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Morphological analysis and optimisation of heterogeneously catalysed reactive distillation of complex chemical systems

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Highlights

- Presentation of a morphological analysis
- Assessment of the sensitivity of the simulations on the choice of the model
- Assessment of the sensitivity of the set-up on the choice of the catalytic internals
- Investigation of the influence of key design parameters on the performance of HCRD
- Useful tool for the design and optimization of reactive separation processes

Introduction: Reactive distillation (RD) has received much attention from industry and academia in the past years as it has many potential advantages compared to conventional processes with sequential arrangement of a reactor and distillation. Up to now, it was commonly assumed that the model based design for heterogeneously catalysed reaction (HCRD) can be done fairly simply even for different types of catalytic internals using an equilibrium stage or rate-based model and accounting for the reaction kinetics. HCRD experiments with two different chemical test systems and with two different types of catalytic internals showed that the two types of internals can give, depending on the test system, significantly different results that cannot be predicted by these simple model approaches. Furthermore, even within one test system, it is possible that the conversion and the concentration profiles of the main products of HCRD processes can be well described by the simple model approaches while these approaches fail to describe the behaviour of the side products. In order to investigate the reason for the different behaviour of the two test systems and the main and side products, a morphological analysis of models for HCRD was carried out. The coordinates of the morphological analysis are a) the type of reactor model (CSTR or PFR) and b) the degree of superposition of reaction and distillation (simultaneous or sequentially alternating). The results show that variations along these coordinates can have, depending on the chosen system, a significant impact on the outcome of HCRD for industrial relevant systems. Hence, there are situations in which details of the actual design of the catalytic internals need to be accounted for in the process model.

The new findings also explain previously not well understood experimental results of HCRD. Additionally, valuable information for the design and optimisation of HCRD processes is gained by the morphological analysis. The morphological analysis cannot only be applied for HCRD but also for other processes in which reaction interacts with distillation (or other separations processes).

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