LABORATORY FOR CHEMICAL TECHNOLOGY
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Supervisor(s)	**Period**	**Funding**
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Modeling of Chamber Reactor used for Light Olefin Oligomerization

Aim

Development of a chamber reactor model that can be integrated in commercial plant simulations. The model should allow accurate designs for future projects and improving the daily operation.

Justification

Light olefin, such as propene, oligomerization is the first step in oxo alcohol production. In the particular process of interest, i.e., the Higher Olefin process, propene is reacted over a solid phosphoric acid catalyst to produce olefins in the C_6-C_{12} carbon number range. Multibed adiabatic reactors, also referred to as 'chamber reactors' are conveniently employed for this reaction when targeting the propene tetramers. At present, their design and optimization relies on a decades' long experience, including a wealth of historical plant data. Yet, some basic understanding such as the per bed performance of the reactor is to be enhanced. A systematic analysis of the relevant elementary phenomena involved in propene tetramerization is at stake. Starting from a laboratory scale analysis of (i) the main reaction kinetics at 'steady state' and (ii) the evolution of the catalyst performance with time, e.g., due to hydration, swelling and or coking, etc. a reliable model for the performance of a single bed will be obtained after including the relevant diffusion phenomena. The 'per bed model' will be embedded in a reactor model accounting for additional catalyst beds of different sizes, interbed quenching, etc.

Program

The planned activities for the PhD program have been logically combined into 3 work packages (WP) focusing on intrinsic kinetics data acquisition, kinetic and reactor bed model construction and chamber reactor simulation and optimization.

1. **Intrinsic kinetics data acquisition**
   An accurate simulation of the chemical conversion at commercially relevant conditions requires an adequate knowledge of the so-called intrinsic kinetics of this chemical transformation, i.e., not disguised by mass or heat transfer phenomena, nor by flow pattern non-idealities. For this purpose, measurements will be performed at conditions leading to a maximum insight in these kinetics and the corresponding reaction mechanism, rather than aiming (in this stage) at a maximized product yield. The following tasks are, hence, planned:
   a. *Determination of adequate operating conditions for intrinsic kinetics measurements*
   b. *Tailoring of the High-Throughput Kinetics (HTK) set-up to the needs for measuring intrinsic propene tetramerization kinetics.*
   c. *Systematic assessment of operating conditions effects on 'steady state' kinetics*
   d. *Analysis of transient effects in propene tetramerization*
2. **Kinetic and reactor bed model construction**
   Having acquired fundamental kinetic information as part of WP1, the gained knowledge can be translated into the corresponding models not only allowing to reproduce these data, but also to adequately extrapolate them towards relevant operating conditions in a realistic configuration.
   a. *Propene tetramerization kinetics model (steady state)*
   b. *Catalyst performance evolution modelling*
   c. *Reactor bed modelling*
3. **Chamber reactor 'simulation' and optimization**
   The final work package aims at bringing the simulation work to the relevant pilot and industrial scale. The starting point being the reactor bed model developed under WP2c, it can be incorporated into a more complex simulation of several reactor beds in series with quenches in between and a recycle stream.
   a. *Chamber reactor model construction*.
   b. *Validation against pilot and historical plant data*
   c. *Optimizing the chamber reactor configuration*