Pilot plant tests allowed validation of the complete reactor model.

The developed reactor model was used to study and optimize the performance of ZoneFlow^{TM} reactors under typical commercial SMR conditions. Comparison with conventional packed bed performance is made and the differences in performance are explained.