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Modelling of structured reactors for a carbon coupling reaction

Aim

Explorative study of structured reactor types for the aldol condensation and selection of interesting designs, based on the compatibility with an existing catalyst. Development of a reactor model for the selected types of structured reactors and comparison with packed bed reactor.

Justification

A fixed bed tubular reactor, packed with catalyst pellets, is probably the simplest continuous flow reactor type we can think of as chemical engineers. Typically, the reactor tubes are relatively long with a small diameter and relatively thin walls, enabling an efficient supply or removal of heat. However, the pressure drop occurring over such a packed bed may become unpractically high. Moreover, non-idealities in the hydrodynamic flow pattern may develop as the reactor tube becomes either too small or too large. These issues can be overcome by structuring the catalyst bed, as part of so-called process intensification, since the ideal behaviour can be approached much better, resulting in an improved performance. The essence of such a structured reactor, is the adequate control over the majorly relevant phenomena in chemical reactor operation, such as the intrinsic reaction kinetics, transport phenomena at the micro scale and hydrodynamics at the macro scale.

In this perspective, we want to explore the possible beneficial effects of such structured reactors for the aldol condensation, an important organic reaction for creating new carbon bonds. Because of the possibility to create larger and more complex molecules, this reaction is very relevant for the pharmaceutical industry and fine chemicals production, or has potential for future applications such as the valorisation of biomass derived platform molecules in bio-refineries. After extensive research, a heterogeneous catalyst, an aminated polymeric resin, has been developed which performs well in a lab-scale continuous flow setup. This catalyst could be applied in a conventional packed bed tubular reactor, but also allows shaping into a monolith or foam type structured catalyst. Therefore, in this thesis, we would like to investigate what influence the reactor type, i.e. packed versus structured bed reactor, has on its performance in the process.

Program

First, the state-of-the art on structured reactors in literature will be explored and the most interesting designs for the case study of continuously operated aldol condensations, e.g. a monolith or foam type reactor, will be selected. Subsequently, a reactor model will be developed for the selected structured reactor types by applying conservation equations for mass, energy and momentum. Finally, a comparison will be made with the conventional fixed bed tubular reactor and guidelines can be proposed for further process optimisation.

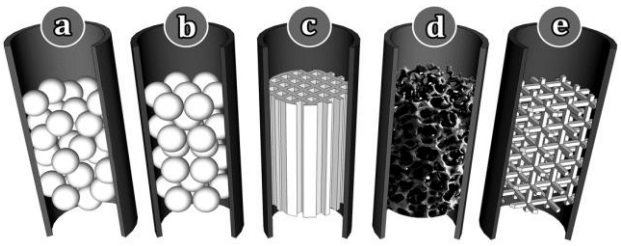

Figure 1: Comparison of packed bed reactors (a,b) with structured reactors (c-e). (Schwieger et al. 2016)

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