

472c Design and Operation of Simulated-Moving-Bed Reactors

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Integrated units like reactive distillation or reactive chromatography can offer additional degrees of freedom which allow achieving higher process performance by altering the internal concentration profiles. Especially in the scope of equilibrium limited reactions, such integrated reactor-separator processes can increase the efficiency substantially because they make it possible to overcome the equilibrium limited yield and to bring the reaction to full conversion. Up to now, no literature is available about the operation of reactive chromatography on an industrial scale, although the advantages in comparison to conventional reactor-separator sequences have been shown experimentally for various reactions, e.g. the production of bisphenol A, the synthesis of methyl acetate, the isomerisation of glucose. Recently, a patent for the production of vitamin C via simulated-moving-bed reactors (SMBR) has been issued. Reliable and matured design procedures are available for purely separative simulated-moving-bed processes and are extensively used in industry, and recently a design method analogue to the "Triangle Theory" has been published for simulated-moving-bed reactors (SMBR). This design method has been verified experimentally in a mini-plant unit and is used in this work as a starting point for further optimization with a detailed model. The necessary model parameters have been obtained from batch column experiments which have been fitted using a detailed model. The minimization of the error between batch column experiments and simulations has been accomplished using a genetic algorithm. The validity to use these fitted parameters for the design of SMBR units has been presented earlier. The adsorptive and catalytic properties of several commercial ion-exchange resins with varying chemistry, acidity, and functionalization have been measured for an industrial synthesis of type $A + B \rightleftharpoons C + D$. The effect of the different stationary phase properties on the efficiency of the SMBR, particularly on the solvent requirement (i.e. moles solvent/ moles of product) is presented. Using the obtained data in a commercially available flowsheet simulator, the conventional, sequential reactor-separator process is compared with the integrated process incorporating a SMBR. These two processes are compared with respect to the overall amount of energy needed per unit product.