



NOTE

Investigation on Numerical Simulation of Acetone and Ethanol Separation from Water by Using Membrane

AZAM MARJANI^{1,*} and SAEED SHIRAZIAN²

¹Department of Chemistry, Islamic Azad University, Arak Branch, Arak, Iran

²Department of Chemical Engineering, Islamic Azad University, Arak Branch, Arak, Iran

*Corresponding author: E-mail: a-marjani@iau-arak.ac.ir

(Received: 14 December 2010;

Accepted: 28 March 2011)

AJC-9785

A mass transfer model was developed to investigate liquid separation in membranes. Axial and radial diffusion inside the tube, through the membrane and within the shell side of the contactor were considered in the model. The system studied in this work is a hollow-fiber membrane based extractor of ethanol and acetone from aqueous solutions using near-critical carbon dioxide. Simulations of extraction percentages of ethanol and acetone show an average difference of 15.66 and 2.55 % with the experimental data, respectively.

Key Words: Membrane, Acetone, Ethanol, Mass transfer, Dense gas.

Porocritical process is used to extract liquids by a hollow-fiber membrane contactor. 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 inert¹⁻⁴.

The main purpose of the present study is to develop and solve a 2D mathematical model for porocritical process. The model is then validated using experimental data reported by Bothun *et al.*¹ for extraction of ethanol and acetone from aqueous solutions.

Formulation of mass transfer: 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 through which the liquid flows with a fully developed laminar parabolic velocity profile. The fiber is surrounded by a laminar gas flow in an opposite direction.

The continuity equation for each species in a reactive system can be expressed as⁵:

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

where C_i , J_i , R_i , V and t are the concentration, diffusive flux, reaction rate of species i , velocity and time, respectively. 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 (FEM) 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.*¹.

Tables 1 and 2 show the simulated and experimental extraction percentage as a function of the liquid feed flow (F) and the dense gas and liquid feed flow (S/F) mole ratio. Comparing the extraction percentages calculated for ethanol and acetone, better accuracy is found for acetone separation. This could be accounted for considering two aspects: better prediction of transport properties and correct estimation of the vapour-liquid equilibrium in the ternary acetone- CO_2 -water system. For both systems studied greater accuracy of the model was obtained at lower values of the liquid feed flow (F) and for dense gas extraction flow (S), since the S/F ratio remains constant ($S/F = 3$) for most of the experimental measurements⁵. Simulations of extraction percentage of ethanol and acetone show an average difference of 15.66 and 2.55 % with the experimental data, respectively. Simulation results show that this mass transfer model is more accurate than other models.

TABLE-1
COMPARISON BETWEEN EXPERIMENTAL AND SIMULATED
(PRESENT WORK) ETHANOL EXTRACTION VALUES FROM
AN AQUEOUS SOLUTION USING THE SINGLE FIBER
POROCRITICAL EXTRACTION SYSTEM
P = 69 bar; T = 298 K; Feed solution concentration = 10 %w/w

F (mL/min)	S/F	Extraction (EXP) (%)	Extraction (MOD) (%)	Error (%)
0.15	3	15.2	16.04	5.5
0.25	3	10.4	11.01	5.9
0.50	3	4.7	5.53	17.6
1.00	3	9.9	5.21	47.3
0.10	10	31.9	32.55	2.0

TABLE-2
COMPARISON BETWEEN EXPERIMENTAL AND SIMULATED
(PRESENT WORK) ACETONE EXTRACTION VALUES FROM
AN AQUEOUS SOLUTION USING THE SINGLE FIBER
POROCRITICAL EXTRACTION SYSTEM
P = 69 bar; T = 298 K; Feed solution concentration = 10 %w/w

F (mL/min)	S/F	Extraction (EXP) (%)	Extraction (MOD) (%)	Error (%)
0.15	3	96.1	98.03	2.0
0.25	3	89.6	87.61	2.2
0.50	3	68.9	67.04	2.7
1.00	3	67.9	65.63	3.3

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 model was developed for non-wetting conditions, taking into consideration axial and radial diffusion in the tube, membrane and shell sides of the contactor. From the values of

these operating parameters, the hydrophobicity or hydrophilicity of the membrane used as contractor could generate more or less important modifications in the performance of the process. 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 reported by Bothun *et al.*¹. The simulation results indicated that the extraction of solute increased with decreasing liquid velocity in the tube side. On the other hand, extraction percentages of solutes when the solutions circulate within the fiber are greater than that solution circulate within the shell.

Nomenclature

A	Cross section of tube (m ²)
C	Concentration (mol/m ³)
D	Diffusion coefficient (m ² /s)
F	Liquid feed flow (m ³ /s)
J _i	Diffusive flux of species i (mol/m ² s)
P	Pressure (Pa)
r	Radial coordinate (m)
S	Solvent flow rate (m ³ /s)
T	Temperature (K)
z	Axial coordinate (m)

REFERENCES

1. G.D. Bothun, B.L. Knutson, H.J. Strobel, S.E. Nokes, E.A. Brignole and S. Díaz, *J. Supercrit. Fluids*, **25**, 119 (2003).
2. A. Birtigh, A Regeneration der Fluidphase bei der Gasextraktion, Ph.D. Thesis, Technical University of Hamburg, Germany (1995).
3. S. Sarrade, G.M. Rios and M. Carles, *J. Membr. Sci.*, **114**, 81 (1996).
4. G. Afrane and E.H. Chimowitz, *J. Membr. Sci.*, **116**, 293 (1996).
5. R.B. Bird, W.E. Stewart and E.N. Lightfoot, *Transport Phenomena*, John Wiley & Sons, New York, edn. 2 (2002).