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Modeling and Economic Optimization of a Hollow Fiber Membrane Module for CO_2 Separation Using Collocation Methods and Genetic Algorithms †

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Abstract: Hollow fiber membranes are frequently used to remove CO_2 gas during the gas sweetening process due to their advantages such as cost-efficiency, simplicity of operation and maintenance, and compact size. Permeate flux behavior, which is governed by various factors such as membrane features and operating conditions, has a significant impact on the performance of membrane separation. The majority of existing research studies focused on enhancing the permeability and selectivity of membranes. The configuration and operation of membrane modules have received scant attention in investigation. The geometrical layout and operational parameters of a membrane module were taken into account as a multivariable optimization problem in this study. The total annual cost serves as the objective function. A construction expenditure based on the size of the membrane plant plus an operational expense related to energy usage make up the total cost. The module dimensions (fiber diameter, fiber length, and packing density) and operating conditions (inlet pressure) were taken into consideration as the design factors in the optimization problem. The membrane area and energy consumption, which are directly related to the overall cost, were calculated using a model to simulate the membrane plant. To simulate multicomponent gas transport through hollow fiber modules, a membrane model with a high prediction accuracy was adapted from a previous work and solved numerically using an orthogonal collocation method. The optimization process was carried out using a genetic algorithm. This study also investigated how different parameters affect the overall cost. The accuracy of the self-developed computation program was checked with the results obtained from ChemBrane. The relative difference in the results obtained from our program and ChemBrane is less than 1%, suggesting the applicability of our model and program. The proposed optimization process is able to find the conditions of the module that meet the requirement of CO_2 concentration of effluent while minimizing the cost. The results suggest that the use of polyamides has a lower cost than the use of cellulose acetate membranes.

Keywords: modeling; optimization; CO_2 separation; membrane module; collocation method; genetic algorithm

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1. Introduction

Hollow fiber membranes are frequently used to remove CO_2 gas during the gas sweetening process due to their advantages such as cost-efficiency, simplicity of operation and maintenance, and compact size [1]. Permeate flux behavior, which is governed by various factors such as membrane features and operating conditions, has a significant impact on the performance of membrane separation [2]. The majority of existing research studies focused on enhancing the permeability and selectivity of membranes. The configuration and operation of membrane modules have received scant attention in investigation [3].

In this study, a model was built based on conventional models concerning component flow and pressure drop along a device's length. The Matlab software was utilized for programming the model to determine the solutions using an orthogonal collocation method. The optimization process involved creating an economic objective function derived from the calculations and estimations of both investment and annual operation costs [4]. The optimization of the entire process and a comparison between two membrane materials, cellulose acetate (CA) and polyimide (PI), were conducted by evaluating the annual operating costs. To achieve the objectives of this study, the optimization process employed a genetic algorithm which shows several advantages, including flexibility, stability, and inclusive scanning options, for solving optimization problems [5].

2. Methodology

2.1. Mathematical Model

The model used in this study was adapted from the work described in [4]. The model was built based on several hypotheses, including:

The module operates in a counter-current mode.

The membrane operates under static conditions.

The input flow is directed through the shell of the device to decrease the influence of pressure on membrane deformation. There are no sweep gases utilized in the model simulation.

The entire model operates under isothermal conditions.

On both the inlet and permeate sides, the flow is assumed to be an ideal plug flow.

The details of the mathematical model are as follows:

- Feed side flow rate:

$$\frac{d(u_{xi})}{dz} = n\pi D_o Q_i (P_F x_i - P_P y_i) \tag{1}$$

- Permeate-side flow rate:

$$\frac{d(v_{yi})}{dz} = n\pi D_o Q_i (P_F x_i - P_P y_i) \tag{2}$$

The pressure drop on both sides is estimated using the Hagen–Poiseuille equation [4] as follows:

- Feed-side pressure drop:

$$\frac{dP}{dz} = \frac{192 n D_o (D + n D_o) \mu_m R T u}{\pi (D^2 + n {D_o}^2)^3 P} \tag{3}$$

- Permeate-side pressure drop:

$$\frac{dp}{dz} = \frac{128 \mu_m R T v}{n \pi n {D_i}^4 p} \tag{4}$$

The collocation method was employed as it can discretize systems of ordinary differential equations. The values at the nodes have to satisfy the boundary conditions. A self-developed program was created in Matlab, which runs by using the fsolve tool that is based on Newton's method to facilitate the generation of solutions for such a system.

2.2. Process Simulation

The settings used in the simulation are as follows:

- The simulation is isothermal and maintains a temperature of 30 °C, with a permeate outlet pressure of 1 bar.

- The flow rate is 50 kmol/h.
- The fiber length is 1.2 m, with an inner and an outer diameter of 150 µm and 200 µm, respectively.
- The feed stream is dehydrated, with a 1% N_2 content, and hydrocarbons higher than C_3 are ignored due to their low permeability, as their large kinetic diameter impedes membrane transport.
- According to current technical standards, the maximum CO_2 concentration of the retained stream after the separation process must be less than 2.5%.
- The cross-sectional area of the module housing is twice the total cross-sectional area for hollow fiber membranes.
- The total membrane contact area is optimized to meet the required output CO_2 content, and the design parameters are calculated according to their relationship.
- PI and CA membranes are utilized in the simulation.
- The device shell is the input for the reverse flow structure.

The detail of the process parameters are summarized in Table 1.

Table 1. Case of process simulation.

Case	Components of Feed Current (%)					P_F [bar]
	CO_2	Methane	Ethane	Propane	N_2	
	10.0	77.4	7.7	3.9	1.0	60
Membrane type	Permeability [mol/(m^2.Pa.s)] [6]					
PI	3.283×10^{-8}	1.641×10^{-9}	1.094×10^{-9}	5.469×10^{-10}	3.283×10^{-9}	
CA	1.691×10^{-8}	1.127×10^{-9}	3.758×10^{-10}	3.381×10^{-10}	1.127×10^{-9}	

2.3. Cost Estimation

In the design process of membrane equipment for separating CO_2 from natural gases, it is crucial to consider the economic aspect. The economic costs of such equipment are estimated based on the operating costs and equipment investment costs, while also taking into account annual depreciation and inflation. The objective is to reduce costs while still ensuring the separation efficiency of the entire process. To optimize this objective, the process implements genetic algorithms to determine the most suitable solution. By comparing between two types of membranes, CA and PI, it is found that the search range and variable range can vary depending on the stated objective, while also considering which type of membranes gives the best separation efficiency at the lowest cost.

Operating costs: The proposed system's operating costs mainly come from the energy consumption of the compressor (E). Assuming the number of operating hours is 8000 h per year (corresponding to 24 h/day for 333 days), the energy cost ($OPEX$) of the system at an industrial electricity price of \$0.0934/kWh [7] is

$$OPEX = 0.0934 \times E \times 8000$$

Investment costs: These costs include the cost of buying the compressor, the cost of constructing the membrane module, and the cost of purchasing ancillary equipment.

Compressor purchase cost (C_{TM}): This cost was calculated according to the economic model described in [8]. Setting a service life of 20 years, the estimated initial purchase cost (C_p) of a machine with a capacity of 450–3000 kW under standard conditions using the CAPCOST tool [9] is

$$\log_{10} C_p = 2.2891 + 1.3604 \log_{10} E - 0.1027 (\log_{10} E)^2$$

To calculate the total investment (C_{TM}), the coefficients of 15.9 (adjusted for high-pressure operation using nickel-based materials) and 1.18 (taxes and installation costs) and

p_1 (inflation rate) = 1.2687 were added according to the CEPCI 2021/2017 [10]; the following formula is obtained:

$$C_{TM} = 1.18 \times 15.9 \times p_1 \times C_p$$

Membrane module cost (C_m): This cost was calculated based on membrane area A. This factor greatly depends on the design parameters of the device and the type of membrane used. A membrane has a lifespan of 5 years, and the value of a m^2 membrane is in the range of USD 40–200. A common value of USD 200/m^2 was selected.

Cost of auxiliary equipment: Sethi [11] divides the components of a membrane system into 4 groups and provides the calculation for the investment costs of each group as follows:

1. Piping and valves:

$$C_{PV} = 6000\ A^{0.42}$$

2. Control tools:

$$C_{IC} = 1500\ A^{0.66}$$

3. Frame and wall of the equipment:

$$C_{TF} = 3100\ A^{0.53}$$

4. Other auxiliary:

$$C_{MI} = 8000\ A^{0.57}$$

Based on the above investment costs, the annual replacement cost (CRC) is estimated as follows:

$$CRC = 0.02 \times (C_{TM} + p_1 \times (C_{PV} + C_{IC} + C_{TF} + C_{MI}))$$

The objective function of the optimization problem is as follows:

$$F = OPEX + CRC$$

2.4. Optimization Using a Genetic Algorithm

Considering that the model operates under static conditions, the variables related to the optimization process include the following:

Design variables: hollow fiber inner diameter, hollow fiber length, and feed flow pressure.

Fixed variables: feed flow rate, separation flow outlet pressure, and osmolality of each component.

The optimization problem parameters and investigation range are summarized in Table 2.

Table 2. Optimal problem parameters and investigation range.

Parameter	Value
Flow rate (mol/s)	125/9
Permeate outlet pressure (Pa)	100,000
Feed pressure (Pa)	4,000,000–9,000,000
Fiber inner diameter (m)	0.0001–0.0003
Fiber length (m)	0.5–2

Dependent variable: this variable is calculated based on the relationship between the parameters, including the number and the outer diameter of the hollow fiber used.

In this study, the optimization problem was built based on the process simulation case of the membrane model to separate CO_2 from natural gases, and the original hypotheses were kept. The output results must meet the technical requirements of CO_2 concentration with the lowest operating cost.

The objective function of the problem is as follows:

$$\min(F) = OPEX + CRC$$

The parameters of the genetic algorithm are as follows: the population size is set to 100, with the selection operator following the rotation method. The hybridization operator uses the one-point cutting mechanism, and the probability of cross-matching is 1.0. The mutation operator has a probability of 0.3, and the number of generations is set at 100.

To minimize the total annual cost, a fitness function was defined:

$$\text{fitness} = \left\{ \begin{matrix} 0, & \text{if the anual total cost } > 5 \times 10^6\,\$ \\ 5 \times 10^6\,\$ - \text{anual total cost}, & \text{otherwise} \end{matrix} \right\}$$

3. Results and Discussions

The simulation results of the self-developed program were compared with the results obtained from ChemBrane, which are presented in [4]. Based on the comparison results, the program gives accurate results with an acceptable level of error (the relative difference is in the range of 5%). In general, the model can be applied in the prediction and simulation of gas separation.

Optimization of the process was achieved by varying the design parameters, such as pressure (ranging from 40 to 90 bar), fiber inner diameter (ranging from 100 to 300 µm), and fiber length (ranging from 0.5 to 2 m). The operating mode is under a counter-current flow. The optimal results for both the CA and PI membranes are presented in Figures 1 and 2, respectively.

The lowest operating cost obtained using the CA membrane is 2615 $\times$ 10^6 USD/year, under the operating conditions of 40 bar in terms of pressure, 297.65 µm for the inner diameter, and a hollow fiber length of 0.5 m. The membrane area used is 3,350,830 m^2, and the final product's CO_2 concentration is at 2.506, meeting the process's technical requirements.

With the PI membrane, the optimal solution results in the lowest operating cost of 2575 $\times$ 10^6 USD/year. The device operates at a pressure of 40 bar, and has a fiber diameter of 300 µm and a fiber length of 0.5176 m. The membrane area used is 1,753,258 m^2, and the final product's CO_2 concentration is at 2.498, meeting the technical requirements.

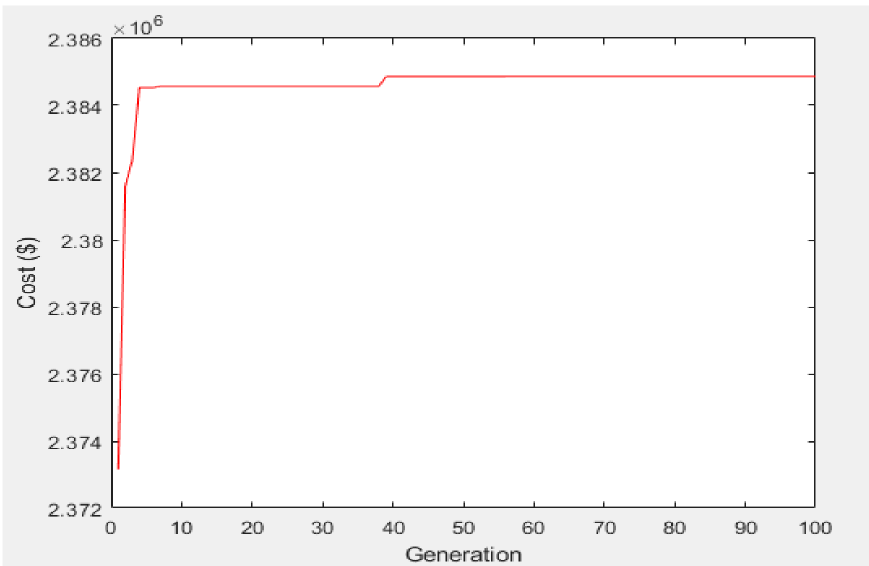

Figure 1. Optimizing operating costs for CA membrane equipment.

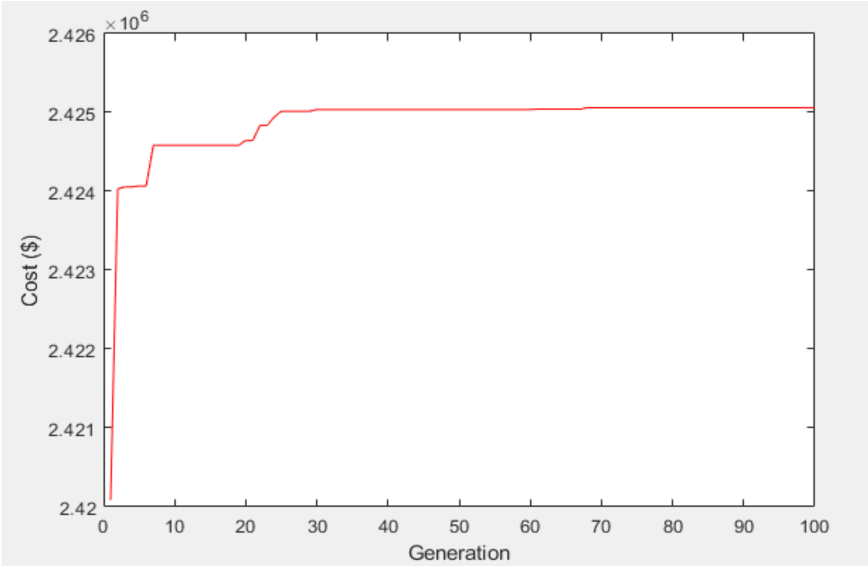

Figure 2. Optimizing operating costs for PI membrane equipment.

Comparing the annual operating costs of the two membranes, it can be concluded that using PI membranes is much more cost-effective than using CA membranes. The membrane area used decreases by 1,597,572 m^2 or approximately 47.68%, resulting in the cost savings of approximately 40,000 USD/year. A PI membrane has good separation efficiency and high optimization, making it the preferred choice to use in CO_2 separation projects, especially for gas separation projects of the same type.

4. Conclusions

The present study involves the simulation of a hollow fiber membrane device. An system of ordinary differential equations was devised for precise modeling of the membrane module. The equations take into account varying flow properties along the membrane and the associated drop in pressure. An economic model that encompasses both capital and operating costs was utilized to evaluate the performance of the membrane plant. This study focused on analyzing the impact of the operating and design parameters, such as the inlet pressure and membrane module geometry, on the economic costs of membrane application. Furthermore, these parameters were scrutinized for two types of membrane materials to understand their influencing trends. Optimization using a genetic algorithm determined that the system should employ PI membranes, operated at optimal pressures and design parameters. However, further investigation is warranted to obtain a more comprehensive understanding of the optimization problem while considering all other relevant parameters. This study underscores the importance of designing, selecting, and implementing strategies in line with the process and permeation flow requirements and their interaction with system parameters. The methodology presented in this work can be extended to the general design of a given process based on the governing equations.

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