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).

\[
\begin{bmatrix}
Q(K) & D(K) & D(K) \\
B(K-2) & Q(K-2) & D(K-2) \\
... & ... & ... \\
B(K) & Q(K) & D(K) \\
... & ... & ... \\
B(K,N-1) & Q(K,N-1) & D(K,N-1) \\
B(K,N) & Q(K,N) & D(K,N) \\
\end{bmatrix}
\begin{bmatrix}
K(K) \\
K(K) \\
... \\
K(K) \\
... \\
K(K,N-1) \\
K(K,N) \\
\end{bmatrix}
= \begin{bmatrix}
0 \\
0 \\
... \\
0 \\
... \\
0 \\
0 \\
\end{bmatrix}
\]

(1)

\[
\sum_{i=1}^{N} \left[ Q(K) \times \left\{ P_i \times X(R) \times Y(K,i) - P_i \times Y(K,i) \right\} \right] = 0
\]

(2)

\[
Y(K,N) = \frac{\sum_{m=1}^{N+1} Q(m) \times XR(m, N+1)}{\sum_{m=1}^{N+1} Q(m) \times XR(m, N+1)} \left(10^{-8}\right)
\]

(3)

\[
\frac{QL(1)}{L(1)} \left(10^{-8}\right) \quad \text{and} \quad \frac{AV(N)}{V(N)} \left(10^{-8}\right)
\]

(4)

\[
l(K,i) = \frac{V(K,i+1) + \frac{V(i)}{Q(K) \times Delta \times P_i} \times l(K,i)}{1 + \left(\frac{V(i)}{Q(K) \times Delta \times P_i} + \frac{P_i \times V(i)}{l(i)}\right)}
\]

(5)

- 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.

\[
\sum_{i=1}^{N} \left[ Q(K) \times \left\{ P_i \times X(R) \times Y(K,i) - P_i \times Y(K,i) \right\} \right] = 0
\]

(2)

\[
2-2- \text{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)
References


9- Pourafshari Chenar M., Soltanieh M., Matsuura T., “Gas permeation properties of commercial polyphenylene oxide and Cardo-type polyimide hollow fiber membranes,” Separation Purification Technology, xxx, 2006 (Received 27 November 2005, Accepted 27 February 2006)


Figure 1- Comparison of experimental results with simulation for CO$_2$/CH$_4$ separation [10]

Figure 2- Comparison of experimental results with simulation for multi component gas mixture containing H$_2$, CH$_4$, CO$_2$ and C$_2$H$_6$, 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]