Sigma J Eng & Nat Sci 35 (1), 2017, 35-45

Sigma Journal of Engineering and Natural Sciences
Sigma Mühendislik ve Fen Bilimleri Dergisi

Research Article / Araştırma Makalesi

DEVELOPMENT OF USER-DEFINED EXTENSION FOR THE SIMULATION OF MEMBRANE PROCESS IN ASPEN HYSYS

Muhammed AHSAN*[1], Olivia Meyonette SWEENEY[2], Arshad HUSSAIN[3]

[1,3]School of Chemical & Materials Engineering, National University of Sciences and Technology, Islamabad-PAKISTAN
[2]School of Engineering, University of Edinburgh, Edinburgh, EH9 3JL, Scotland-UNITED KINGDOM

Received/Geliş: 25.06.2016 Revised/Düzeltme: 13.12.2016 Accepted/Kabul: 21.12.2016

ABSTRACT

Membrane gas separation has gained an important place in process industry for various applications. ASPEN HYSYS is a widely used commercial simulation software for process flow design. However, there is no built-in unit operation available in ASPEN HYSYS for membrane processes. In this research work, a user-defined extension has been developed and implemented by using commercial process simulators ASPEN HYSYS. The module has been used for the design and simulation of membrane processes. The benefit of this user defined extension is that it can be easily linked with ASPEN HYSYS. A CO_2 selective membrane has been used to separate CO_2 from the flue gas as a case study. This work analyses the effect of two-stage membrane process, using different streams, and having different process configurations. The results have been verified with the data available in the literature. The proposed unit operation extension shows good agreement with published results.
Keywords: Mathematical modeling and simulation, membrane gas separation, ASPEN HYSYS, CO_2 capture.

ASPEN HYSYS İÇİNDE MEMBRAN SÜRECİNİN SİMÜLASYON IÇIN KULLANICI TANIMLI UZATMA GELİŞİMİ

ÖZ

Membran gaz ayırma çeşitli uygulamalar için işlem sektöründe önemli bir yer edinmiştir. ASPEN HYSYS süreç akış tasarımı için yaygın olarak kullanılan ticari simülasyon yazılımıdır. Ancak, membran prosesleri için ASPEN Hysys mevcut yerleşik hiçbir ünitesi çalışma var. Bu araştırma çalışmasında, bir kullanıcı tanımlı uzatma geliştirilmiştir ve ASPEN Hysys ticari işlem simülatörleri kullanarak uyguladı. Modül membran proseslerinin tasarımı ve simülasyonu için kullanılır olmuştur. Bu kullanıcı tanımlı uzatma yararı kolayca ASPEN Hysys ile bağlantılı olmasıdır. Bir CO_2 seçici membran bir vaka çalışması olarak baca gazından CO_2 ayırmak için kullanılır olmuştur. Bu çalışma, farklı akışları kullanarak ve farklı süreç konfigürasyonları sahip, iki aşamalı zar sürecinin etkisini analiz eder. Sonuçlar literatürde mevcut verilerle teyit edilmiştir. teklif birim operasyon uzatma yayınlanan sonuçlarla iyi bir uyum göstermektedir.
Anahtar Sözcükler: Matematiksel modelleme ve simülasyon, membran gaz ayırma, ASPEN HYSYS, CO_2 yakalama.

* Corresponding Author/Sorumlu Yazar: e-mail/e-ileti: ahsan@scme.nust.edu.pk, tel: +92 333 6057 937

1. INTRODUCTION

From the survey of the published literature, Aspen HYSYS is found to be one of the promising software for process flow designing of membrane gas separation processes. It provides a component-based framework that can be easily modified, modernized, and retained to meet changing user necessities [1]. A user-defined membrane model can be applied in conjunction with the Aspen HYSYS solution procedure adapting the Visual Basic (VB) or C++ subroutine [2]. Hussain and Hagg [3] applied a one dimension hollow fiber membrane model in Aspen HYSYS for the feasibility study of CO_2 capture by comparing the process economics of several process configurations. Peters et al. [4] performed a simulation analysis interfaced within Aspen HYSYS to compare the performance and economics of an amine absorption process and a simple membrane unit. He and Hagg [5] also adapted the Aspen HYSYS process simulator with the integration of ChemBrane to evaluate the techno-economic feasibility of their respective membrane systems associated to hollow fiber carbon membranes and fixed site carrier membranes. In this research unit operation extension is implemented to enhance the functionality of an ASPEN HYSYS for membrane gas separation. To the best of our knowledge of the published literature, this is the first attempt where user define extension is implemented along with ASPEN HYSYS for the separation of CO_2 from multicomponent flue gas.

The Global energy demand is constantly growing and the increasing amount of fuels being consumed leads to more pollutants entering the atmosphere. Though globally we are more aware of the environmental danger of this and have stopped releasing some greenhouse gases (GHG) into the atmosphere but CO_2 concentration is still increasing in the atmosphere. Over half of this is due to industrial practice. There are currently many initiatives to control and decrease GHG emissions, these include renewable energy development, reduction of energy consumption, improved efficiency of energy processes and CO_2 capturing. One way to reduce the emission of CO_2, particularly from industrial work, is to capture and store CO_2 [3, 6-8]. There are many separation processes including membranes, adsorption, and absorption, being researched both pre (when CO_2 is removed from the combustion chamber) and post-combustion (when CO_2 is removed from the flue gas). Most of the research is being focused on post-combustion CO_2 capture as this is easy to implement on current power plants, and can be adapted to many industrial processes such as cement and steel industries to lower CO_2 exhaust from furnaces.

Separation of CO_2 from flue gas can be considered as a CO_2/N_2 separation problem for which there are currently many solutions. Amine absorption is considered the best available technology despite it being energy intensive, and having problems with alkanol amine degradation. Uncertainty lies around membrane separation technology due to the sensitivity of the membrane to extreme operation conditions, namely temperature, pressure, and flow rates [9]. However, membranes offer vast potential with low initial investment, small footprint, low energy requirements, ease to scale up and the ability to integrate modular upscaling to existing membrane technology [10-12].

Aspen HYSYS is a comprehensive process modeling tool used by the world's leading oil and gas producers, refineries, and engineering companies for process simulation and process optimization in design and operations. Unfortunately, Aspen Hysys do not have a built-in unit operation for gas permeation. Therefore, the membrane unit operation cannot be added to process flow design in Aspen HYSYS. There are two path to developed a unit operation of a membrane in Aspen HYSYS. 1) User unit operation 2) Unit operation extension. Most of the researcher used first path, but in this research, a unit operation extension for membrane has been implemented and verified. The development of user-defined extension in Aspen Hysys was a difficult task. A sound knowledge of numerical modeling, chemical engineering, membrane gas separation and computer programming is required to develop this extension.

Current research is focused on limiting the uncertainty in the numerical analysis of membrane gas separation. Membrane research groups have developed a CO_2 capture membrane with

facilitated transport which boosts selectivity of 200 and permeance of 1 m^3 (STP)/hr.bar.m^2. The ultra-thin polyvinyl amine supported on polysulfone has promising preliminary results for gas separation [13, 14]. The technical possibility of membrane CO_2 capture has been confirmed the use of two-stage membrane process with efficient process design. The aim of the simulation analysis was to verify the results with data available in the literature [3]. The aim was to achieve 90% CO_2 recovery and 90% purity in permeate which is considered necessary in the application of membrane gas separation [15]. A low CO_2 concentration (10%) was chosen in the feed flue gas to show the technologies applicability in a variety of situations even though membrane gas separation favors higher initial concentration.

2. MATHEMATICAL MODELING

2.1. Principles of Membrane Gas Separation

The function of a membrane is dependent on some parameters, i.e. membrane material, gas components and process conditions. The solution-diffusion model is most commonly used mechanism for gas permeation through polymer membranes [16].

From Fick's law, it is possible to derive the principle flux equation which is valid when the driving force is the difference in partial pressure. Flux (J) is shown by:

$$\frac{q_{pi}}{A_m} = q_{pi} \times \frac{y_{pi}}{A_m} = J_i = \frac{Pi}{l}(p_h x_i - p_l y_i) \quad (1)$$

For gasses permeability is defined as diffusivity multiplied by solubility:

$$P = D\frac{m^2}{s} * S\frac{m^3}{m^3.bar} \quad (2)$$

$$\alpha = \frac{Pi}{Pj} \quad (3)$$

The separation factor "α*" is highly dependent on the mole fraction of a component in the feed.

$$\alpha^* = \frac{\frac{y_i}{y_j}}{\frac{x_i}{x_j}} \quad (4)$$

which is also known as process selectivity. Pressure ratio and selectivity govern gas separation. There is a pressure ratio limited region when pressure is low relative to selectivity. In this study like, the model is based on solution diffusion alone. It does not differentiate between mass transfers from carrier effect or solution diffusion. For the reason, instantaneous reaction equilibrium concentration and carrier concentration are irrelevant in this simulation.

2.2. Process Conditions and Simulation Method

The concentration of CO_2 in flue gas can vary from 7 – 30% depending on the process [17]. Most membrane studies have considered binary separation problem of CO_2/N_2, whereas in this study the flue gas composition is 10% CO_2, 80% N_2, 5% O_2 and 5% H_20. Components of the flue gas with negligible concentrations are in this work, i.e. ash, NO_2 and SO_x. The following process variables have to be considered when dealing with the simulation of membrane processes: feed flow rate, permeate flow rate, temperature, composition, pressure ratio between upstream and downstream, pressure across the membrane and stage cut (θ) being the ratio of permeate flow rate to feed flow rate. The recovery (R) of the desired component (CO_2) can be calculated using the following equation:

$$R = \frac{\theta\, yi}{xi} \quad (5)$$

Where y_i, considered the "purity" is the mole fraction of CO_2 in the permeate stream and x_i is the mole fraction of CO_2 in the feed stream.

For post-combustion studies, the flow rate of flue gas is dependent on the source of emissions, but can often be high. For this study flue, gas flow rate is assumed to be 1×10^6 kg/hr which is realistic and has been reported in [18]. The temperature of the flue gas is 40 ℃ and the pressure 1 bar. In order to maximize the driving force across the membrane, creating a higher-pressure ratio, the flue gas is compressed from 1 to 5 bar before entering the membrane. This simulation was performed with a permeate pressure of 25mbar to 75mbar.

This study considered a facilitated transport membrane, so water vapors can be used as a sweep gas. But in this simulation due to limitations in the membrane interface, sweep gas and recycling streams were not used. The following assumptions are also made [19]: (1) Permeability is independent of pressure and concentration (2) Pressure drop on feed side is negligible (3) Assumed the steady state (4) The membrane is of uniform thickness (5) There are no concentration gradients in perpendicular direction of the membrane (6) The total pressure is essentially constant on each side of the membrane.

CO_2/N_2 selectivity value of 200 is scaled up to 5 bars for facilitated membrane transport. The model used in this study to calculate the performance of a hollow fiber membrane made for CO_2 selectivity is one-dimensional isothermal. An in-house membrane interface coupled with ASPEN HYSYS 7.3 has been used to investigate and confirm the effects of parameters and membrane stage configuration by designing the process flow simulations.

The membrane module can take any number of components and calculate the composition of permeate and retentate streams given permeance and membrane area are defined. Complex simulations can be evaluated as the interface allows any number of modules to be added and can calculate results for countercurrent flow pattern. In this simulation, the membrane was divided into m sections of equal area. In a membrane, feed side molar flux for each component can be calculated by:

$$dF_i = P_i\left(p_h \times y_{if} - p_l \times y_{ip}\right)dA \tag{6}$$

Where dFi is molar flow in feed, Pi is permeance of component i, ph is feed side pressure, yif is feed mole fraction of component i, pl represents permeate side pressure, yip is permeate mol fraction of component and dA the differential membrane area.

The simplest system to solve is co-current flow as permeate and feed conditions are known at the same point in the model (the inlet). Plug flow on both sides of the membrane is assumed. This formula equates to the mole fraction of component i as:

$$y_{if} = \frac{F_{if}}{\sum F_{kf}} \tag{7}$$

In which $\sum Fkf$ is the sum of all components in the feed.

The permeate side mole fraction is also shown by:

$$y_{ip} = \frac{F_{ip}}{\sum F_{kp}} \tag{8}$$

It follows that the permeate balance is:

$$dF_{ip} = -dF_{if} \tag{9}$$

The terms being molar flow in permeate and molar flow in feed respectively.

For co-current flow, the model is a system of coupled linear differential equations. To integrate these equations and compute the final retentate composition a higher order numerical method algorithm is used (Stream gasses are part of the system of equations as they are fed into permeate).

A more intricate solution is needed when a cross-flow model is used. This is because permeate and feed mole fractions are coupled along the whole length of the membrane.

Permeate concentration is given by:

$$y_{ip} = \frac{F_{ipm}}{\sum F_{kpm}} \tag{10}$$

which is equal to all points so is also the outlet permeate. This is solved by iterations over an initial concentration estimate to find the final permeate fraction.

The most efficient system to solve is counter current flow which is used in this study. These complications arise because of the concentration profile on the permeate side and the fact the exit permeate flow is unknown.

There are opposite directions of flow for feed and permeate so the balance is:

$$dF_{ip} = dF_{if} \tag{11}$$

This model can be solved using two different numerical approaches: (1) The flux along the membrane is calculated using the higher order numerical method and iteration over permeate flow is conducted until convergence to a solution is achieved. (2) Successive stages model with permeates approximated [20]. Though similar results were calculated for both approaches but the second method is stronger as it still shows valid results even when component driving forces are very small.

An iterative method is used to solve for the output partial pressures such that mass is conserved over the unit. The membrane unit calculation code attempts to solve for all the components iteratively using the given scheme. Assume output composition is the same as feed composition, and calculate a set of Log Mean Pressures (LMPs). Using these LMPs calculate permeate flow rates and hence output flow rates via a mass balance. Based on these flow rates calculate another set of LMPs. These two sets of LMPs now provide a bracket with the possible extreme values. A bisection search is then performed to home in on the correct answer. At each iteration, new LMPs are calculated at the bisection, and hence permeate flows and another new set of LMPs. The appropriate LMPs that form the new bracket are selected and iterations continue. LMPs are converged when the values calculated on successive iterations differ by less than 0.2 kPa. Additionally, if the calculations do not converge within 200 iterations then the extension returns an error. The solution algorithm of bisection method is as follow:

1. Start
2. Read x1, x2, error (Here x1 and x2 are initial guesses)
3. Compute: f1 = f(x1) and f2 = f(x2)
4. If (f1*f2) > 0, then x1 and x2 are wrong and GOTO (11)

Otherwise, continue.

5. x = (x1 + x2)/2
6. If ($\left|(x1 - x2)/x\right|$ < error), then display x and GOTO (11)
7. Else, f = f(x)
8. If ((f*f1) > 0), then x1 = x and f1 = f.
9. Else, x2 = x and f2 = f.
10. GOTO (5)

(Now the loop continues with new values)

11. Stop

The input data used for process conditions are based on literature [3]. They are outlined below: (1) Feed composition 10% CO_2, 80% N_2, 5% O_2 and 5% H_20. (2) The Permeance values are: $P_{CO2} = 1(m^3(STP)/bar.m^2.hr)$, $P_{O2} = 2x10^{-2}(m^3(STP)/bar.m^2.hr)$, $P_{N2} = 5x10^{-3}(m^3(STP)/bar.m^2.hr)$, $P_{H2O} = 2.25x10^{-9}(m^3(STP)/bar.m^2.hr)$. (3) Compressor adiabatic efficiency assumed at 90%. (4) All Heat exchangers have no pressure change. (5) Vacuum pumps adiabatic efficiency 75%.

2.3. ASPEN HYSYS extensibility

The most powerful features of the ASPEN HYSYS program enables users to add additional unit operations by using either user unit operations or unit operation extensions. Hussain and Hägg [3] applied user unit operations in their study while in this research unit operation extensions is implemented to enhance the functionality of an existing program in a direct and seamless manner. User unit operations and unit operation extensions differ from each other in several ways; the most important difference is the location of the defining code. With a unit operation extension, the defining code exists outside of the ASPEN HYSYS simulation in a separate DLL (Dynamic Link Library); while the defining code for a user unit operation is written and exists within the ASPEN HYSYS simulation.

User unit operations and unit operation extensions both offer the ASPEN HYSYS user an opportunity to increase the functionality of the ASPEN HYSYS program through the addition of custom built unit operations. These two features have differences that direct them towards different areas of application.

One disadvantage of the user unit operation is that the code is not in a compiled form like it is for an extension. This means that the user unit operation code cannot be distributed without possibly distributing confidential and proprietary information. Another limitation is that the views for the user unit operation cannot be modified and customized like the views for extensions.

On another hand, once created, ASPEN HYSYS extensions interact seamlessly with the ASPEN HYSYS interface. Unit operation extensions can be installed just like the ordinary unit operations, they are solved the same way and have similar property views.

2.3.1. ASPEN HYSYS extension structure

An ASPEN HYSYS extension consists of two separate and distinct files. Firstly, the ActiveX server DLL (Dynamic Link Library) file that contains the compiled code and defines the operation of the extension. Secondly, the EDF (Extension Definition File) that acts as the link between the DLL and the ASPEN HYSYS program. The DLL file is the compiled code written in the object-oriented programming language (VB). The EDF file is created using the Hyprotech Extension View Editor (supplied with the ASPEN HYSYS program). The EDF acts as the "translator"; it also acts as a place to declare variables used in the extension and held by the simulation. The EDF can also be referred to as a Container. While the DLL file contains the code that will define the operation of the extension, the EDF will define the appearance of the extension in the ASPEN HYSYS environment. The relationship between the ASPEN HYSYS program, the EDF, and the DLL can be represented graphically in Figure 1.

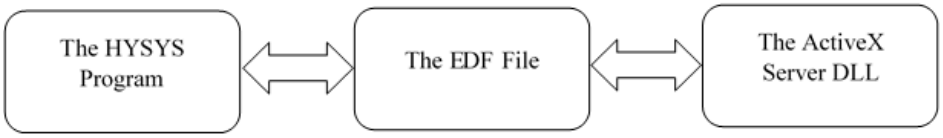

Figure 1. ASPEN HYSYS extension structure

Note that ASPEN HYSYS does not communicate directly with the DLL file; rather, all communication passes through the EDF file. For this reason, it is necessary that all variables that will coexist in both ASPEN HYSYS and the DLL be declared and defined in the EDF. There are six basic steps that outline the procedure for creating an extension for the ASPEN HYSYS program. These six steps are the same for each type of extension; however, what is done for each step will be different depending on the type of extension you are creating.

The six steps to creating an extension are:

1. Create the Extension Definition
2. Create the object views using the Extension View Editor
3. Implement the required methods
4. Register the extension
5. Debug the extension.
6. Distribute the extension.

3. RESULTS AND DISCUSSION

A two-stage membrane separation process gives the possibility of energy efficient CO_2 capture from flue gas. In this study, three different stream gas combinations were analyzed.

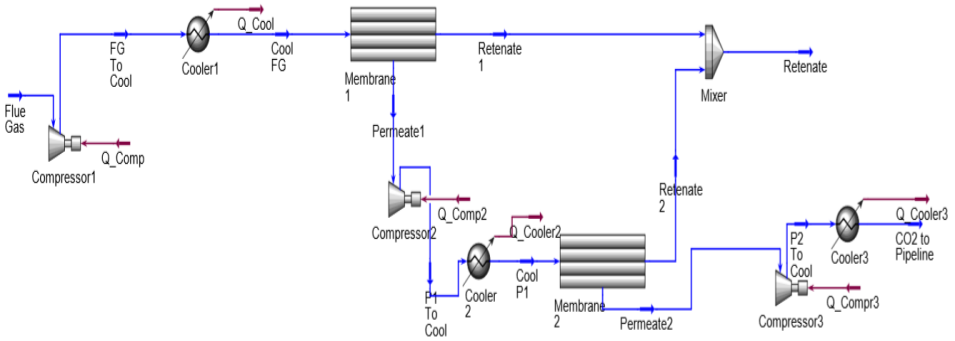

Figure 2. Simplified two-stage membrane separation process

In Figure 2 the flue gas is firstly compressed then cooled to the desired upstream operation conditions (5 bars, 50℃). The gas is then fed into the first membrane. The permeate exits with no water content and is then compressed and cooled once again before entering the second membrane (2 bars, 50℃). The second permeate stream exits the membrane with no water content and a higher CO_2 purity. This final stream is compressed and cooled to a suitable condition for downstream processes/storage (1 bar, 60℃). Both retentate streams are mixed and exit with a composition close to that of the flue gas feed. The results are presented in table 1. The area of both membranes is assumed to be $10m^{2.}$

Table 1. Results of Figure 2 simulation

	Flue Gas (FG)	**FG To Cool**	**Cool FG**	**Retentate 1**	**Cool P1**	**Retentate 2**	**Retentate**	**CO_2 to pipe**
Temp (^{0}C)	40	227.3	50	49.98	50	137.5	38.07	60
Pressure (bar)	1	5	5	4.99	2	1.99	1.99	1
Molar Flow (MMSCFD)	700	700	700	700	5.225×10^{-3}	3.315×10^{-3}	700	1.91×10^{-3}
Mass Flow (kg/hr)	1.022×10^{6}	1.022×10^{6}	1.022×10^{6}	1.022×10^{6}	11.30	7.114	1.022×10^{6}	4.181
N_2	0.8000	0.8000	0.8000	0.8000	0.0307	0.0475	0.8000	0.0016
CO_2	0.1000	0.1000	0.1000	0.1000	0.9597	0.9388	0.1000	0.9960
O_2	0.0500	0.0500	0.0500	0.0500	0.0096	0.0137	0.0500	0.0024
H_2O	0.0500	0.0500	0.0500	0.0500	0.0000	0.0000	0.0500	0.0000

90% purity of CO_2 is achieved in this example.

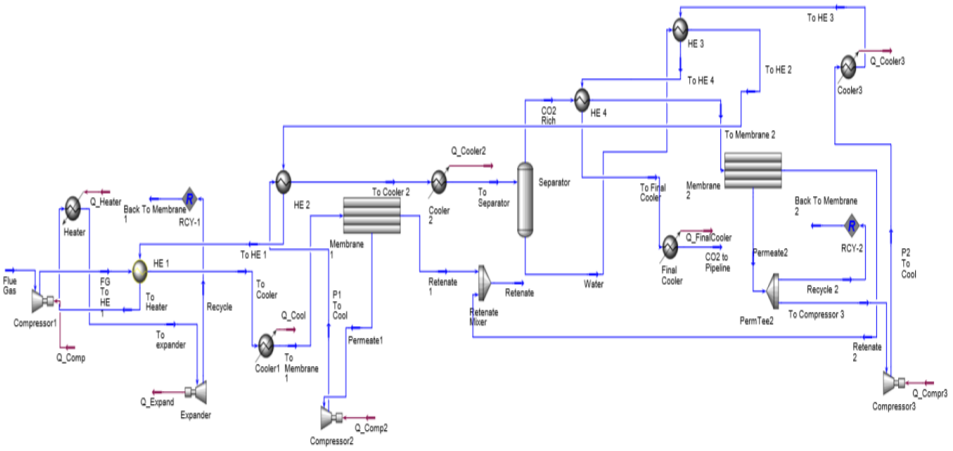

Figure 3. Process flow diagram for CO_2 capture by membrane from flue gas

Figure 3 shows a two-stage membrane gas separation. Like Figure 2 the flue gas is first compressed and cooled to meet downstream requirements (5 bars 50℃) . Permeate 1 stream is compressed to 2 bars then cooled by the heat exchanger and cooler to 3℃ before entering the separator. The stream is CO_2 rich and is passed through a heat exchanger to increase the temperature to 25 ℃ before further separating out of CO_2 can occur in the second membrane. The product of the separator which is passed through a series of heat exchangers, a heater and an expander has the temperature of 50℃ and pressure 0.075 bars. The CO_2 content of permeate 1 for Figure 3 is 61.3% which is much lower than the no stream CO_2 concentration of 95% or the permeate stream concentration (Figure 4) of 75%. The membrane area of both stages is kept at 8.2×10^5 m^2 and 2.32×10^5 m^2 and the pressure ratios are maintained to achieve 90% CO_2 purity and 90% recovery. The permeate passes through a series of heat exchangers to minimize energy consumption and is cooled and compressed to the same conditions as in Figure 2. Although using permeate as stream adds efficient removal of permeate it reduces the CO_2 driving force across the membrane marginally (dependent on CO_2 partial pressures up and downstream).

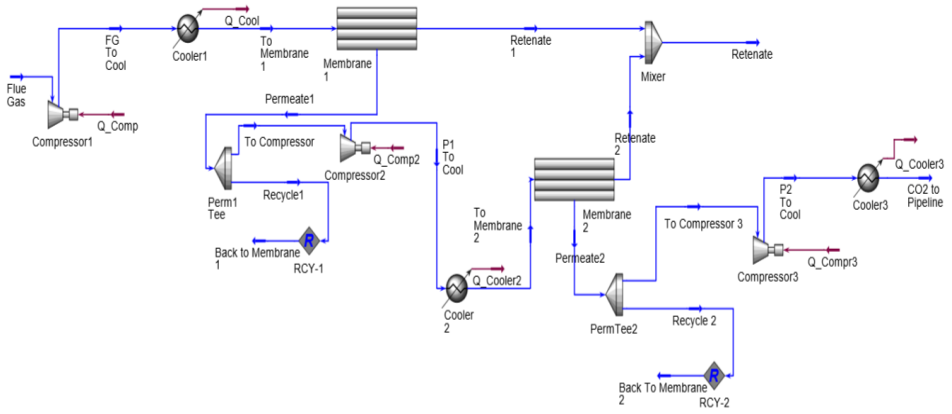

Figure 4. Process flow diagram for CO_2 flue gas capture

In the first stage, 70% of permeate flows to membrane two as feed and the remaining 30% is reused as permeate stream. At the second stage membrane, only 5% is recirculated the rest is cooled and compressed to the same outlet condition as Figure 2 and 4. These percentages of stream correspond to 5% of feed flow rate from each membrane respectively. The membrane area of both stages is kept at 1.6×10^6 m^2 and 4.6510^5 m^2. Other than this the setup of Figure 4 is much the same as of Figure 2. Flue gas is cooled and compressed before entering membrane one, permeate which continues to membrane two is also cooled and compressed (2 bars, 25℃) before entering. The retentates are mixed and exit. The outlet stream results for Figure 3 and 4 are compared with the literature data and shown in Table 2 and 3 respectively.

Table 2. Comparison of results of CO_2 to pipeline stream for Figure 3

CO_2 to Pipeline	**Literature [3]**	**This Simulation**	**Difference %**
Temperature (^{0}C)	60	60	0
Pressure (bar)	1	1	0
Molar Flow (MMSCFD)	65.56	44.5	32.1
Mass Flow (kg/hr)	141877	96350	32.1
N_2	0.02	0.0172	14.0
CO2	0.96	0.9609	0.1
O_2	0.02	0.0219	9.5
H_2O	0	0	0

Table 3. Comparison of results of CO_2 to pipeline stream for Figure 4

CO_2 to Pipeline	**Literature [3]**	**This Simulation**	**Difference %**
Temperature (^{0}C)	60	60	0
Pressure (bar)	1	1	0
Molar Flow (MMSCFD)	68.46	44.5	35.0
Mass Flow (kg/hr)	146109	95650	34.5
N_2	0.05	0.029	42.0
CO_2	0.92	0.939	2.1
O_2	0.03	0.032	6.7
H_2O	0	0	0

Table 4. Comparison between simulation results of three different systems

CO_2 to Pipeline	**Figure 2**	**Figure 3**	**Figure 4**
Temperature (^{0}C)	60	60	60
Pressure (bar)	1	1	1
Molar Flow (MMSCFD)	1.91×10^{-3}	44.5	44.5
Mass Flow (kg/hr)	4.181	96350	95650
N_2	0.0016	0.0172	0.029
CO2	0.9960	0.9609	0.939
O_2	0.0024	0.0219	0.032
H_2O	0	0	0

The results substantiate the previous findings. The compositions are nearly identical which confirms it is possible to achieve 90% CO_2 purity from flue gas with a CO_2 concentration of 10%. The flow rates are slightly lower in both cases, this is because in this study it has not been

possible to recirculate the stream so CO_2 removal has not been added, for this reason, 90% CO_2 recovery has not been achieved. For Figure 3, 75% recovery was achieved and Figure 4, 73%. It is important to note that the temperature and pressure of permeate 1 stream in all cases has a vital impact on the system convergence. Membrane area and pressure ration has not been varied but held constant. Outline of the findings are as follow: (1) Larger membrane area is needed for lower pressure ratio. (2) Little difference between membrane area for no stream or permeate stream. (3) Permeate purity increases with pressure ratio. (4) Low-pressure ratio means more energy is required. (5) Permeate stream requires less energy at higher pressures. (6) Permeate as stream only feasible at high pressure.

4. CONCLUSION

A unit operation extensions along with ASPEN HYSYS has been proven to describe the separation performance of the membrane module under three different process flow design cases. The precision of the results obtained by the model has been compared and validated with published data, in which the model shows good agreement with published results. The case study was focused on the separation of CO_2 from flue gas using unit operation extension in ASPEN HYSYS. This study showed that CO_2 separation with high purity is achievable from the post combustion flue gas. This simulation has been conducted using realistic parameters and operation design to simulate a real flue gas process. The model results for different membrane systems have been validated by comparing with the literature data. The results of this research work suggested a scope of unit operation extension for process flow design in membrane technology. The study of membrane unit operation extension related to the recovery and productivity may be carried out in subsequent studies.

Acknowledgements / Teşekkür

The authors would like to thank the AspenTech Customer Support for their guidance in this research work.

NOMENCLATURE

q_{pi} Flowrate of gas permeate ($\frac{m^3}{h}$)
P_i Permeability of gas ($\frac{m^3.m}{m^2.h.bar}$)
l Thickness of membrane *(m)*
p_h Feed side pressure *(bar)*
p_l Permeate side pressure *(bar)*
x_i Feed side mol fraction
y_i Permeate side mole fraction
A_m Membrane area *(m^2)*
α Selectivity
$\alpha*$ Separation factor
D Fickian's diffusion constant

REFERENCES / KAYNAKLAR

[1] Aspen Technolgy Inc. (2010) Aspen HYSYS customization guide. Burlington, USA.
[2] Lock S, Lau K, Ahmad F, Shariff A. (2015) Modeling, simulation and economic analysis of CO_2 capture from natural gas using cocurrent, countercurrent and radial crossflow hollow fiber membrane, Int. J. Greenhouse Gas Control, 36,114-134.

[3] Hussain A, Hägg M-B. (2010) A feasibility study of CO_2 capture from flue gas by a facilitated transport membrane, J. Membrane Sci., 359,140-148.

[4] Peters L, Hussain A, Follmann M, Melin T, Hägg M-B. (2011) CO_2 removal from natural gas by employing amine absorption and membrane technology—A technical and economical analysis, Chem. Eng. J., 172,952-960.

[5] He X, Hägg MB, Kim TJ. (2014) Hybrid FSC membrane for CO2 removal from natural gas: Experimental, process simulation, and economic feasibility analysis, AIChE J., 60, 4174-4184.

[6] Yu C-H, Huang C-H, Tan C-S. (2012) A review of CO_2 capture by absorption and adsorption, Aerosol Air Quality Res., 12,745-769.

[7] Zamani Pedram M, Omidkhah M, Ebadi Amooghin A. (2014) Synthesis and characterization of diethanolamine-impregnated cross-linked polyvinylalcohol/ glutaraldehyde membranes for CO_2/CH_4 separation, J Ind. Eng. Chem., 20, 74-82.

[8] Yan S, Zhao S, Wardhaugh LT, Feron PH. (205) Innovative use of membrane contactor as condenser for heat recovery in carbon capture, Env. Sci. Technol., 49,2532–2540

[9] Song C, Kitamura Y, Li S. (2014), Energy analysis of the cryogenic CO_2 capture process based on Stirling coolers, Energy, 65,580-589.

[10] Boot-Handford ME et al. (2014) Carbon capture and storage update, Energy Env. Sci., 7,130-189.

[11] Salih AAM, Yi C, Hu J, Yin L, Yang B. (2014) Preparation of vinyl amine-co-vinyl alcohol/polysulfone composite membranes and their carbon dioxide facilitated transport properties, J Appl. Polym. Sci., 131(6), 40043.

[12] Chen B, Ruan X, Jiang X, Xiao W, He G. (2016) Dual-membrane Module and its Optimal Flow Pattern for H_2/CO_2 separation, Ind. Eng. Chem. Res., 55,1064-1075.

[13] Hussain A. (2012) A Single Stage Membrane Process for CO_2 Capture from Flue Gas by a Facilitated Transport Membrane, Sep. Sci. Tech., 47,1857-1865.

[14] Hussain A, Nasir H, Ahsan M. (2014) Process design analyses of CO2 capture from natural gas by polymer membrane, J. Chem. Soc. Pakistan., 36,411-421.

[15] Luis P, Van der Bruggen B. (2013) The role of membranes in post-combustion CO_2 capture. Greenhouse Gases, Sci. Technol., 3,318-337.

[16] Wijmans JG, Baker RW. (1995) The solution-diffusion model: A review, J Membrane Sci., 107, 1-21.

[17] Davison J, Thambimuthu K. (2004) Technologies for capture of carbon dioxide. Proceedings of the Seventh Greenhouse Gas Technology Conference.

[18] Bounaceur R, Lape N, Roizard D, Vallieres C, Favre E. (2006) Membrane processes for post-combustion carbon dioxide capture, A parametric study, Energy., 31,2556-2570.

[19] Ahsan M, Hussain A. (2014) Comparing Numerical Methods for Multicomponent Gas Separation by Single Permeation Unit, Chiang Mai J. Sci., 41,184-199.

[20] Coker DT, Freeman BD, Fleming GK. (1998) Modeling multicomponent gas separation using hollow-fiber membrane contactors, AIChE J., 44, 1289-1300.