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Reactive and hybrid separations of chemicals and bioactive substances: Modeling and optimization

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Abstract

Distillation, absorption and extraction belong to the oldest and most mature separation technologies. They require often big columns and are energy intensive. In the chemical processing industry these separations are applied usually for the purification of the products, recycling of solvents or catalysts, etc. and are placed as a last step of a production process, after the chemical reactor(s). The integration of separation and reaction in one single unit operation offer high potentials for process optimisation and has been recognized as an important method for process intensification. Despite of that potential, **reactive separation** processes, like reactive distillation, reactive extraction and reactive absorption are sometimes recognize by industry as niche solutions only. One of the reasons for that situation is a lack of validated modelling methods of columns for reactive separations or limited knowledge of the model parameters. This paper shows the modelling approaches of different complexity for some reactive separations, gives the recommendations for the most suitable simulation methods and illustrates the necessity for the harmony between the accuracy of the experimental

model parameters and the depth of the modelling methods. Simulation results are validated through industrial case studies of catalytic distillation and reactive absorption.

Another method to intensify the processes is the combination of several separations into so called **hybrid separations**. They potentially allow to replace the industrially applied processes like azeotropic, extractive and pressure-swing distillation, contributing to the energy saving. They may also be applied in the production of bioethanol. The combination of distillation and membrane separations is a classical example of hybrid separations which is not yet established in chemical industry due to low permeate fluxes, short membrane lifetime or the lack of general design methodology and detailed process know-how. The paper presents a flexible and robust simulation tool for simulation of a hybrid process consisting of a (reactive) distillation column and pervaporation or vapour permeation. Various modelling approaches and different modelling complexities for both unit operations are implemented taking into account all non-ideal effects for the membrane separation. The influence of decisive operational parameters on dewatering (pilot scale) and on membrane area and operational costs (industrial scale) is illustrated. Even though this hybrid membrane process is not yet competitive, the benefits are very likely to prevail in the nearest future. Binary and ternary lab-scale pervaporation experiments have been performed to determine relevant model parameters and to validate the model. The agreement between simulation and experiment is satisfactory.

Tha idea of hybrid separations may be also applied for the **bioseparations**. The paper presents a case study of simulation and optimisation of the downstream process for purification of human serum albumin by using ion exchange membrane adsorbers. Models of different complexity for relevant unit operations such as ultrafiltration, chromatography and membrane adsorbers have been combined in order to generate the complete, generic downstream process model. Despite of model complexity the process model proves robust numerical convergence properties and offers valuable model flexibility. An optimal process setup for the unconventional process is achieved.