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Mathematical modelling of membrane gas separation using the finite difference method

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ABSTRACT

Membrane gas separation has been recognized as the main technology that is used in chemical engineering for hydrogen recovery, air separation, natural gas sweetening, helium recovery, natural gas dehydration, and so on. Membrane-based gas separation processes have great potential for these industrial applications because of their environmental friendliness, energy efficiency and ease of scale up. Mathematical modelling of the membrane-based gas separation process can be useful to predict the performance of such separation processes. An improved mathematical model has been implemented in this research for the separation of a binary gas mixture using a membrane separator. The finite difference method (FDM) is applied to predict the membrane gas separation behaviour. The method is helpful as it involves the least effort and computational time because algebraic equations are used instead of differential equations. Different configurations, such as single stage and double stage, are used in this study. The results of the FDM simulation are compared with the simulation results of the model and the experimental data of several membrane systems.

1. Introduction

Gas separation using a membrane is an effective substitute for traditional processes because of its operational ease, economic viability, low maintenance, low energy consumption, small size and dependable performance. Polymeric membranes have established uses in different processes in industry, such as oxygen enrichment of air, recovery of carbon dioxide, volatile organic compound recovery, air dehumidification, helium recovery from natural gas, natural gas sweetening, landfill gas upgrading, nitrogen production, hydrogen recovery from refinery and syngas ratio adjustment, and ammonia synthesis purge gases. Significant hard work has been performed to synthesize membrane materials of high permeability. The complete operating conditions and process design are also vital for the effective and economical application of membrane gas separations [1]. It is challenging to find an effective mathematical technique with an ideal design and operating environment. Modelling and simulation of the membrane gas separation process is a feasible way to obtain important data on the economics, design and operation of the separation process with a low budget. Several features in membrane gas separation, such as economic evaluation, permeation analysis and module design, have been investigated using several forms and structures [2]. Most of the models relate to binary systems, and only a few of them are based on multicomponent systems [3–5]. To overcome the numerical difficulties in solving boundary value problems, numerous changes and different numerical methods have been suggested to solve the model equations [6–8]. The purpose of these models is introducing additional assumptions and simplifying the governing equations that lead to estimated solutions with less computational time and effort.

In the problem of binary gas mixtures, at low permeabilities, the results appear to be inaccurate [9]. Under some operating conditions, the gas diffusion is very fast inside the substrate pores compared to bulk transport [10–13]. The solution requires the estimation of different operating variables, such as the residue concentration at the exit. Asymmetric hollow fibre membranes with a cross flow or co-current configuration were considered for binary gas separation without studying the pressure build-up within the fibre lumen [14,15]. The Runge–Kutta method was used to simplify the problem to an initial value problem to calculate the dependent variable data. A model depending on an initial

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theoretical formulation [16,17] was proposed, and the basic differential equations were solved by applying the orthogonal collocation technique [18]. A system of non-linear equations was reduced by implementing this approach, and a composition profile was used to find the convergence. Substantial information has been reported by different researchers [16,19–27] to discuss the main features in making a pure product with membranes. For several membrane systems, a single-stage configuration is adequate and requires a minimal cost [21,28]. However, other complex designs are financially acceptable as the level and expenditures of the process increase. Numerical solutions for performing separation with a permeate or residue determined that the product recovery and purity could be increased by residue recycling [29].

In this research, a finite difference (numerical) method (FDM) is suggested for asymmetric membranes to solve model equations, which create a boundary value problem. An iterative scheme is implemented, as the quantities at any precise end of the hollow fibre membrane separator were not known. The numerical method is used for several flow conditions. The model results are compared with experimental values, and its robustness is confirmed. The model can be applied to several membrane gas separation systems. Implementing the proposed mathematical model, air separation, natural gas sweetening and helium recovery from natural gas have been studied. Commercially, different values of feed are being used for membrane gas production, as decided by the module configuration and cost of the separation process. The configurations considered here include single-stage and two stages in series. The outcomes are shown in terms of the purity and recovery of a specific gas. There is a complicated relationship between an optimization study and the process parameters or the complex parametric study that is mandatory for good knowledge of the module configurations and economics of the process.

2. Mathematical modelling

The flow direction of the gas streams is parallel and in the opposite direction on both sides of the membrane. Fig. 1 shows the schematic of the countercurrent flow in a membrane separator.

The feed with a specific flow rate Q^f enters the unit and is divided into two streams: Q^p on the permeate side and Q^0 leaving on the residue side. These streams have mole fractions of x_f, y_p and x_o, respectively.

Hence, we can write the overall mass balance as

$$Q^f = Q^p + Q^0 \tag{1}$$

Q^f is the feed flow rate, Q^0 is residue flow rate and Q^p is the permeate flow rate. We can also write the component balance as

$$Q^f x_f = Q^p y_p + Q^0 x_0 \tag{2}$$

The stage cut is defined as

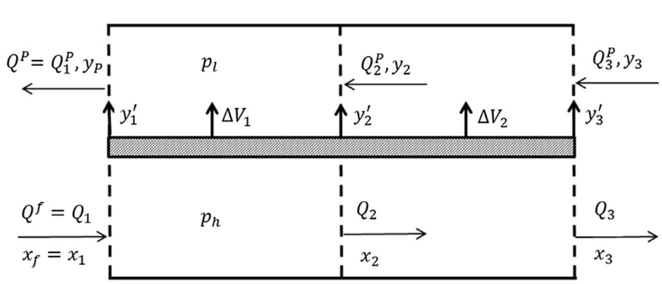

Fig. 1. Schematic of the countercurrent flow in a membrane separator used in FDM.

$$\theta = \frac{Q^p}{Q^f} = \frac{Q^f - Q^0}{Q^f} \tag{3}$$

The ideal separation factor (selectivity) is defined as

$$\alpha = \frac{P_A}{P_B} \tag{4}$$

P_A Is permeability of gas A and P_B is the permeability of gas B.

The pressure ratio is defined as

$$\gamma = \frac{p_l}{p_h} \tag{5}$$

Parameterp_l is the low pressure on the permeate side and p_h is the high pressure on the feed side.

The following assumptions are made during the mathematical modelling.

- The values of permeability are similar to those of the pure species.
- The permeabilities considered are independent of pressure.
- The steady state is assumed.
- The membrane of uniform thickness is considered.
- The total pressure is essentially constant on each side of the membrane.
- There are no concentration gradients in the perpendicular direction of the membrane.
- Plug flow is considered.

Using the finite difference method (FDM) [30] and taking the increment area ΔA_m, the mass balances on both streams can be written as

$$\Delta Q^p = Q_{in} - Q_{out} \tag{6}$$

$\Delta Q^p, Q_{in}$, Q_{out} are the flow rate of the permeate flow of an increment, flow rate entering the increment and flow rate leaving the increment, respectively.

The value of y'_{in} (permeate at the beginning of increment) can be calculated from the equation

$$y'_{in} = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \tag{7}$$

$$a = 1 - \alpha$$

$$b = -1 + \alpha + \frac{1}{\gamma} + \frac{x_{in}}{\gamma}(\alpha - 1)$$

$$c = \frac{-\alpha\, x_{in}}{\gamma}$$

Additionally, the value of y'_{out} (permeate at the end of the increment) is calculated similarly by using x_{out}forx_{in}.

Then, balancing A,

$$\Delta Q^p y'_{av} = Q_{in} x_{in} - Q_{out} x_{out} \tag{8}$$

where

$$y'_{av} = (y_{in} + y_{out})/2$$

Placing Q_{out} from Eq. (6) into (8),

$$\Delta Q^p = Q_{in} \frac{(x_{in} - x_{out})}{(y'_{av} - x_{out})} \tag{9}$$

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