Steady-state multicomponent gas diffusion in conical tubes and pores

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Tube reactors are packed with a porous substrate that carries active sites to heterogeneously catalyze gas phase reactions. In case of fast reactions, it is mass transport that limits the process. The rate determining step (RDS) is the diffusive transport between the educt-rich bulk phase and the product-rich region directly in dead-end pores of the substrate (Figure 1). Under the presence of more than two gas species, as it is the case for most chemical reactions, multicomponent effects have to be taken into account when talking about diffusion. In a previous study, we showed that multicomponent gas diffusion in the transient two-bulb diffusion experiment is significantly delayed by the geometry of test tubes that may be taken as the simplest abstraction of a pore [1]. This delay, a *diffusion-hindrance effect*, increases with the degree of pore tapering, i.e., aspect ratio of inlet and outlet opening cone diameter.

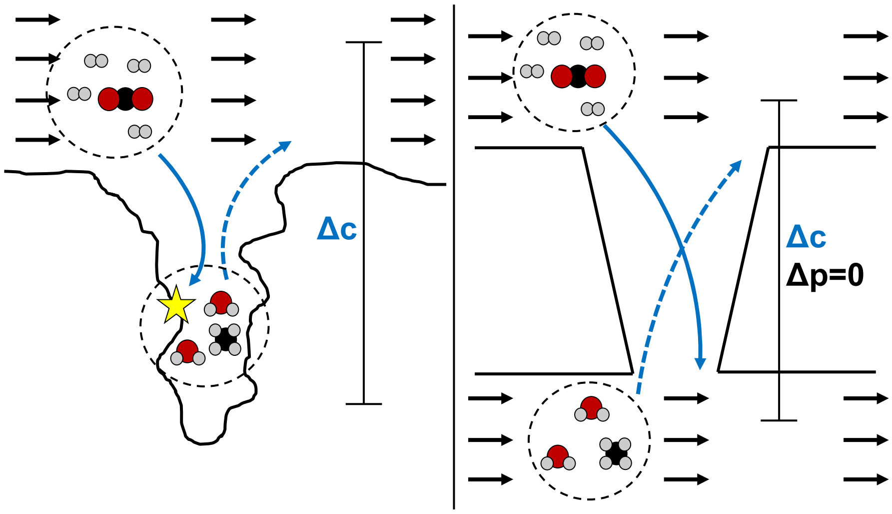

Figure 1: Schematic of the diffusive transport step in a dead-end pore and its abstraction that is realized experimentally and described by our model.

Here we show that the same *diffusion-hindrance effect* also exists for steady-state conditions in gas phase reactions. We experimentally realized the draft shown on the right-hand side of Figure 1 that mimics the abstraction of the transport process in a single pore (left-hand side of Figure 1). By varying the cone angle of the test duct that connects the both regions with different gas mixtures, we can study the impact of the geometry of confinements in which diffusion takes place. The model that was developed and validated in this work enables us to find tailored catalyst pore geometries for specific cases in order to demonstrate the potential of the reduction of mass transport limitation in heterogeneous catalysis.

References

[1] T. Veltzke, L. Kiewidt, J. Thöming: *Multicomponent gas diffusion in nonuniform tubes*. AIChE Journal. **61**, 1404-1412 (2015).