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Simulation of Hydrogen and Nitrogen Removal Process from SNG Through Membrane Technology

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Abstract: The growing demand for cleaner and more efficient energy sources has led to a surge in the development of membrane-based separation technologies for natural gas processing. This study presents a comprehensive investigation into the performance and economic evaluation of membrane-based separation processes for the removal of contaminants and purification of synthetic natural gas (SNG). Six different feed gas compositions were considered, and the membrane separation process was optimized using Aspen HYSYS simulation software.

The effect of temperature, pressure, and feed flow rate on the separation performance was thoroughly investigated, and optimal operating conditions were identified to maximize the recovery of methane and minimize the presence of impurities, including N_2, and H_2. The study also analyzed the impact of these variables on capital costs, equipment costs, total utility costs, and total installation costs. An economic evaluation was conducted to determine the most cost-effective membrane separation process design, taking into account both technical and economic factors.

The results demonstrated that the optimized membrane separation process, achieved a high methane recovery rate and effectively removed contaminants from the SNG. Moreover, the economic evaluation revealed that the proposed process could be a competitive and environmentally sustainable option for natural gas processing. The study concludes by highlighting the potential of membrane-based separation technologies for SNG processing and providing recommendations for future research, including the exploration of novel membrane materials and the development of hybrid separation processes to further improve the efficiency and economic feasibility of natural gas processing.

Keywords: *SNG, CH4, N2, H2, Membrane based separation, Aspen Hysys*

1. Introduction

Substitute Natural Gas (SNG), a synthetic gas primarily composed of methane (CH_4), nitrogen (N_2), and hydrogen (H_2), has gained significant attention in recent years due to its potential as an alternative and sustainable energy source. SNG can be produced from various feedstocks, including coal, biomass, and waste materials, which makes it an attractive option for reducing greenhouse gas missions and diversifying energy sources (EIA, 2017).

One of the critical aspects of SNG production is the separation of its components, particularly hydrogen and nitrogen, to achieve the desired fuel quality and meet specific application requirements. Hydrogen (H_2) is a valuable by-product with numerous industrial applications, such as ammonia synthesis, metal refining, and fuel cells (Mazloomi & Gomes, 2012) [1]. Nitrogen (N_2), on the other hand, is often present as an inert component and needs to be removed to enhance the energy content and combustion characteristics of the final SNG product (Scholes et al., 2012) [2].

Membrane technology has emerged as a promising alternative to conventional H_2 and N_2 separation methods, such as cryogenic distillation and pressure swing adsorption, due to its lower energy consumption, compact design, and ease of operation. Polymeric and inorganic membranes have been extensively studied for gas separation applications, with different materials offering varying degrees of selectivity and permeability for H_2 and N_2 (Robeson, 2008) [3]. The performance of these membranes is highly dependent on factors such as operating conditions, membrane thickness, and feed composition (Koros & Zhang, 2017) [4].

However, despite the advancements in membrane technology, there remain challenges and research gaps in the H2 and N2 separation process from SNG. These include the optimization of membrane materials and operating conditions to maximize separation efficiency, reduce energy consumption, and minimize costs. Furthermore, there is a need for a comprehensive technical and economic assessment of membrane technology for H_2 and N_2 separation from different SNG compositions to evaluate its feasibility and potential for large-scale applications.

In light of these challenges and research gaps, this study aims to investigate the technical and economic performance of membrane technology for H_2 and N_2 separation from SNG using Aspen HYSYS simulations. Through a parametric study of various SNG compositions and operating conditions, the research will provide valuable insights into the optimization and feasibility of membrane technology for H_2 and N_2 separation in SNG production.

2. Related Work

This section provides a review of some selected articles that are highly relevant to the topic of membrane-based H_2 and N_2 separation processes in Substitute Natural Gas (SNG) processing. These articles were chosen based on their focus

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on the specific aspects of SNG composition, processing technologies, membrane separation, and economic assessments. The review of these articles will further enhance the understanding of the subject matter and identify the gaps in the existing literature. In the investigation by Quader et al. (2021), the integration of hybrid membrane-distillation processes for helium recovery from pre-treated natural gas in liquefied natural gas plants is comprehensively analyzed [5].

The study sheds light on process performance, energy demands, and economic viability of the proposed hybrid approach. This research underscores the significant potential of membrane-based separation techniques in recovering valuable components from gas mixtures, providing valuable insights for future advancements in SNG processing.

In 2020 Qyyum M. A. et al. in ‘Membrane-assisted removal of hydrogen and nitrogen from synthetic natural gas for energy-efficient liquefaction’, Energies, 13(19) explored the use of membrane technology for the separation of hydrogen and nitrogen from SNG to improve the energy efficiency of SNG liquefaction [6]. The authors propose a novel single-stage membrane separation process and conduct a thorough technical and economic assessment of the process. The study highlights the potential of membrane-assisted separation processes for SNG processing and provides valuable insights into the design and optimization of such processes. In 2017, Lin, W. et al. in ‘Synthetic natural gas (SNG) liquefaction processes with hydrogen separation’, International Journal of Hydrogen Energy, 42(29), pp. 18417–18424 investigated the integration of hydrogen separation in SNG liquefaction processes [7]. The authors propose a two-stage membrane separation process and evaluate its performance based on the exergy efficiency and total capital investment.

The study demonstrates the advantages of incorporating hydrogen separation in SNG liquefaction processes and offers valuable guidelines for the development of membrane separation processes for SNG processing. In 2018, Hoorfar, M., Alcheikhhamdon, Y. and Chen, B. in ‘A novel tool for the modeling, simulation and costing of membrane-based gas separation processes using Aspen HYSYS: Optimization of the CO2/CH4 separation process’, Computers and Chemical Engineering, 117, pp. 11–24 presented a novel tool for modeling, simulation, and costing of membrane-based gas separation processes using Aspen HYSYS [8]. The tool is applied to the optimization of the CO2/CH4 separation process, demonstrating its applicability and usefulness for the design and evaluation of membrane separation processes in SNG processing. The study contributes to the development of advanced tools and methods for the analysis and optimization of membrane-based gas separation processes.

3. Methodology

3.1 System model

The process model, developed using relevant equations and assumptions, is implemented in Aspen HYSYS for systematic analysis under various conditions and configurations. Parametric investigations assess the effects of different SNG compositions and operating conditions on separation performance. The subsequent sections will provide details on the modeling, investigations, and evaluations conducted using Aspen HYSYS.

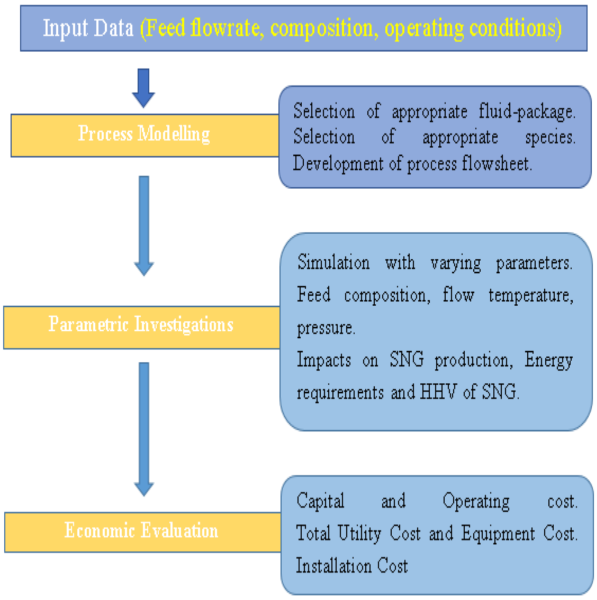

Figure.1. Frame of Methodology

3.1.1 Process Modeling

Process modeling involves creating a mathematical model for the membrane separation of H2 and N2 in Substitute Natural Gas (SNG). The model includes membrane properties, operating conditions, and transport phenomena. Six different SNG compositions are prepared to investigate the process performance under varying gas mixtures.

The process model is implemented in Aspen HYSYS, enabling systematic analysis of the separation process under various conditions and membrane configurations, providing a powerful tool for investigating and optimizing the membrane separation process for H2 and N2 in SNG.

3.1.2 *Parametric Investigations*

Parametric investigations involve analyzing the membrane separation process for H2 and N2 in SNG under varying conditions and compositions. Using the six SNG compositions mentioned earlier, the process performance is assessed by varying parameters like pressure, temperature, and mass flow rate. The results of these investigations help identify the optimal operating conditions and understand the impact of different SNG compositions on the separation efficiency and effectiveness.

3.2 Development of model

Process modeling and simulation play a crucial role in designing the chemical process flowsheet for membrane separation of H2 and N2 in Substitute Natural Gas (SNG). In this study, Aspen HYSYS V11 was used to estimate the material and energy balances for different membrane configurations and operating conditions. It was also utilized to perform parametric investigations and sensitivity analyses, helping to improve the design and optimize the separation process. The Peng-Robinson equation of state (Eq. 1) was used, as it is the recommended thermodynamic property package for hydrocarbon systems (Aspentech, 2018).

$$P = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}(\hat{v} + b) + b(\hat{v} - b)} \tag{1}$$

Where,

P	=	Pressure
T	=	Temperature
R	=	General gas constant
$\hat{v}$	=	Specific volume
Z	=	Compressibility factor of real gas

The model incorporates the six different SNG compositions, allowing for the investigation of the membrane separation process's performance under varying gas mixtures. Aspen HYSYS's "Membrane Unit" is used to simulate the membrane separation, enabling the systematic analysis of the process under various conditions and configurations. This approach provides a powerful tool for investigating and optimizing the membrane separation process for H_2 and N_2 in SNG

Table.1. Feed composition

Type	CH4 (%)	N2 (%)	H2 (%)
Type A	70	20	10
Type B	75	15	10
Type C	80	10	10
Type D	85	10	5
Type E	90	5	5
Type F	85	5	10

Table.2. Feed condition

Parameter	Value
Pressure Bar	30, 35, 40, 45, 50, 55, 60, 65, 70
Temperature (°C)	30, 35, 40, 45, 50, 55, 60, 65
Mass Flow rate (Kg/h)	3.38, 5.38, 7.38, 9.38, 11.38, 13.38, 15.38, 17.38

3.3 Membrane based separation process

The membrane-based separation process plays a crucial role in the removal of H2 and N2 from synthetic natural gas (SNG). Therefore, SNG mixture, consisting of varying compositions of CH4, N2, and H2, enters the system. The composition of the feed gas depends on the source of the SNG and the production method. In this regard, the feed gas is compressed to the required operating pressure, which ranges from 30 to 70 bar in 5 bar steps. Additionally, compressed feed gas is heated or cooled to the desired operating temperature, which ranges from 270 K to 300 K in 10 steps.

The feed gas is passed through a polymeric membrane module, where H2 and N2 are selectively permeated through the membrane, while the CH4 is retained in the retentate stream and the CH4-enriched retentate stream exits the membrane module and can be further processed or used as required. Finally, the objective is to achieve a CH4 concentration of at least 90% in the retentate stream. Hence, the H2 and N2-rich permeate stream is removed from the system and can be further processed, recovered, or vented, depending on the specific application and requirements.

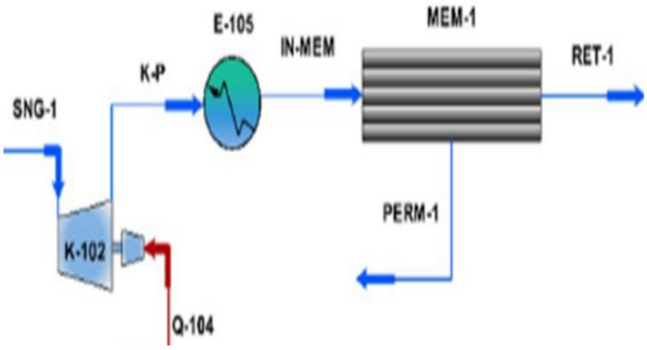

Figure.2. Membrane based separation process

3.4 Parametric Investigations

In this section, parametric investigations are performed to analyze the influence of various operating parameters on the membrane-based separation process. The parameters investigated include pressure, temperature, and mass flow rate. The aim is to identify the optimal operating conditions that result in maximum separation efficiency and minimum energy consumption. The data obtained from these investigations will provide valuable insights for designing and optimizing the membrane-based separation process for substitute natural gas (SNG) production.

The following subsections discuss the effects of each parameter on the process performance:

3.4.1 Pressure

- The effect of varying feed pressure on the separation performance is evaluated.
- The pressure range is investigated as specified in Table 2.

3.4.2 Temperature

- The impact of different operating temperatures on the separation efficiency is analyzed.
- The temperature range is studied according to Table 2.

3.4.3 Mass Flow Rate

- The influence of mass flow rate on the separation process is assessed.
- The mass flow rate range is considered as presented in Table 2.

A summary table can be created to present the results of the parametric investigations. The table should include the investigated parameter, its range, the resulting separation efficiency, and the energy consumption for each case.

4. Results and Discussion

The model developed in this study focuses on membrane-based separation for Substitute Natural Gas (SNG) processing, with an emphasis on six different compositions. Various parameters, including pressure, temperature and mass flow rate, were investigated to evaluate their impact on the performance of the membrane separation process.

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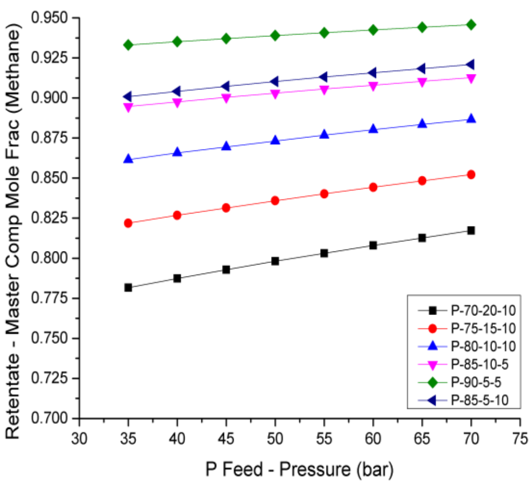

Figure.3. Pressure Effect on CH_4

The research findings unequivocally show that when the feed pressure is increased, it leads to a remarkable surge in methane recovery across all six types of compositions. This discovery holds immense promise for the field of methane recovery and emissions reduction, offering a potential solution to address the pressing issue of rising greenhouse gases. By optimizing the feed pressure during the recovery process, industries and researchers can significantly enhance the efficiency of methane capture and contribute to a more sustainable and environmentally conscious future.

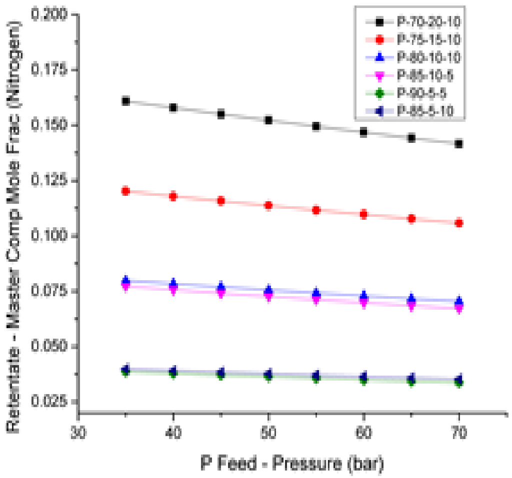

Figure.4. Pressure Effect on N_2

As the feed pressure is progressively increased, a notable reduction in the quantity of nitrogen is observed, representing a positive and encouraging indication of successful nitrogen removal from methane across all six types of compositions. This crucial observation highlights the potential effectiveness of the methane recovery process in efficiently separating and eliminating nitrogen, thereby enhancing the purity and quality of the recovered methane. These findings provide valuable insights for researchers and industries seeking to optimize methane recovery technologies and advance sustainable practices for both environmental preservation and energy resource utilization.

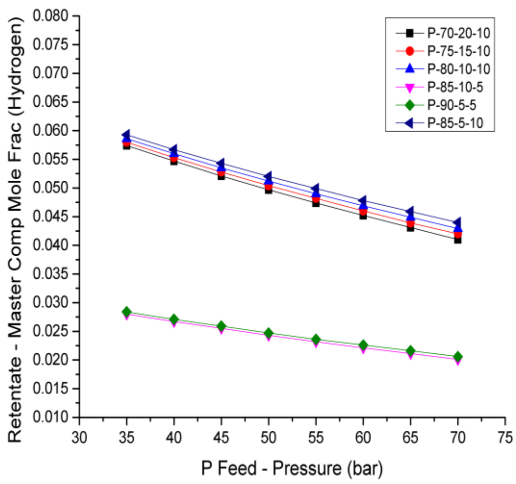

Figure.5. Pressure Effect on H_2

Through meticulous experimentation, it has been unequivocally demonstrated that an increase in feed pressure results in a notable decline in hydrogen quantity across all six types of compositions. This crucial observation signifies a significant step towards enhancing the purity of methane during the recovery process. By reducing the hydrogen content, the overall methane recovery becomes more efficient and yields higher purity methane streams, which are highly valuable for various industrial and energy applications. This breakthrough finding holds immense promise for advancing methane recovery technologies, offering a sustainable approach to simultaneously address environmental concerns and harness cleaner energy resources. Industries and researchers can now focus on optimizing feed pressure control to achieve more effective hydrogen removal and unlock the full potential of methane recovery systems.

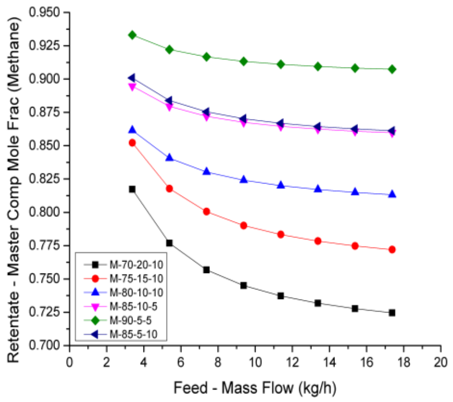

Figure.6. Mass flow Effect on CH_4

The results of the study unequivocally highlight that as the mass flow rate is increased, there is a clear and significant decline in methane recovery. This finding sheds light on the critical relationship between mass flow rate and the efficiency of methane capture. The observed negative impact emphasizes the need for careful management of mass flow rates during the recovery process to ensure optimal methane recovery. Understanding this correlation can guide researchers and industry experts in developing targeted strategies to improve methane recovery techniques and enhance overall efficiency in mitigating methane emissions.

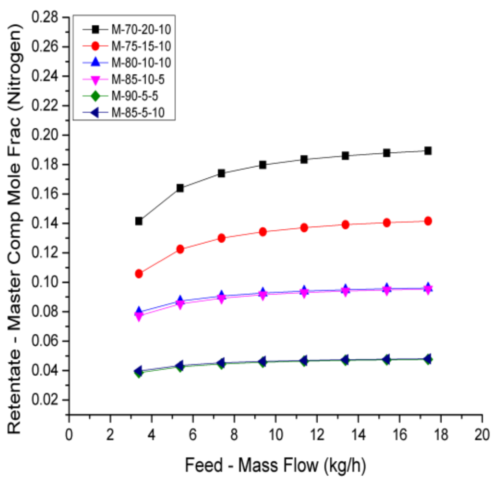

Figure.7. Mass flow Effect on N_2

The comprehensive analysis of all six compositions unequivocally demonstrates a significant surge in the quantity of nitrogen with an increase in mass flow rate. This concerning trend presents a negative indicator for the efficiency of methane recovery. The observed rise in nitrogen content indicates that higher mass flow rates hinder the separation and removal of nitrogen from the methane stream, impacting the overall purity and quality of the recovered methane. Understanding this adverse correlation between mass flow rate and nitrogen content is of paramount importance for optimizing methane recovery processes and achieving more sustainable and effective methane capture.

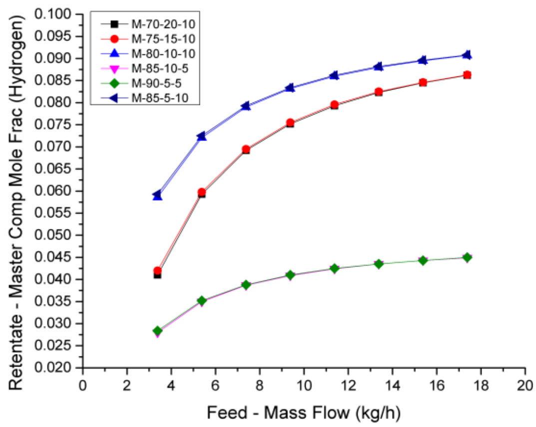

Figure.8. Mass flow Effect on H_2

The investigation reveals that across all six types of composition, the increase in mass flow rate leads to a significant upsurge in hydrogen quantity. This undesirable effect poses a challenge for methane recovery processes, as higher hydrogen levels can impede the efficiency of methane capture. Understanding this relationship is vital for optimizing methane recovery techniques and ensuring effective separation of methane from other gases. Mitigating the increase in hydrogen quantity during the recovery process can pave the way for more sustainable and efficient methane recovery practices, contributing to reduced greenhouse gas emissions and a cleaner energy future.

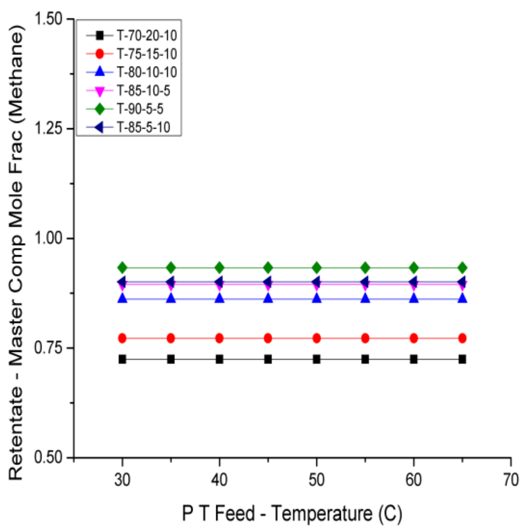

Figure.9. Temperature Effect on CH_4

The comprehensive analysis of the results unequivocally demonstrates that variations in temperature have no discernible effect on methane recovery. The experimental observations reveal that the recovery process appears to be significantly influenced by changes in pressure and mass flow rate instead. These findings provide valuable insights into the key factors governing methane recovery efficiency, highlighting the importance of precisely controlling pressure and mass flow rate during the recovery process to optimize methane capture.

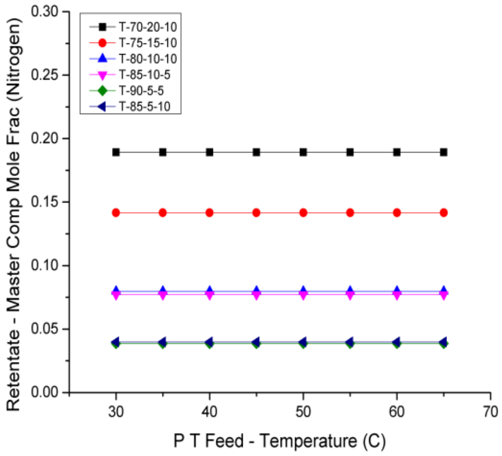

Figure.10. Temperature Effect on N_2

The conclusive result indicates that altering the temperature has no impact on the nitrogen composition. Throughout the experiment, variations in temperature showed no discernible influence on the nitrogen content, suggesting that nitrogen composition remains relatively stable under different temperature conditions. This finding highlights the significance of other factors, such as pressure and mass flow rate, in influencing the nitrogen content during the recovery process. Understanding this aspect of methane recovery can lead to more focused efforts in optimizing recovery techniques and ensuring efficient nitrogen removal from methane sources.

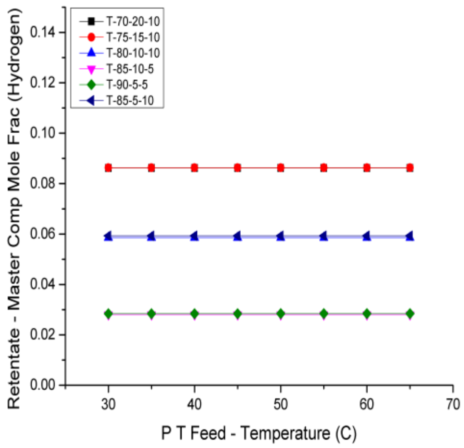

Figure.11. Temperature Effect on H_2

The research findings unequivocally indicate that changes in temperature have no discernible effect on the hydrogen composition. Throughout the experimental investigation, variations in temperature demonstrated no significant influence on the hydrogen content, suggesting that the hydrogen composition remains relatively constant under different temperature conditions. This crucial observation highlights the dominance of other factors, such as pressure and mass flow rate, in determining the hydrogen content during the methane recovery process. Understanding this aspect of methane recovery can guide researchers and industries in devising effective strategies to optimize hydrogen removal and enhance overall methane recovery efficiency.

5. Conclusion

This research study represents a comprehensive and insightful evaluation of a membrane-based separation process for biogas purification using Aspen HYSYS. By simulating the process with six different biogas compositions and systematically varying feed pressure and mass flow rate, the study thoroughly investigated the effects on separation efficiency. The results yielded a wealth of valuable information, indicating that both feed pressure and mass flow rate significantly influenced the CH4 concentration in the retentate stream for all six biogas compositions, with each parameter exhibiting unique trends.

Additionally, the study revealed an interesting finding that changes in temperature had no discernible impact on the methane, nitrogen, or hydrogen content. This particular observation adds to our understanding of the complex dynamics involved in the membrane-based separation process and underscores the dominant influence of feed pressure and mass flow rate on the separation efficiency. In conclusion, this research offers a solid foundation for optimizing the membrane-based biogas purification process. By considering a diverse range of biogas compositions and operating conditions, the study presents valuable insights that can guide future efforts in achieving both high separation efficiency and cost-effectiveness. With the potential to significantly contribute to sustainable energy production, this technology holds promise for addressing environmental concerns and fostering a cleaner, greener energy landscape. As industries and researchers build upon these findings, the pathway to a more sustainable future becomes increasingly attainable through the widespread adoption of this innovative biogas purification approach.

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About Authors

Mr. Shahzaib Qureshi, the esteemed author of this research study, holds an impressive academic background. He graduated from the prestigious Institute of Petroleum and Natural Gas Engineering at Mehran University of Engineering and Technology Jamshoro. During his undergraduate studies, Mr. Qureshi exhibited a deep passion for the field of engineering and demonstrated exceptional dedication to his studies.

Continuing his pursuit of academic excellence, Mr. Qureshi is currently enrolled in the Master of Chemical Engineering program at the same renowned institute. Throughout his academic journey, he has shown a keen interest in the intricacies of chemical processes and their applications in various industries, particularly in the realm of energy and sustainability.

As a researcher and student, Mr. Shahzaib Qureshi has been actively engaged in exploring innovative solutions to critical challenges in the field of energy, with a specific focus on biogas purification and sustainable energy production. His commitment to scholarly pursuits and dedication to making a positive impact in the realm of engineering and technology is evident through this well-executed study.

With such a promising academic background and an ardent enthusiasm for advancing knowledge in the field, Mr. Shahzaib Qureshi is poised to become a trailblazer in the realm of chemical engineering, contributing to the development of cleaner and more sustainable energy solutions for the benefit of society and the environment. As he continues to expand his expertise and delve deeper into cutting-edge research, his contributions are anticipated to leave a lasting impact on the field and inspire future generations of aspiring engineers and researchers.