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Kinetics evaluation and large-scale reactor model development for 2,3-butanediol dehydration into 1,3-butadiene

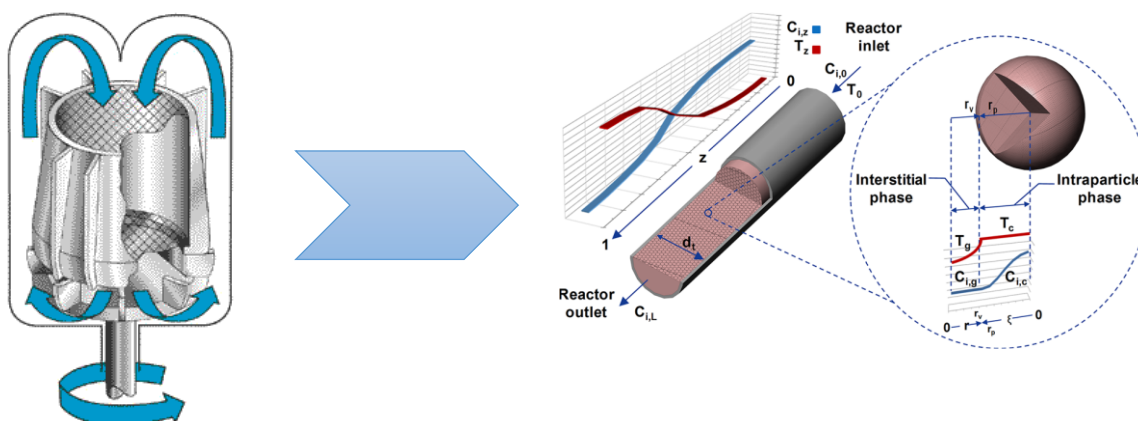
Aim

Construction of a reactor model for 1,3-butadiene production from 2,3-butanediol. After performing a well-selected set of experiments, a LHHW kinetic model needs to be constructed using the available intrinsic kinetic data. The constructed model should be able to describe effect of operating conditions on the reaction kinetics. Finally, the constructed kinetic model should be combined with heat and mass transfer aiming at the development of a large-scale fixed bed reactor model that can be used for optimization purposes and assessing process efficiency of two-step production process versus one-step production process.

Justification

1,3-Butadiene is the key building block for synthetic rubber production. The current butadiene production, as a coproduct from ethylene via thermal cracking, is recently declining due to a shift in typically employed feedstocks to lighter molecules. Pressing environmental concerns urge for the exploration of more sustainable, c.q., bio-based, routes for 1,3-butadiene production.

This master thesis will be performed within the framework of the SPICY and the GREEN-B2B projects which entail a collaboration between industrial partners and research institutes (KU Leuven, UGent, UHasselt, BBEPP and VITO), aiming to answer the above challenges on the Flemish level. More particularly, SPICY aims at the sustainable production of existing polymers and discovery of novel biopolymers. The production of these biobased 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 master thesis topic. GREEN-B2B, on the other hand, focuses on the production of 1,3butanediol by fermentation, followed by its chemocatalytic conversion into 1,3butadiene.



Program

- Completion of an experimental intrinsic kinetics data set for 1,3-butadiene production from 2,3butadiene.
- Construction of a LHHW kinetic model using existing intrinsic kinetic data to simulate the effects of partial pressure, temperature and space time.

- Development of a large-scale 1D reactor model using the constructed kinetic model and taking into account heat and mass transfer effects.
- Overall comparison of two step versus one step process for 1,3-butadiene production process.