Catalytic Fixed Bed Reactors – Experimental and Numerical Reactor Diagnostics and Knowledge Based Optimization

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Catalysis and Reaction Engineering are key technologies for our modern society. Catalytic reactors produce transportation fuels, base chemicals for polymers, fertilizers, and pharmaceuticals, they are used for energy conversion and they clean emissions from mobile and stationary sources. Academic and industrial researchers around the globe optimize existing and search for new catalytic processes to meet current and future challenges. This business is competitive and sometimes frustrating. Promising catalysts often do not perform well outside the lab and improvements to established catalytic processes are incremental. One reason for this is that catalysts are dynamic. Like a chameleon changes color and pattern to adapt to its habitat, catalysts change their structure and reactivity as function of local temperature and concentration conditions in the reactor. While a chameleon still behaves like a chameleon, a catalyst in a technical reactor might behave totally different than in a well defined laboratory testing unit. In most applications, the processes inside the catalytic reactor remain hidden. Reactors are normally non-transparent, operate at high temperature and pressure conditions and contain toxic, flammable or even explosive chemicals. Figuratively speaking, the reactor is a „black box“ (Fig. 1). Measurements are restricted to inlet and outlet flows, mathematical models are often too simplified and reactor optimization is based on trial and error.

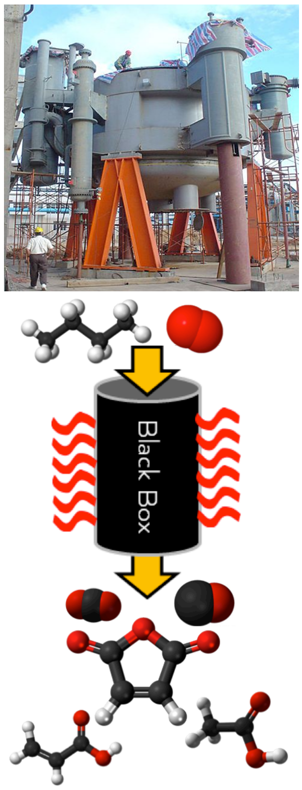

Fig. 1 The Catalytic Reactor as Black Box.

The Institute of Chemical Reaction Engineering at Hamburg University of Technology develops experimental and simulation methods to resolve the physical and chemical processes in catalytic fixed bed reactors. The experimental methods range from measurement of concentration and temperature profiles in reactors to spatially resolved operando characterization of the catalyst in the reactor by Raman spectroscopy. In the field of reactor simulation we generate catalyst packings by DEM simulations and compute the flow-, concentration- and temperature field inside the reactor by particle resolved CFD methods (Fig. 2). The knowledge gained from measurements and simulations leads to strategies to improve the performance of the reactor, e.g. by increasing the yield of the target product and minimizing the formation of waste products.

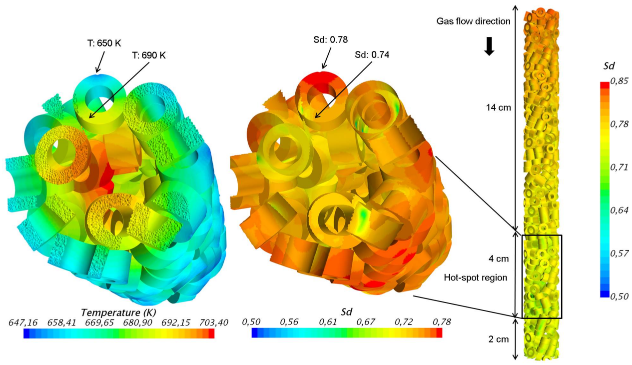

Fig. 2 Particle Resolved CFD Simulation of Temperature and Differential Selectivity in a Fixed-Bed Reactor for n-Butane Oxidation to Maleic Anhydride on a Vanadyl Pyrophosphate Catalyst.