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

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Abstract. The hollow fiber membrane is frequently used to remove CO_2 gas in gas sweetening process due to its advantages such as cost-effiency, simplicity of operation and maintenance, 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 current research focuses on enhancing the permeability and selectivity of membranes. The configuration and operation of the membrane module have received scant attention in investigations. The geometrical layout and operational parameters of a membrane module are taken into account as multivariable optimization problem in this study. The annual cost serves as the objective function. A construction expenditure based on the size of the plant plus an operational expense related to energy usage make up the cost. The module dimensions (fiber diameter, fiber length, packing density) and operating conditions (inlet pressure) were taken into consideration as design factors in the optimization problem. The membrane area and energy consumption, which are directly related to the overall cost, are calculated using the model to simulate the membrane plant. To simulate multicomponent gas transport through hollow fiber modules, a membrane model with high prediction accuracy is adapted and solved numerically using collocation methods. The optimization is carried out using the genetic algorithm. It is also discussed 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 between our program and ChemBrane is less than 1%. It suggests the applicability of our model and program. The optimization problem is finding the condition of the module that meet the requirement of CO_2 concentration of the effluent while minimizing the cost. The results suggest that the use of polyamide consumes lower cost than cellulose acetate membrane.

1. INTRODUCTION

The hollow fiber membrane is frequently used to remove CO_2 gas in gas sweetening process due to its advantages such as cost-effiency, simplicity of operation and maintenance, 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 current research focuses on enhancing the permeability and selectivity of membranes. The configuration and operation of the membrane module have received scant attention in investigations [3].

In this study, a model is built based on conventional models concerning component flow and pressure drop along the device's length. The Matlab software was utilized for programming the model to determine solutions using orthogonal collocations method. The optimization process involves creating an economic objective function derived from 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, the optimization employed a genetic algorithm that has several benefits, including flexibility, stability, and inclusive scanning options for the optimization problem [5]

2. METHODOLOGY

2.1. Mathematical model

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

The module operate in counter-current mode.

The membrane operates in a static condition.

The input flow is directed through the shell of the device to decrease the pressure's influence 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 ideal plug flow.

The details of the mathematical model are as follows.

Feed side flow rate:

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

In which,

Permeate side flow rate:

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

The pressure drop in both side is estimated using Hagen–Poiseuille equation [4]:

Feed side pressure drop:

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

Permeate side pressure drop:

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

The collocation method was employed to discretize the system of ordinary differential equations. The values at the nodes have to sastify the boundary conditions. A program was self-developed in Matlab and runs the fsolve tool that bases on Newton's method for facilitating the solution of the 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 1.2m, with inner and outer diameters of 150μm and 200μm, 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 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 fibers.
- The total membrane contact area is optimized to meet the required output CO_2 content, and design parameters are calculated through their relationship.
- The PI and CA membranes are utilized in the simulation.
- The device shell is the input for the reverse flow structure.

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}Pas)] [6]					
PI	3.283e-8	1.641e-9	1.094e-9	5.469e-10	3.283e-9	
CA	1.691e-8	1.127e-9	3.758e-10	3.381e-10	1.127e-9	

2.3. Cost estimation

In the design process of membrane equipment for separating CO_2 from natural gas, the economic aspect is crucial to consider. The economic problem of this equipment is built 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 problem implements genetic algorithms in determining the most suitable solution. Comparing between two types of membranes, CA and PI, the search range and variable survey can vary depending on the stated objective, while also considering which membrane gives the best separation efficiency at the lowest cost.

Operating costs: the system mainly comes from the energy consumption of the compressor. Assuming the number of operating hours is 8000h per year (corresponding to 24h/day during 333 days), the energy cost (OPEX) of the system at the industrial electricity price of $0.0934/kWh [7] is:

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

Investment cost: includes the cost of buying the compressor, the cost of the membrane module and the cost of ancillary equipment.

Compressor purchase cost (C_{TM}): 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:

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

To calculate the total investment (CTM), add the coefficients 15.9 (adjusted for high-pressure operation using nickel materials), 1.18 (taxes and installation costs) and pl (inflation rate) = 1.2687 according to CEPCI 2021/2017 [10], the following formula is obtained:

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

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

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

1. Piping and valves:

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

2. Control tools:

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

3. Frame and wall of equipment:

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

4. Other auxiliary:

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

From the investments, the annual replacement cost of CRC is estimated as follows:

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

The objective function of the problem:

$F = OPEX + CRC$

2.4. Optimization by Genetic Algorithm

Considering the model operating under static conditions, the variables related to the optimization process include:

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

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

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

Build the optimal problem based on process simulation case of the membrane model to separate CO_2 from natural gas and keep the original hypotheses. Output results must meet the technical requirements of CO_2 concentration with the lowest operating cost.

The objective function of the problem:

$\min(F) = OPEX + CRC$

The parameters of genetic algorithm is as follows: the population size is set to 100, with the selection operator following the rotation method. The hybridization operator uses the one-point cut 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.

Due to the minimization of the annual total cost, the fitness fuction was defined as:

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

Table 1 Optimal parameters and survey range

Parameter	**Value**
Flow rate (mol/s)	125/9
Permeation outlet pressure (Pa)	100000
Feed pressure (Pa)	4000000-9000000
Fiber inner diameter (m)	0.0001-0.0003
Fiber lenght (m)	0.5-2

3. ResultS and discussionS

The simulation results of the self-developed program are compared with the results obtained from ChemBrane which is presented in [4]. From 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 prediction and simulation in gas separation.

Optimization of the process is achieved by varying 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 2m). The operating mode is counter-current flow. The optimal results for both CA and PI membranes are presented in Figure 5 and Figure 6, respectively.

The lowest operating cost obtained using CA membrane is 2,615*10^6 USD/year, under the operating conditions of 40 bar pressure, 297.65 µm inner diameter, and a hollow fiber length of 0.5m. The membrane area used is 335,0830 m^2, and the finished product CO_2 concentration is at 2.506, meeting the process's technical requirements.

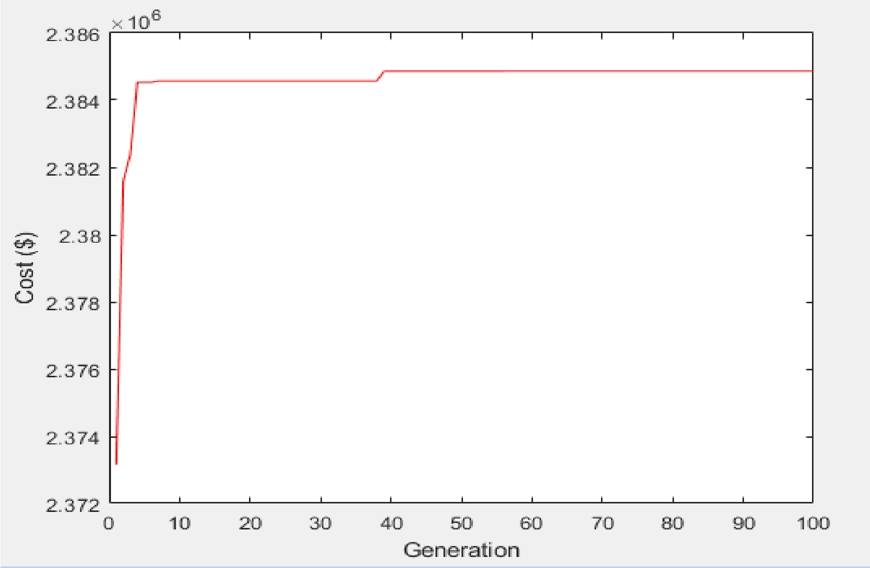

Figure 1 Optimizing operating costs for CA membrane equipment

With PI membrane, the optimal solution resulted in the lowest operating cost of 2,575*10^6 USD/year. The device is operating at a pressure of 40 bar, a fiber diameter of 300 µm, and a fiber length of 0.5176 m. The membrane area used is 175,3258 m^2, and the finished product CO_2 concentration is at 2.498, meeting the technical requirements.

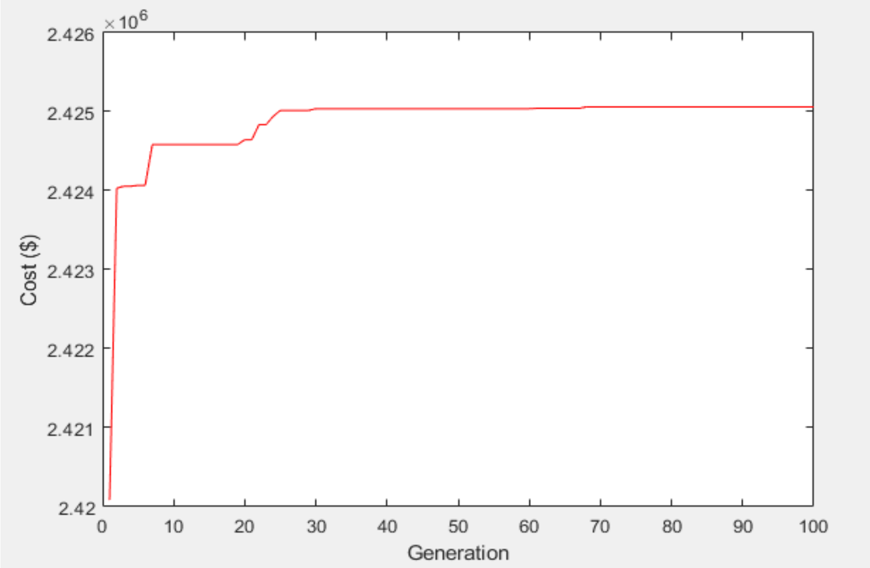

Figure 2. Optimizing operating costs for PI membrane equipment.

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 decreased by 159,7572 m^2 or approximately 47.68%, resulting in cost savings of approximately 40,000 USD/year. The PI membrane has good separation efficiency and high optimization, making it the preferred choice 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 elaborate system of conventional differential equations has been devised for precisely modeling the membrane modulus. The equations take into account the varying flow properties along the membrane and the associated drop in pressure. An economic model that encompasses both capital and operating costs was utilized for evaluating the performance of the membrane plant. The study focused on analyzing the impact of operating and design parameters, such as inlet pressure and membrane module geometry, on the membrane application's economics. Furthermore, these parameters were scrutinized for two types of membrane materials to understand their influence trends. Optimization using genetic algorithms determined that the system should employ PI material 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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References

1. Bernardo P. and Drioli E., *Membrane gas separation progresses for process intensification strategy in the petrochemical industry.* Petroleum Chemistry, 2010. **50**(4): p. 271-282.
2. Nguyen T.-A., Yoshikawa S., and Ookawara S., *Steady State Permeate Flux Estimation in Cross-Flow Ultrafiltration of Protein Solution.* Separation Science and Technology, 2014. **49**(10): p. 1469-1478.
3. Mores P.L., Arias A.M., Scenna N.J., Caballero J.A., Mussati S.F., and Mussati M.C., *Membrane-Based Processes: Optimization of Hydrogen Separation by Minimization of Power, Membrane Area, and Cost.* Processes, 2018. **6**(11): p. 221.
4. Chu Y., Lindbråthen A., Lei L., He X., and Hillestad M., *Mathematical modeling and process parametric study of* CO_2 *removal from natural gas by hollow fiber membranes.* Chemical Engineering Research and Design, 2019. **148**: p. 45-55.
5. Mitchell M., *Genetic Algorithms: An Overview*, in *An Introduction to Genetic Algorithms*. 1998, The MIT Press. p. 1-31.
6. Baker R., *Future directions of membrane gas-separation technology.* Membrane Technology, 2001. **2001**(138): p. 5-10.
7. U.S. Energy Information Administration, *Monthly Electric Power Industry Report.* 2023: Washington, DC 20585.
8. He X., Chu Y., Lindbråthen A., Hillestad M., and Hägg M.-B., *Carbon molecular sieve membranes for biogas upgrading: Techno-economic feasibility analysis.* Journal of Cleaner Production, 2018. **194**: p. 584-593.
9. Turton R., Shaeiwitz J.A., Bhattacharyya D., and Whiting W.B., *Analysis, Synthesis, and Design of Chemical Processes*. 2018: Prentice Hall.
10. Maxwell C. *Cost Indices*. 2023 Available from: https://toweringskills.com/financial-analysis/cost-indices/.
11. Sethi S., *Transient permeate flux analysis, cost estimation, and design optimization in crossflow membrane filtration*. 1997, Rice University.