Numerical Modeling of the Original and Advanced TEMKIN Reactor for Catalysis Experiments in Laboratory Scale

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Abstract

1. Introduction
Chemical processes are often characterised by a strong interaction between reaction kinetics and transport phenomena. Selective hydrogenation of acetylene, used to remove disruptive acetylene traces in steam cracker ethylene streams, represents a well-known example. The process is using special catalysts with a thin catalytically active shell (figure 1). Normally, catalysis experiments for the development and optimisation of these catalyst types are time- and cost-intensive. Therefore, Temkin and coworkers developed a special reactor design for the direct testing of industrial type catalysts (figure 1).[1]

Based on the concept of the linearly alternating catalyst and inert pellets inside a small tube, our working group developed an advanced version of this reactor where the catalyst pellets are aligned in the centre of separate small cavities (figure 1).[2]

2. Use of COMSOL Multiphysics®
A COMSOL Multiphysics® model is used to simulate the complex mass and energy transport inside these two different reactor designs to evaluate and compare their performance in the catalysis experiments. The small and clearly defined structural design of the TEMKIN-reactors makes it possible to directly transfer the geometry into a computer model. The COMSOL model is separately accounting for the different transport laws in the domains of free fluid and porous catalysts (figure 2). The spatially resolved concentrations are used to calculate the reaction rates in the catalytically active regions of the catalyst pellet so that concentration gradients and their impact on kinetics can be studied. The intrinsic kinetics of the acetylene hydrogenation have already been investigated using an integral fixed bed reactor so the reaction system and rate laws are mostly familiar.[3]

Simulations are validated by pulsed tagging and catalysis experiments using our advanced TEMKIN-reactor (figure 3). The testing set-up consisted of four separate TEMKIN-reactor modules in a tap-connection arrangement coupled with an online gas-phase chromatograph.

3. Results
Simulations confirm good isothermal conditions due to an efficient and fast transport of the

reaction heat. Furthermore simulations concerning the comparison between the original and advanced version of the TEMKIN-reactor clearly confirm advantages of our advanced version in comparison to the original, mainly caused by reducing the size of dead zones.

3. Conclusions

Although the computational demands of such direct numerical simulations are presently still very high, this work is able to show the advantages in the development and optimization of laboratory scale reactors.

Reference

1. M. I. Temkin and N. V. Kulkova., "Laboratory reactor with ideal displacement", Kinetics and Catalysis, 10, 461-463 (1969).
2. a) Süd-Chemie AG, "Temkin-Screening-Reaktor", Patent DE200920003014, (2010).
b) T. Schulz, Thesis, TU Darmstadt, in preparation.
c) M. Kuhn, M. Lucas, P. Claus,"Advanced TEMKIN Reaktor: Testung von industriellen Schalenkatalysatoren im Labormaßstab", Chemie Ingenieur Technik, submitted.
d) D. Götz, M. Kuhn, P. Claus, "Numerical Modelling and Performance Studies of the original and advanced TEMKIN Reactor in Laboratory Scale Testing of Industrial Egg Shell Catalysts for the Selective Hydrogenation of Acetylene", Chemical Engineering Research and Design, under review.
3. Axel Pachulski, Rainer Schödel and Peter Claus. "Kinetics and reactor modeling of a Pd-Ag/Al2O3 catalyst during selective hydrogenation of ethyne." Applied Catalysis A: General, 445, 107-120 (2012).
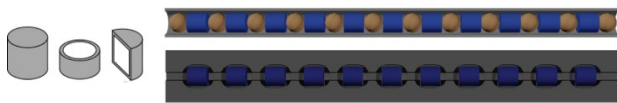
Figures used in the abstract

Figure 1: Left: Cylindrical catalyst pellet and cutplanes showing the thin active shell (grey areas). Right: Cut through the original (above) and advanced (below) TEMKIN reactor.
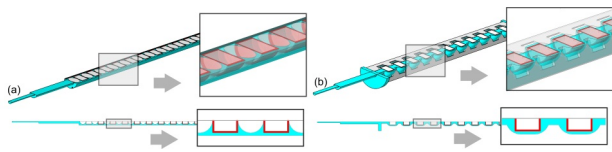
Figure 2: Three- and two-dimensional geometry models of the original (a) and advanced (b) TEMKIN reactor.
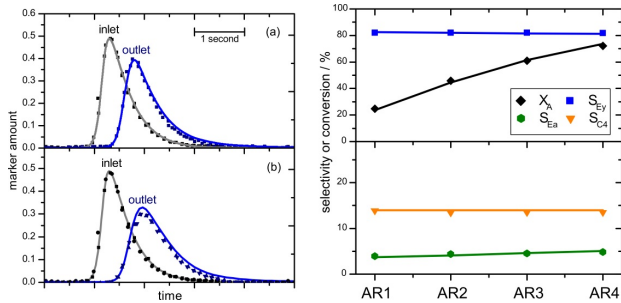

Figure 3: Comparison of experiment and simulation for the pulse tagging (left a: solid pellets b: porous pellets) and catalysis (right) experiments.
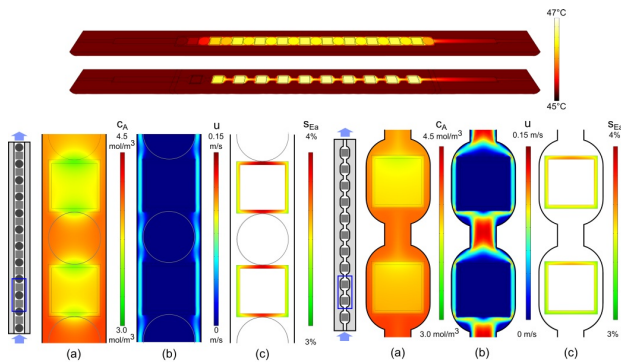

Figure 4: Above: Temperature distribution in the reactor when assuming typical reaction conditons. Below: Colour-coded representations of a section (framed in the reactor scheme) in the original (left) and advanced (right) TEMKIN reactor showing the acetylene concentration in the first module (a), gas velocity (b) differential ethane selectivity in the active shell (c).