Gas separation simulation in hollow fiber membrane modules for multi component mixtures: Calculation of the performance and required area

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1- Summary

In this study, simulation of multi component gas mixtures separation with hollow fiber polymeric membranes was investigated. With this simulation, required membrane area for a specific separation for all of flow patterns can be calculated and the best flow pattern with minimum required area and maximum performance can be chosen. With this model, the effect of flow pattern, pressure losses and sweep gas on membrane performance and its required area can be investigated. Results of simulation have shown good consistency with experimental data from literature.

2- Extended Abstract

2-1- Mathematical modeling

- Counter current flow

For simulation, each fiber was divided in to N equal stages and mass balance and permeation equations for each component in each stage were written. These equations were coupled with each other to form a tridiagonal matrix which should be solved by Thomas algorithm (Equation 1). The initial guesses needed for matrix solving were calculated with the aid of cross flow pattern equations. Related equations were solved by Jacobian method (Equation 2). As the initial guess for solving these nonlinear equations, in all stages except stage N, the composition of component in the previous stage was used. In stage N equation (Equation 3) was used as the initial guess. After this, the matrix was solved until convergence (Equation 4).

- Cocurrent flow

In this case, there is no need for matrix solving, and the governing equation (equation 5) for each component, was solved until convergence.

$$\begin{bmatrix} C(K,1) & D(K,1) & & & & \\ B(K,2) & C(K,2) & D(K,2) & & & \\ ..... & .... & ..... & ..... & ...... & \\ & B(K,i) & C(K,i) & D(K,i) & ...... & \\ ...... & ..... & ...... & ...... & ...... & \\ & & B(K,N-1) & C(K,N-1) & D(K,N-1) & \\ & & & B(K,N) & C(K,N) & \end{bmatrix} \begin{bmatrix} l(K,1) \\ l(K,2) \\ .... \\ l(K,i) \\ .... \\ l(K,N-1) \\ l(K,N) \end{bmatrix} = \begin{bmatrix} V(K,0) \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -D(K,N)\times l(K,N+1) \end{bmatrix} \quad (1)$$

$$Y(K,i) - \frac{Q(K)\times\left(P_f \times XR(K,i) - P_v \times Y(K,i)\right)}{\sum_{i=1}^{R}\left(Q(K)\times\left(P_f \times XR(K,i) - P_v \times Y(K,i)\right)\right)} = 0 \quad (2)$$

$$Y(K,N) = \frac{Q(K)\times XR(K,N+1)}{\sum_{m=1}^{R} Q(m)\times XR(m,N+1)} \quad (3)$$

$$\left|\frac{\Delta L(1)}{L(1)}\right| \langle 10^{-8} \text{ and } \left|\frac{\Delta V(N)}{V(N)}\right| \langle 10^{-8} \quad (4)$$

$$l(K,i) = \frac{V(K,i+1) + \left(1 + \frac{V(i)}{Q(K)\times DeltaA \times P_v}\right)\times l(K,i)}{1 + \left(\frac{V(i)}{Q(K)\times DeltaA\times P_v} + \frac{P_f}{P_v}\times\frac{V(i)}{L(i)}\right)} \quad (5)$$

2-2- Results

Comparison of the simulation results with experimental data for binary and multi component gas mixtures have shown good consistency between them. This can be seen in following figures. (feed pressure 100 psig, permeate pressure 1 atm)

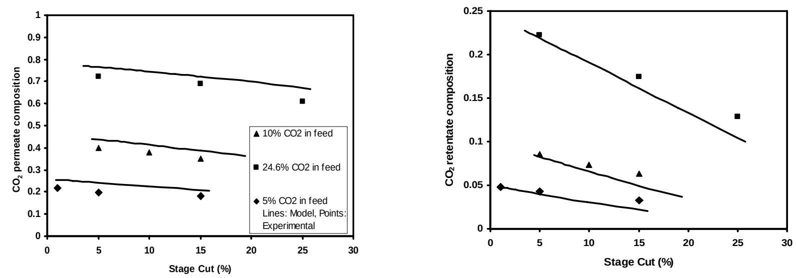
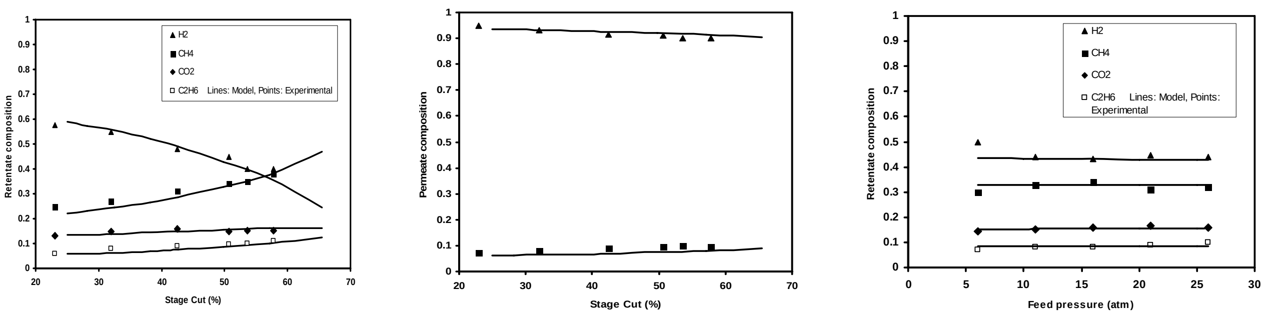


Figure 1- Comparison of experimental results with simulation for CO_2/CH_4 separation [10]



(a) (b) (c)

Figure 2- Comparison of experimental results with simulation for multi component gas mixture containing H_2, CH_4, CO_2 and C_2H_6, feed pressure 20 bar, effect of stage cut on a) retentate composition, b) permeate composition and c) effect of feed pressure on retentate composition [11]

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