Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale,
Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

System scale design and mesoscale modeling for natural gas dehydration process

Zhehao Jin[a], Zhongde Dai[b], and Yiyang Dai[a]*

[a] Sichuan University, School of Chemical Engineering, Chengdu, Sichuan Province, China.
[b] Sichuan University, School of Carbon Neutrality Future Technology, Chengdu, Sichuan Province, China.
* Corresponding Author: daiyy@scu.edu.cn.

ABSTRACT

Triethylene glycol (TEG) or mono-ethylene glycol (MEG) absorption are the commercial technologies for natural gas dehydration processes. Nevertheless, the necessity of regenerating solvents under high temperatures results in environmental footprint and complex operation. Membrane with advantages in small footprint and high feasibility operation in hostile conditions is considered as promising technology for natural gas dehydration processes. In this work, system scale design and mesoscale modelling are synchronously adopted to optimize natural dehydration process design. Aspen HYSYS with ChemBrane extension is used for natural gas dehydration process. Taking pressure ration, membrane area and sweep gas flowrate as decision variables for minimizing specific process cost is optimized through NSGA-II algorithms. The minimum specific cost of < 3.06×10^{-2} \$/m^3 natural gas is estimated to achieve the separation requirement of <100 ppm. Then, the module length, and membrane thickness of the hollow fiber membrane design is investigated using Computational fluid dynamics (CFD), which better configures the simulation results and concentration, velocity profile to analyze the simulation results. The system scale engineering design and mesoscale modelling provide an in-depth insight into natural gas dehydration process.

Keywords: Natural gas dehydration, System scale design, Mesoscale design

1. INTRODUCTION

Natural gas (NG) proves to be a notably secure energy commodity during its transportation, storage and utilization processes [1]. Natural gas must be dried before enters distribution pipelines, otherwise it may corrode pipelines or form hydrocarbon [2]. Triethylene glycol (TEG) or mono-ethylene glycol (MEG) absorption are the commercial method for NG dehydration. However, the volatile organic compounds especially benzene, toluene, ethylbenzene, and xylenes will vent during absorption processes [3] and complex operating and control system restrict its application in remote and harsh environment [4,5]. Gas separation membrane with small footprint and no necessity for frequent parameter adjustments [6,7] is an attractive alternative for natural gas dehydration.

At the laboratory scale, the selectivity of water/methane can reach several thousand or even tens of thousands [8–12]. The gutter layer exists in membrane shows significant resistance to water vapor permeation which leads to the disparity in selectivity between laboratory-scale and pilot-scale conditions[13]. Lin et al. [13]evaluated a spiral-wound module for natural gas dehydration processes, results show that a low selectivity of 47 at 30-60 bar under field testing. However, the optimization of crucial parameters such as pressure ratio, sweep gas flowrate, and membrane area was not addressed in the aforementioned researches. He et al. conducted a hybrid membrane process for natural gas dehydration and sweeting, sensitivity analysis taking outlet pressure of each stage membrane as decision variable to minimize the specific NG processing cost. The research gap exists in the impact of flow and diffusion patterns of membrane is not been fully conducted.

In this work, a system scale design using Aspen HYSYS software with ChemBrane [14,15] extensions is used for natural gas dehydration process modeling, and pressure ratio, sweep gas flowrate, membrane area as decision variables to minimize the processing cost. The fluid

dynamic simulation of gas separation membranes is modeled by coupling laminar flow module and transport of concentrated species module. The effect of velocity distribution field and concentration field at the mesoscale on membrane efficiency are discussed.

2. METHODLOGY

2.1 Simulation basis

The natural gas produced from a natural gas processing plant in Qinghai Province, China. The natural gas with a total molar flowrate of 2571.29 kmol/h in water saturated at 308K, 4500kPa. The water content in the residue side of the gas separation membrane system must below 100ppm. Aspen HYSYS in conjunction with ChemBrane [15] was used to simulate the process conditions. The membrane used has a water vapor permeance of 983 gpu and water/methane selectivity of 47, the detailed information of other components permeance is shown in Table 2. The system scale design minimizes the specific cost of the natural gas dehydration process, taking pressure ratio, membrane area, and sweep gas flowrates as decision variables. Furthermore, the mesoscale design delves into the influence of parameters such as the inner and outer diameter and aspect ratio of the membrane on its performance. By examining the influence of different parameters across two distinct scales on membrane performance, aim to provide enhanced guidance for membrane structural design and industrial parameter selection.

Table 1. Typical compositions of gas streams at natural gas processing plant.

Component	Molar flowrate(kmol/h)	Molar fraction (%)
Methane	2502.5	0.9733
Ethane	1.77	0.0007
Propane	0.64	0.0003
Hydrogen	0.10	0.00004
Water	3.74	0.0015
Carbon dioxide	18.61	0.0072
Nitrogen	36.05	0.014
Helium	0.15	0.00006
Oxygen	7.70	0.003

Table 2. Gas permeance of membranes.

Component	Gas permeance(mol(STP)/(m^2·h·kPa))
Methane	0.023
Ethane	0.046
Propane	0.071
Water	1.217

2.2 System scale Design

2.2.1 Process description

Natural gas dehydration process was conducted by HYSYS integrated with ChemBrane unit. The natural gas with saturated water content is gradually condensed through the cooler and then introduced into a gas-liquid separator to remove condensed water and heavy hydrocarbons. Subsequently, sent to the dehydration membrane unit, where the nitrogen gas used as sweep gas. The membrane unit operated in counter-current form and outlet natural gas water content need be less than 100 ppm. By system design, the appropriate pressure ratio, membrane area, and sweep gas flowrates can be determined to maximize the process economics. However, the system design is unable to determine parameters such as the inner and outer diameter thickness, aspect ratio, and distribution form of the membrane.

2.2.3 Process parameters optimization

The most critical parameters in gas separation membranes unit are pressure ratio, sweep gas flowrate, and membrane area, as these factors directly determine the hydrocarbon loss and cost associated with dehydration processes. The membrane cost of \$50 per m^2 was used to estimate the dehydration membrane unit cost and a life time of the membrane was 5 years [14]. The cost functions regarding the heat exchanger, and separator are neglected. An annual interest rate of 7% was used for the calculation of annual capital cost. The price of electricity is 0.05\$/kWh used for operating cost of the compressors. The specific process cost model is shown in equation (1) [16].

$$CC^s = \frac{Capital\ related\ cost + OPEX}{Total\ NG\ production} \quad (1)$$

Figure 1. displays the schematic diagram of the optimization process. The range of variables is initially obtained through sensitivity analysis. Subsequently, generate the initial values of variables and input into the Aspen HYSYS software. Optimize the specific process cost while ensuring outlet natural gas water content is below 100 ppm. Provided that the obtained values do not meet the pre-defined criteria, the new parameters will be generated for next iteration.

2.3 Mesoscale modeling

2.3.1 Computational fluid dynamic (CFD) simulation model

To date, the CFD simulation about natural gas dehydration process through membrane technology has not been reported. The optimized parameter values obtained through system design are incorporated into CFD model. In system design, the calculation can be performed by inputting the defined membrane area. At the CFD scale, the impact on membrane performance can be investigated by adjusting parameters such as the inner and outer

diameters, aspect ratio, and distribution of individual hollow fiber membranes. Modeling the mass transfer process and flow pattern of natural gas dehydration using the COMSOL software. Figure 2. illustrates the membrane structure in the simulations, encompassing the feed gas side, selective membrane, porous layer, and permeate side. The simulation process is conducted with the utilization of laminar flow module and transported of the concentrated spices. Given that the flow patterns and diffusion characteristics of the gas significantly influence this process, it is crucial to preserve the reliability of the flow pattern and diffusion mechanisms while simplifying the model. The following assumptions are considered during modeling.

1. The modeling is under steady-state conditions and in adiabatic conditions;
2. The diffusion mechanism is Fick's law;
3. The simulated fluid is Newtonian-type fluid and adheres to the ideal gas assumption;
4. The driving force for the transportation is pressure difference between feed and permeate side;
5. Hollow fiber membrane has uniform outer and inner diameters.

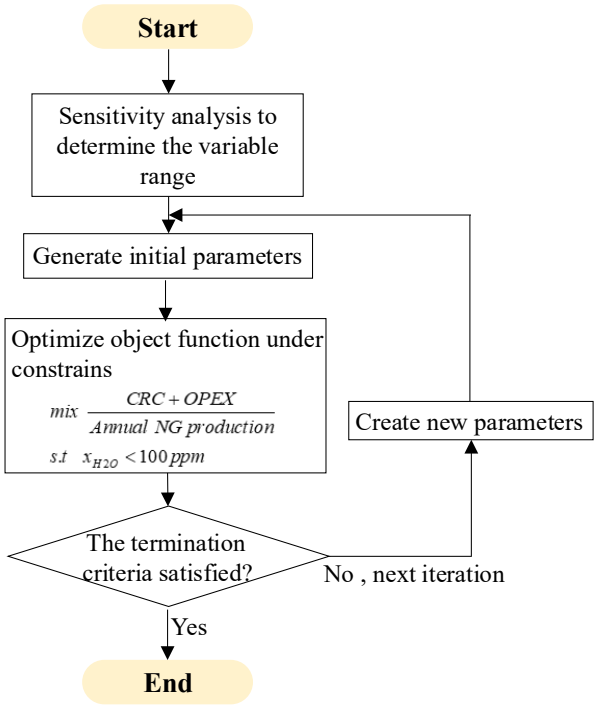

Figure 1. Schematic diagram of optimization process.

2.3.2 Numerical methods

The natural gas dehydration membrane modeling governing equation with the boundary conditions were solved utilizing COMSOL Multiphysics (6.2) software with the finite element method. Figure 2. displays the detailed mesh partitioning of the modeling, encompassing 404,487 degrees of freedom. The time required to solve a set of governing equations is 180 seconds. Table 3. presents pivotal parameters in CFD simulations, including the temperature and pressure distribution in both side of the membrane [17].

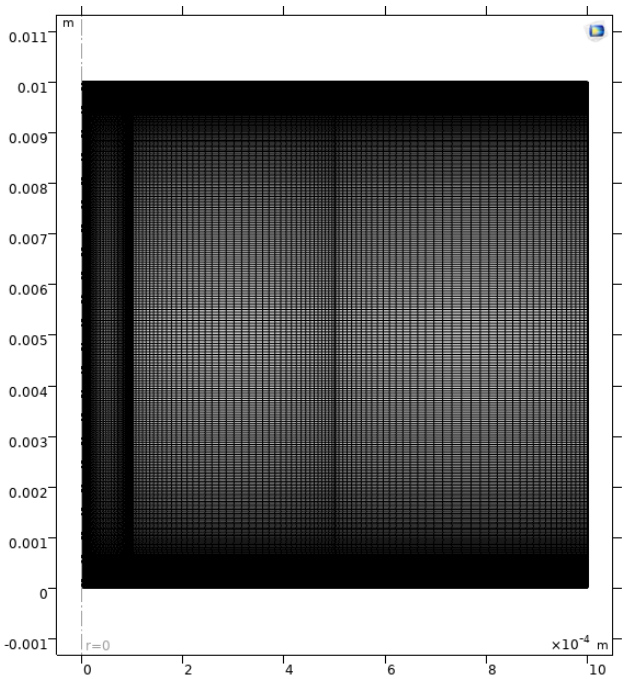

Figure 2. Mesh partitioning of the proposed model.

Table 3. The key input parameters for the proposed model.

Parameters	Value	units
Temperature of inlet gas	323	K
Pressure of feed	45	Bar
Pressure of sweep gas	0.8	Bar
Permeance of CH_4	0.023	mol(STP)/(m^2·h·kPa)
Permeance of H_2O	1.217	mol(STP)/(m^2·h·kPa)
Diffusion coefficients of CH_4	2.32×10^{-5}	m^2/s
Diffusion coefficients of H_2O	1.66×10^{-5}	m^2/s
Dynamic viscosity of CH_4	1.058×10^{-5}	Pa·s
Dynamic viscosity of H_2O	1.3×10^{-5}	Pa·s

3. RESULTS AND DISCUSSION

3.1 Process parameters optimization results

The optimization process selects specific costs as the objective function, using pressure ratio, membrane area, and sweep gas usage as decision variables, and applies the NSGA-II algorithm for optimization. The optimization range of decision variables is determined based on the results of sensitivity analysis.

Table 4. Decision variables ranges of the optimization process.

Decision variables	Optimization range
Pressure ratio	[30,60]
Membrane area	[650,950]
Sweep gas flowrate	[150,300]

The optimization process involves selecting the point with the minimum process cost to be incorporated into the operation. In this case, the permeate pressure is 0.8 bar, the membrane area is 850 $m^{2,}$ and the amount of sweep gas used is 150 kmol/h.

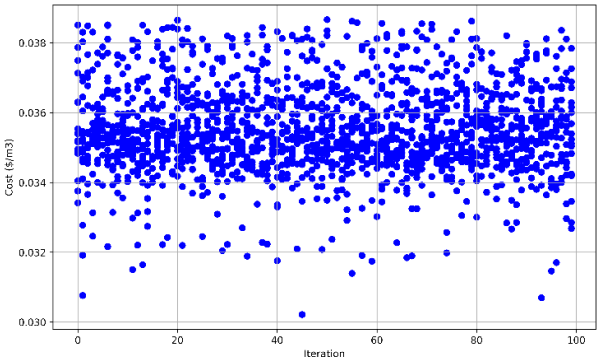

Figure 3. Optimization process scatter distribution.

At 4500 kPa, saturated natural gas passes through heat exchanger 1 (HX-1) and heat exchanger 2 (HX-2) to gradually lower the temperature before being sent to the gas-liquid separator (Sep). After removing condensate water and some heavy hydrocarbons, the gas is warmed up by HX-1 and then directed into a gas separation membrane unit for deep dehydration. By incorporating optimized parameters into the model, the water content in the outlet natural gas is 96 ppm, meeting the dehydration requirements, with a hydrocarbon loss rate of 3.00% and the specific cost of the process is 0.0306 $/$m^3$.

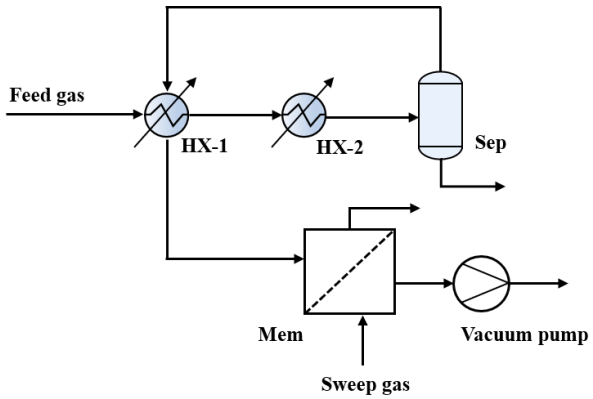

Figure 4. The flowchart of the natural gas dehydration process.

3.2 CFD simulation results

The velocity field and concentration field of water profile in the gas separation membrane are shown in Figures 5-6.

The velocity profile exhibits a parabolic distribution form, with the maximum flow velocity of 0.063m/s at the center of the pipe, while the velocity is reduced to 0.023m/s at the pipe wall due to the frictional force acting between the membrane selective layer. Furthermore, it is evident that the velocity remains undeveloped at the entrance zones of the feed side, with full development occurring as distance from the entrance increases. This observation underscores the significance of inlet effects on fluid flow hydrodynamics on the feed side. The velocity distribution on the shell side is determined through the solution of the Navier-Stokes equations and material balance equations.

Figure 6. describes the water concentration in the feed side of the feed side. The molar concentration of water in the natural gas feedstock decreased from 1.2 mol/m^3 to 0.18 m^3/s at the outlet, successfully meeting the dehydration requirement of less than 100 ppm in the outlet natural gas. Moreover, the dehydration process exhibited a rational design as evidenced by the gradient changes in concentration curve, which showed good consistency with simulations performed using Aspen HYSYS software.

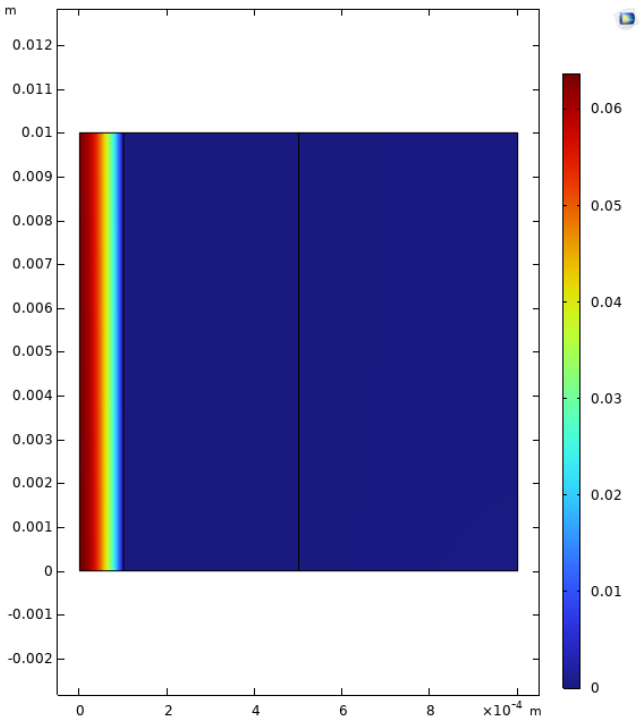

Figure 5. Field of velocity in the gas separation membrane

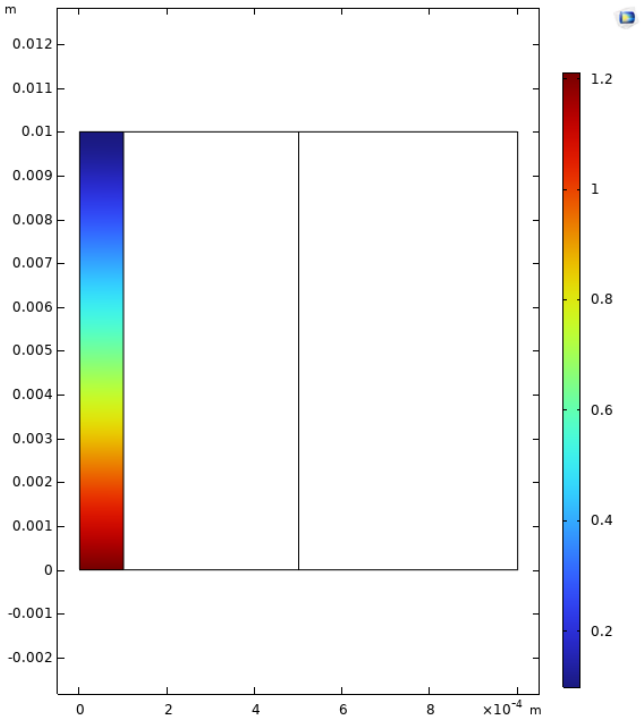

Figure 6. Concentration field of water in the feed side of the gas separation membrane.

4 CONCLUSION

The study employs a simultaneous approach of system scale design and mesoscale modeling to enhance the efficiency of natural dehydration process design. The natural gas dehydration process is conducted using Aspen HYSYS with ChemBrane extension. Decision variables such as pressure ratio, membrane area, and sweep gas flowrate are considered to minimize the specific process cost through optimization with NSGA-II algorithms. A minimum specific cost of 3.06×10-2 $/m^3 natural gas is projected to meet the separation requirement of 100 ppm. Subsequently, Computational Fluid Dynamics (CFD) is utilized to analyze the hollow fiber membrane design from the velocity and concentration profile, resulting in improved simulation outcomes. The integration of system scale engineering design and mesoscale modeling offers a comprehensive understanding of the natural gas dehydration process.

ACKNOWLEDGEMENTS

The authors would like to thank the Sichuan Science and Technology Program for their financial support (Grant No. 2021YFH0116).

REFERENCES

1. S. Faramawy, T. Zaki, A.A.-E. Sakr, Natural gas origin, composition, and processing: A review, Journal of Natural Gas Science and Engineering 34 (2016) 34–54. https://doi.org/10.1016/j.jngse.2016.06.030.
2. X. He, I. Kumakiri, M. Hillestad, Conceptual process design and simulation of membrane systems for integrated natural gas dehydration and sweetening, Separation and Purification Technology 247 (2020) 116993. https://doi.org/10.1016/j.seppur.2020.116993.
3. K. Ohlrogge, J. Wind, T. Brinkmann, Membrane Technology for Natural Gas Processing, in: 2002: p. SPE-75505-MS. https://doi.org/10.2118/75505-MS.
4. K. Dalane, Potential applications of membrane separation for subsea natural gas processing: A review, Journal of Natural Gas Science and Engineering (2017).
5. H. Lin, S.M. Thompson, A. Serbanescu-Martin, J.G. Wijmans, K.D. Amo, K.A. Lokhandwala, T.C. Merkel, Dehydration of natural gas using membranes. Part I: Composite membranes, Journal of Membrane Science 413–414 (2012) 70–81. https://doi.org/10.1016/j.memsci.2012.04.009.
6. R.W. Baker, K. Lokhandwala, Natural Gas Processing with Membranes: An Overview, Ind. Eng. Chem. Res. 47 (2008) 2109–2121. https://doi.org/10.1021/ie071083w.
7. R.W. Baker, Future Directions of Membrane Gas Separation Technology, Ind. Eng. Chem. Res. 41 (2002) 1393–1411. https://doi.org/10.1021/ie0108088.

8. M. Mulder, Basic principles of membrane technology, Springer science & business media, 2012.
9. V. Barbi, S.S. Funari, R. Gehrke, N. Scharnagl, N. Stribeck, SAXS and the Gas Transport in Polyether-b lock-polyamide Copolymer Membranes, Macromolecules 36 (2003) 749–758.
10. S.J. Metz, M.H.V. Mulder, M. Wessling, Gas-permeation properties of poly (ethylene oxide) poly (butylene terephthalate) block copolymers, Macromolecules 37 (2004) 4590–4597.
11. T. Watari, H. Wang, K. Kuwahara, K. Tanaka, H. Kita, K. Okamoto, Water vapor sorption and diffusion properties of sulfonated polyimide membranes, Journal of Membrane Science 219 (2003) 137–147.
12. J.S. Chiou, D.R. Paul, Gas permeation in a dry Nafion membrane, Industrial & Engineering Chemistry Research 27 (1988) 2161–2164.
13. H. Lin, S.M. Thompson, A. Serbanescu-Martin, J.G. Wijmans, K.D. Amo, K.A. Lokhandwala, B.T. Low, T.C. Merkel, Dehydration of natural gas using membranes. Part II: Sweep/countercurrent design and field test, Journal of Membrane Science 432 (2013) 106–114. https://doi.org/10.1016/j.memsci.2012.12.049.
14. X. He, Y. Chu, A. Lindbråthen, M. Hillestad, M.-B. Hägg, Carbon molecular sieve membranes for biogas upgrading: Techno-economic feasibility analysis, Journal of Cleaner Production 194 (2018) 584–593. https://doi.org/10.1016/j.jclepro.2018.05.172.
15. D. Grainger, Development of carbon membranes for hydrogen recovery, (2007).
16. Y. Chu, X. He, Process Simulation and Cost Evaluation of Carbon Membranes for CO2 Removal from High-Pressure Natural Gas, Membranes 8 (2018) 118. https://doi.org/10.3390/membranes8040118.
17. D.J. Jasim, T.J. Mohammed, H.N. Harharah, R.H. Harharah, A. Amari, M.F. Abid, Modeling and Optimal Operating Conditions of Hollow Fiber Membrane for CO2/CH4 Separation, Membranes 13 (2023) 557. https://doi.org/10.3390/membranes13060557.