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Non-equilibrium modelling of simulated moving bed processes for separation of Xylenes in petrochemical industry

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Industrial adsorptive separation processes have been largely employed for separations in the petrochemical industry. Conventional fixed bed adsorption desorptionseparationis a batch process. As opposed to conventional adsorptive separations, continuous adsorptive separation processes, presents advantages in terms of productivity. Simulated Moving Bed (SMB) technology is a highly selective adsorption desorption process of continuous separation which is often employed in the separation of complex mixtures.This technology has been applied over four decades in the petrochemical industry and currently enjoying preparative an production scale separation of sugars, proteins, pharmaceuticals, fine chemicals, flavorings, foods and enantiomers. This work focuses on mathematical modeling and simulation of SMB systems to be used for xylene isomers separation, which is extensively used in petrochemical industries. Production of polyester fibers and polyethylene terephthalate are the main examples. The operation methodology of SMB is highly complex in nature. Therefore, generally, a model-based control scheme is used so as to obtain a stable operation and better understood SMB process. A great deal of theoretical work has been carried out for developing useful simulation procedures for design and process development purposes. There are several models to be used for adsorptive separations whether it is at the analytical scale or at the preparative/production scale. The ideal model, the equilibrium dispersive model, the transport dispersive model and the general rate (GR) model, which may be also called non-equilibrium model, are the main examples. The GR model is widely acknowledged as being the most comprehensive among such models available in the literature as it accounts for axial dispersion and all the mass transfer resistances, e.g., external mass transfer of solute molecules from bulk phase to the external surface of the adsorbent, diffusion of the solute molecules through the particle, and adsorption-desorption processes on the site of the particles. The solution of the GR model based SMB governing equations involves the employment of advanced numerical techniques. The solution algorithm usually employs linear adsorption isotherm conditions. This is largely due to the highly complex nature of the resulting equations whennon-linear adsorption isotherms integrated into SMB modeling studies. Özdural et al. proposed a new algorithm for the numerical solution of non-equilibrium packed-bed adsorption with non-linear adsorption isotherms. Contrary to the generally employed practices, this methodology is not governed by the solution of coupled partial differential equations.The number of partial differential equations to be solved reduces to one. In the present study this technique is extended to SMB systems and applied to Langmuir type nonlinear adsorption isotherm model for xylenes. The solution of the present model predicts the concentration profiles of the components along the columns. For separation of xylenes in petrochemical industry, the present non-equilibrium modelling of SMB under non-linear adsorption isotherms allows a strong perspective and facilitates scale-up procedures.

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