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NOTE

Simulation of Ethanol and Acetone Extraction from Aqueous Solutions in Membrane Contactors

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In this work a 2D mathematical model was developed to study liquid extraction by membrane contactors. The equations of model were solved by numerical method based on finite element method. The system studied in this work is a hollow-fiber membrane based extractor using near-critical carbon dioxide. Simulations results were compared with the experimental data and showed good agreement. This mass transfer model is more accurate than other models and represents a general approach which can be applied in other membrane separation.

Key Words: Solvent-extraction, Modeling, Mass transfer, Numerical simulation, Dense gas.

Supercritical fluid (SCF) is a compound which is subjected to temperatures and pressures more than the critical values. The supercritical fluid indicates valuable properties as well as a high solubilizing capacity for solvent-extraction processes because of the transition between gas and liquid phases and its high density. The most popular compound which is used as supercritical fluid in separation processes is carbon dioxide because it is non-toxic, inexpensive and inert[1-5].

The main purpose of the present study is to develop and solve a 2D mathematical model for porocritical process. The model considers axial and radial diffusion in the tube, membrane and shell compartments of the contactor. It also considers convection in the tube and shell sides. The model is then validated using experimental data reported by Bothun *et al.*[6] for extraction of ethanol and acetone from aqueous solutions.

Model developments: The continuity equations for three sections of contactor were obtained and solved to predict the concentrations of solute along the contactor. The model is developed for a hollow fiber (Fig. 1), through which the liquid flows with a fully developed laminar parabolic velocity profile.

The continuity equation for each species in a reactive system can be expressed as:

$$\frac{\partial C_i}{\partial t} = -(\nabla \cdot C_i V) - (\nabla \cdot J_i) + R_i \qquad (1)$$

where C_i, J_i, R_i, V and t are the concentration, diffusive flux, reaction rate of species i, velocity and time, respectively. Either Fick's law of diffusion or Maxwell-Stefan theory can be used for the determination of diffusive fluxes of species i.

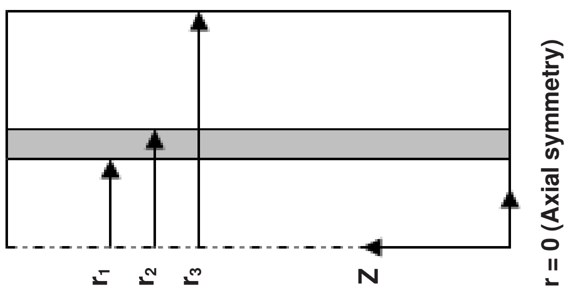

Fig. 1. Model domain

The mass transfer equations related to tube, membrane and shell side of contactor with the boundary conditions were solved using COMSOL Multiphysics software, which uses finite element method for numerical solutions of differential equations.

Validation of the mass transfer model: Calculations of the extraction percentage using the simulation developed in this work were compared with the experimental data reported by Bothun *et al.*[6]. Figs. 2 and 3 show the simulated and experimental extraction percentage as a function of the liquid feed flow. Comparing the extraction percentages calculated for ethanol and acetone, better accuracy is found for acetone separation. Simulation results show that this mass transfer model is very accurate.

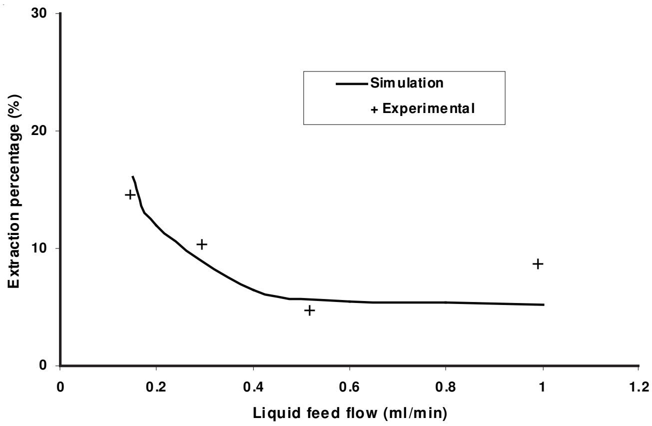

Fig. 2. Extraction percentage values of ethanol from aqueous solutions (10 %w/w) obtained from experiments (Bothun *et al.*[6]) and simulation (this work)

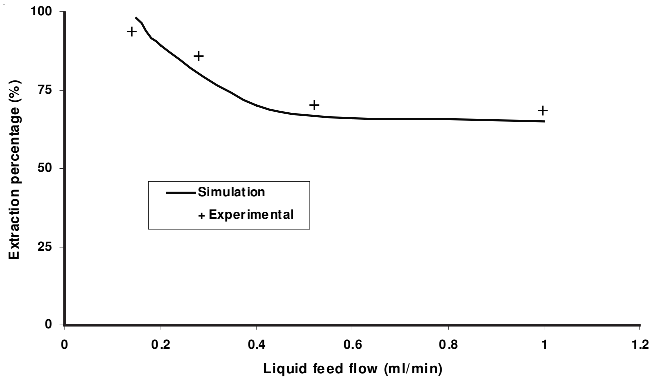

Fig. 3. Extraction percentage values of acetone from aqueous solutions (10 % w/w) obtained from experiments (Bothun *et al.*[6]) and simulation (this work)

Conclusion

A 2D mathematical model was developed to study the removal of compounds from aqueous solutions in hollow fiber membrane contactors. The model predicts the steady state solute concentration in the contactor by solving the conservation equations. The mass transfer model was validated by comparing results of extraction percentages of ethanol and acetone from aqueous solutions obtained from simulations with experimental data. The simulation results indicated that the extraction of solute increased with decreasing liquid velocity in the tube side.

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