Chemical Reaction and Heat Transfer Simulation in a LOHC Dehydrogenation Reactor

Creation of a physico-chemical based model for perhydro-benzyltoluene dehydrogenation to enable a rational reactor design and scale-up strategies

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Abstract

Hydrogen release from the Liquid Organic Hydrogen Carriers (LOHC) is a highly volume-expanding, multiphase reaction with a high heat demand [1]. Pt on a porous AlOx support is used as catalyst for dehydrogenation. Since reactor design requires a deep understanding of the complex interplay between heat transfer, hydrodynamics, and catalyst kinetics, past design strategies have primarily relied on empirical data and experimental validation [2].

A spatially resolved model allows us to detect dead zones in the reactor, hot-spots, which might lead to increased formation of by-products and the wetting behavior of the catalyst, which is crucial for catalytic activity. This qualitative understanding has already led to significant improvements in the design of the heat transfer surfaces. The progress of perhydro-benzyltoluene (H12-BT) conversion (DoDH) and the catalyst temperature (T) is shown in Figure 1 as an experiment and in Figure 2 as a simulation.

Methodology

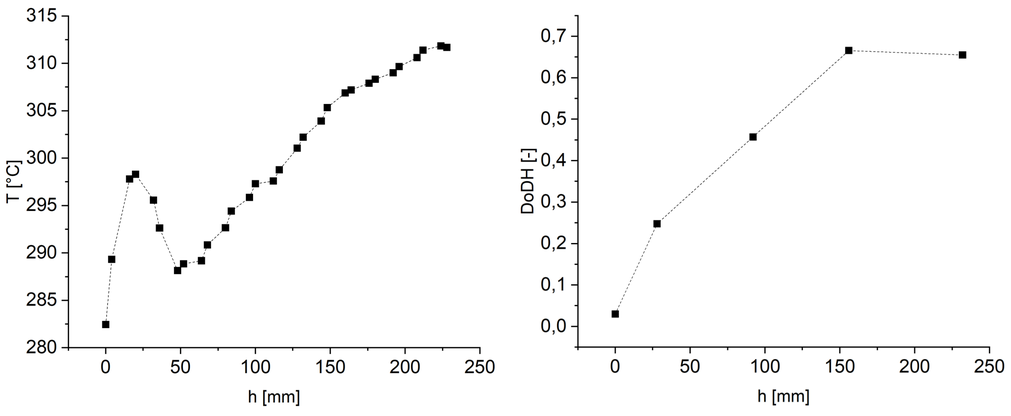

Figure 1. Experimental plot of T-profile (left) and DoDH (right).
Reaction: 3 L/h H12-BT @ 320 °C and 4 bara.

Experiment

1.4 kg of 0.3 wt-% Pt/AlOx catalyst in a cubic stainless-steel reactor of 128 mm x 80 mm x 230 mm with electrical heating rods of Ø 8 mm.

Model

Materials: Literature correlation of density, viscosity, heat capacity and thermal conductivity of reactants and solid walls.
Chemistry: $C_{14}H_{26}$ <=> $C_{14}H_{14}$ + 6 H_2 with defined reaction rate, equilibrium and reaction enthalpy.
Darcy's Law: Inflow and particle diameter of porous media.
Transport of Diluted Species: Inflow concentration.
Heat transfer in Porous Media: Heat sources and losses.

Results

Compared to our experimental data, the simulation significantly overestimates the extent of the reaction. We suspect this is due to insufficient modeling of the complex hydrodynamics and wetting behavior of the catalyst. This issue stems from the highly dynamic three-phase system, in which the released hydrogen increase the total volume flow up to a hundred times than the initially liquid LOHC. To address this, we will integrate more accurate effective heat transfer coefficients and chemical reaction kinetics considering hydrodynamic effects, which we have recently determined experimentally at our institute [3, 4].

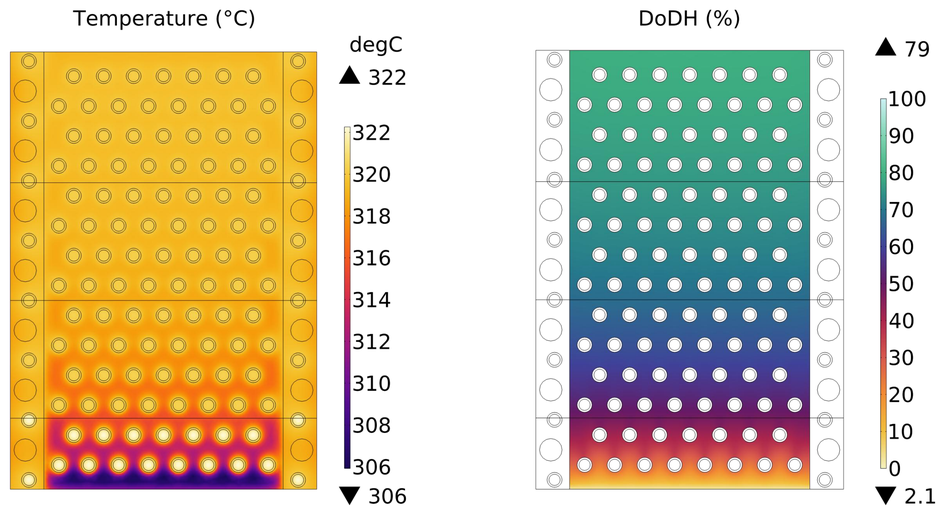

Figure 2. Simulation of T (left) and DoDH (right) using COMSOL®.
Reaction: 3 L/h H12-BT @ 320 °C and 4 bara.

REFERENCES

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