LABORATORY FOR CHEMICAL TECHNOLOGY
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Coach	Supervisor(s)	Funding
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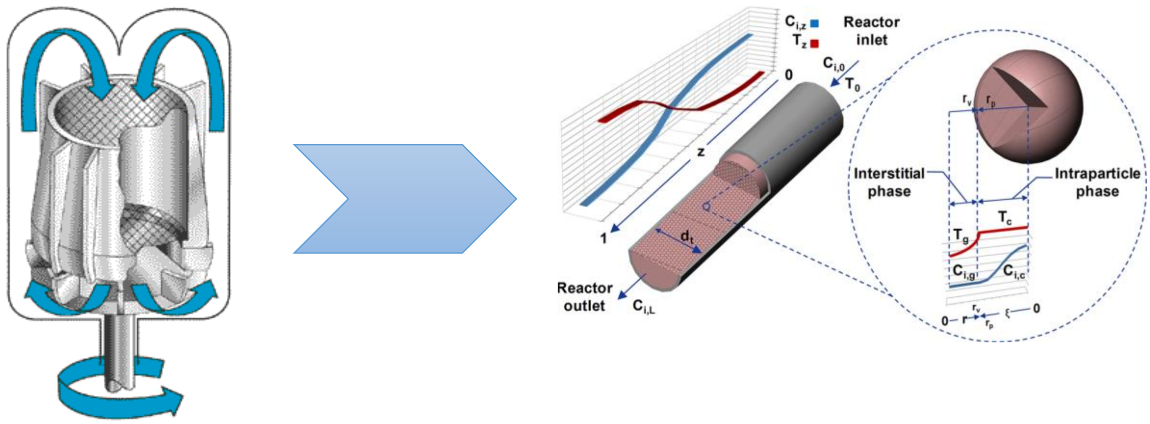
Kinetic study and reactor model development for the dehydration of 2,3-butanediol into 1,3-butadiene

Aim

Construction of a LHHW kinetic model using available intrinsic kinetic data. The constructed model should be able to describe effect of operating conditions on the reaction kinetics. Application of the constructed kinetic model within a large-scale fixed bed reactor model, also accounting for heat and mass transfer, that serves optimization purposes.

Justification

1,3-Butadiene is the key building block for synthetic rubber production. The issues related to the pressing environmental concerns are leading to look into a more sustainable bio-based production process for butadiene production. Furthermore, there is a recent change in feedstock in the current butadiene production process, as a coproduct in the production of ethylene. In some industries, there is already a shift in feedstock from naphtha to shale gas to enhance process efficacy but lead to a decrease in 1,3-butadiene production.
This master thesis will be performed within the framework of the SPICY Project, which is a collaboration between industrial partners and research institutes (KU Leuven, UGent, UHasselt, BBEPP and VITO), aiming to answer these questions and demands on the Flemish level. This will be achieved *via* the sustainable production of existing polymers and discovery of novel biopolymers. The production of these bio-based polymers starts from sugars, *via* biochemical conversion to precursor molecules, such as 2,3-butanediol. The further chemical conversion of this molecule into a monomer, 1,3-butadiene is the subject of this research.



Program

- ➢ Literature survey of the conversion of 2,3-butanediol to 1,3-butadiene with the specific focus on Sc_2O_3 and similar rare earth metal oxides, kinetics and reactor modeling.
- ➢ Construction of a LHHW kinetic model using intrinsic kinetic data to simulate the effects of partial pressure, temperature and space time.
- ➢ Development of a large-scale 1D reactor model using the kinetic model constructed and taking into account heat and mass transfer effects.

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