Numerical simulations of dead zone formation in the catalytic flow-through membrane reactor

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The use of catalytic membranes in chemical reactor engineering has significantly improved the reactor performance. Therefore, mathematical modelling and numerical simulations of catalytic membrane reactors are important for optimal parameter design increasing the selectivity and yield of certain products in chemical reactions. In this talk, the mathematical model of the flow-through catalytic membrane reactor is presented. The model is based on coupled nonlinear convection-diffusion-reaction equations with temperature-dependent reaction rate constants. The series reactions in the reactor are characterized by the power-law kinetics of fractional order which until now has been rarely investigated in the literature. Under specific reaction and process conditions the reactant can be depleted and a dead-zone can be formed in the membrane reactor. The numerical simulation of this phenomenon requires special solvers. The key idea in this presentation is to construct an appropriate time-marching scheme for solving the steady-state model equations. The effects of parameters such as reaction order, Peclet number, and Thiele modulus on solution profiles and formation of dead-zones are studied numerically. The simulation results show how these parameters influence the appearance and size of the dead zone for the non-isothermal multi-reaction systems.