iJRASET
International Journal For Research in
Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 10 **Issue:** IX **Month of publication:** September 2022

DOI: https://doi.org/10.22214/ijraset.2022.46552

Dynamic Simulation and Process Design Analysis of Syngas Purification and The Utilization of Gas Permeation

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Abstract: Syngas generation from alternative energy sources, notable methanation, is currently gaining popularity. The technique saves energy by converting it into a chemical product. It is not suited for use directly in distribution grids, where a greater purity of methane is necessary for maximum power density. Various syngas purification levels should be supplied for various methane grades (for heat, power, and automotive fuels uses). Water damages the mechanical components of an engine, thus it must be removed before it can be utilized as a fuel. CO_2 removal should also be performed to increase methane heat quality and minimize pollution. This research evaluated the performance of a syngas purification system using a flash separator and hollow fiber membranes. A flash separator model condensed the water from the wet feed. The CO_2 removal from methane was then investigated using hollow fiber membranes. As a consequence, Aspen Plus® V8.6 includes a FORTRAN user model for unit operations. The greatest result was filtering methane up to 98 percent vol. using a two stage pervaporation system with recycling streams. The model scheme may help in the implementation and quality evaluation of a complex methanation plant system.

Keywords: Simulation, Process, Design, CO_2, Purufication, Syngas

I. INTRODUCTION

Catalytic methanation was fully detailed in one of the authors' past investigations (Sharifian and Harasek, 2015). Water is roughly 50% of the product stream, followed by methane (33%), carbon dioxide (12%), and other 5%. (CO and H_2). Syngas may be refined for use as a heat and energy source, as well as motor fuel. Purification is essential to remove CO_2 and water from gasoline, since water damages engine mechanical components. Also, removing CO_2 from the atmosphere improves methane thermal quality and reduces pollution. This gas combination cannot be utilized directly in distribution systems due to the need for greater methane purity. Purification of methane after the reactor is essential for grid connection. The purification step aims to obtain a methane content of over 98 percent and a residual component content of less than 2%. This study employed a pervaporation membrane to purify methane. Membrane may be used to separate homogenous mixes in a steady state. In one of several recent research on gas permeation systems, Razavi et al. (2016) modeled CO_2 removal from N_2. Darebkhani et al. conducted a semi-empirical investigation on CO_2 removal from injected CH4 (2018). Dalane et al. (2019) developed a membrane-based subsea natural gas dehydration model in Aspen HYSYS.

II. SYNGAS PURIFICATION

A. *Separation of Flash (water removal)*

To remove water from a gas mixture, use flash separation. This usage is more helpful when gas components have different thermodynamic characteristics than water. The liquid phase is removed using gravity to settle at the bottom of a vertical cylinder. The feed (liquid or gas) is flashed into vapor and liquid in a vapor–liquid separator. The vapor phase exits the flash column through the gas outlet valve, keeping liquid droplets out. Figure 1 depicts the impact of temperature variations on a methanation product stream using a flash separator column at 50 bar pressure.

The molar concentration of water in the vapour state decreases with decreasing temperature. Also, at relatively low temperature, the mole fraction of methane as the main product rises.

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.538
Volume 10 Issue IX Sep 2022- Available at www.ijraset.com

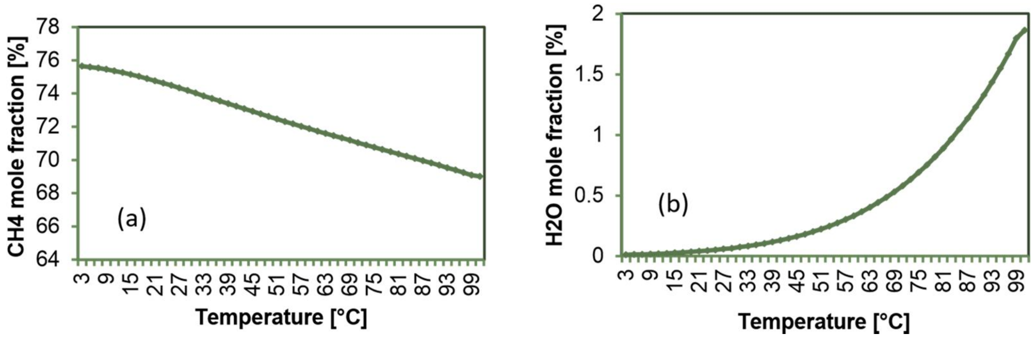
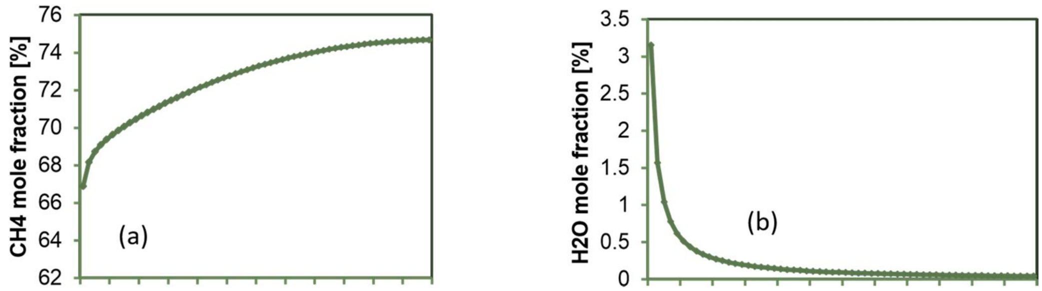


Fig 1: Moles of CH_4 and H_2O in the vapor phase, 50 bar pressure, and different temperatures

Figure 2 shows the impact of pressure changes on purifying performance at 4°C. Increasing the operating pressure reduces the water mole fraction in the vapor stream while increasing the methane mole fraction.



1 6 11 16 21 26 31 36 41 46 51 56 1 5 9 131721252933374145495357 Pressure [bar] Pressure [bar]

Fig 2: Moles of component (a) CH_4 and (b) H_2O in vapor phase, 4°C and different pressures

B. Separation Of Gas By Membrane

The content of methane rose by up to 80% following the initial purification process of eliminating water (see Table 1).

The next step is to purify methane using a membrane separator. Nevertheless, membrane gas separation technology has just been developed over the last 30 years. Membrane gas separation has various benefits, including low maintenance costs, little environmental impact, and easy plant operation (Drioli and Romano, 2001). • extracting organic vapor from contaminated air; • recovering methane from landfill gas (Rautenbach and Welsch, 1993); (Rautenbach and Welsch, 1993). (Chung et al.)

It is known that several mathematical models and computation techniques for multicomponent gas separation systems provide the best realistic portrayal of multi - component separation processes in hollow fiber membranes (Pan, 1986).

Table 1: The components' percentages after water removal

Component	Symbol	Percentage [%]	
		before flash	after flash
Water	H_2O	45-55	0-1
Methane	CH_4	27-35	75-85
Carbon dioxide	CO_2	5-15	5-15
Hydrogen	H_2	1-5	1-5
Carbon monoxide	CO	0-1	0-2

This study used an asymmetrical hollow fibre gas modules for multi - component mixture separation and a commercialized simulator (Aspen Plus® V8.6). A multi - component pervaporation system has been devised and proven for use in syngas purification after the methanation procedure in a flowsheet (Sharifian et al., 2016).

C. Strategy of Design

Process design is part of the assessment process in chemical systems. A pervaporation process' design includes a correct operating state and module configuration.

A one stage pervaporation separator for purifying methane after water removal is the most common and simplest configuration. However, multistage setups with a recycling flow are often employed in industrial size systems. A multiphase application is made up of two or three components that are linked in different ways to improve product purity while minimizing loss percentages. There are several examples of CO_2 removal from natural gas in varied flow patterns, uses, and architectures (He et al. 2014). Ohs et al. Module computation requires inner and outer diameters, active length, species permeance, and real pressure values on both sides. Table 2 lists the acceptable features for a typical module used in a gas upgrading system. Aspen Plus® is a commercial and user-friendly approach that enables define all flowsheet parameters. Our example is taken from our information sheet on the pilot scale system. However, future research may specify these variables depending on system needs, desired product conditions, and feed mix.

Table 2: Modules for gas upgrading systems

Parameter	Value
Membrane type	asymmetric hollow fiber membrane
Flow pattern	co-current flow
Inner diameter [μm]	300
Outer diameter [μm]	500
Active length [m]	0.5
Permeance [10^{-10} mol/s m^2 Pa]	CO_2: 311.4 CO: 12.8 H_2: 971.0 CH_4: 12.4 H_2O: 3348.2

Following four configurations were selected to simulate the membrane's efficacy in purifying methane in a power-to-gas system. A multistage system, in addition to the single stage permeator, is crucial when deciding on a separation method. Figure 3 shows three different two-stage permeator designs. Figure 3 a) has no recycling flow; it is the simplest method for enhancing the primary component in retentate flow. Figures 3b and 3c show a recycling flow to decrease permeate product losses.

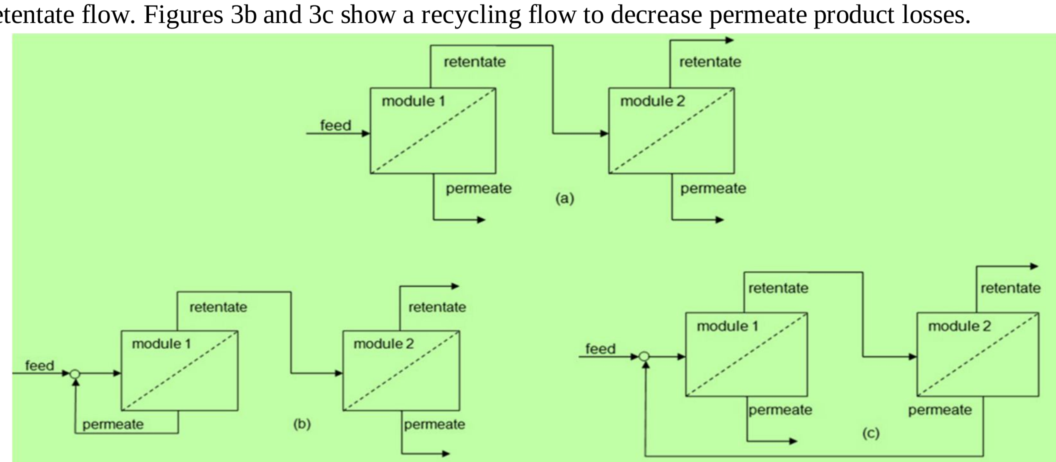


Fig 3: Design arrangement of 2-stage permeator system (b, c) with or (a) without recycling stream

Figure 3 shows the Aspen Plus process settings used to investigate the methanation post-processing process. As a principal product, methane is highly purified. The carbon dioxide content in the exhaust stream is low. A high quantity of methane is found in the outflow stream of the first design (Table 3). Among all designs, it leaks the most methane.

The second design has the lowest methane percentage in the outflow and the poorest overall performance. The third arrangement meets our criteria in a practical way. As a consequence, the final one is now part of the flowsheet.

Studies show that two-stage separation systems lose less CH_4 than single-stage separation systems. As a consequence, the initial permeate stream is rich in CO_2 and H_2, ready to be added to the new feed stream to start the methanation reaction. Also, the second module's permeate stream may be recycled before the first permeator.

Table 3: Performance evaluation of two-stage permeators for syngas purification (Figure 3)

Design configuration	CH_4 fraction [%]	CH_4 loss [%]	CO_2 mole fraction [%]
a	98.5	10.0	0.10
b	95.7	7.2	0.13
c	98.0	8.1	0.11

III. COMPREHENSIVE FLOWSHEET

After the methanation process, a complete flowsheet integrates a gas upgrading system. Many models and requirements exist for this system. The PENG ROB technique is now the default property method in Aspen Plus® V8.6 Properties. This property technique is comparable to RK-SOAVE. It is highly recommended for petrochemical and gas processing systems. The PENG-ROB technique may also be used to determine non-polar or moderately polar combination qualities. Carbon dioxide, hydrogen sulfide, and hydrogen are examples of hydrocarbons.

A. Blocks Specification

The flowsheet (Figure 4) includes a pre-heater to boost the feed temperature to the operating set point. This was achieved using an isentropic single stage compressor unit operating model, COMPR.

Flowsheet of a heat exchanger To prepare the reactant, a pre-heating step is necessary. After the methanation process, the product stream temperature must be lowered to 4°C to remove water. The HEATER block handles these single or multiphase computations. The heater produces one exit stream, with or without water. A heat stream from another block might provide the need. If the user only specifies one specification (temperature or pressure), the duty specification is the total of the inlet heat streams. Other than that, the heater relies on the incoming heat stream to calculate net heat duty.

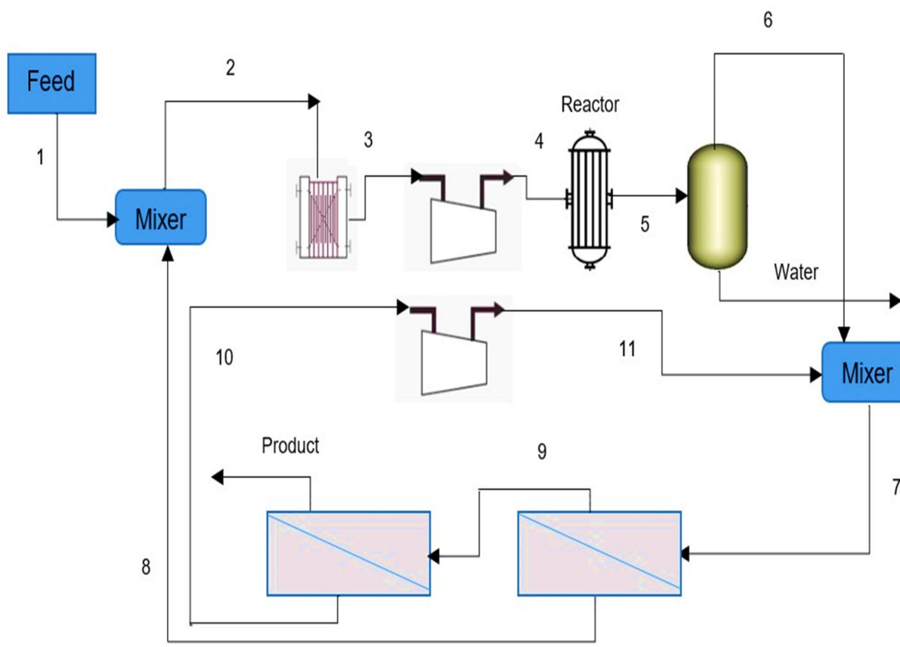


Fig 4: Schematic diagram of methanation and natural gas purification using Aspen Plus® V8.6 flowsheet

The RGIBBS reactor model was used for methanation. As noted earlier (Sharifian and Harasek, 2015), this model accurately confirmed CO2 and CO hydrogenation.

RGIBBS assumes that all species of solution are diffused in all stages. This research looks at both vapor and liquid phases. Also, the model is supposed to regard all components as products. The Setup specification's products sheet may be adjusted to assign species to each solution step. Optional thermodynamic property techniques for each phase. This model's principal working conditions are 250°C and 10 bar pressure.

In the flowchart is the MIXER (Figure 4). The mixer combines the material (or heat) and work streams.

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Volume 10 Issue IX Sep 2022- Available at www.ijraset.com

Table 4: Figure 4 Streams Specification

Stream NO	1	2	4	5	6	7	8	9	10	Product
Mole Fraction CO_2	0.2	0.197	0.197	0.001	0.015	0.013	0.09	0.005	0.04	trace
CO	0	trace	trace	Trace	trace	trace	trace	trace	trace	trace
H_2	0.8	0.797	0.797	0.017	0.075	0.085	0.60	0.041	0.387	0.018
CH_4	0	0.005	0.005	0.332	0.923	0.901	0.39	0.956	0.605	0.982
H_2O	0	trace	trace	0.649	trace	trace	trace	trace	trace	trace
Total mole flow, kmol h^{-1} 4.02		4.07	4.07	2.47	0.54	0.56	0.04	0.52	0.02	0.50
Temperature, ˚C	25	24	250	250	4	4	4	4	4	4
Pressure, bar	1	1	10	10	50	50	1	50	1	50

After methanation, water removal is necessary. FLASH is included in Aspen Plus collection and can be used to calculate 2- or 3-phase equilibrium. Three-phase FLASH creates vapor, liquid, and additional water decant streams. With this model, you may mimic flash separations, evaporators, knock out drums, and other single stage separators, including vapor-liquid deputation. Changes in operating conditions will achieve this separation (mostly pressure and temperature). In our test, we must remove water from the natural gas stream. As a consequence, high pressure and low temperature are necessary to liquefy the product stream's high water content (60 percent). Flash separation occurs at 50 bar and 4°C, with the waste water stream at the bottom and the enriched vapor product at the top.

The USER model purification block is accessible under the CUSTOMIZE ribbon Manage Library (membrane separation system). This study used a two-stage module purification process with recycling streams from the first block to the methanation process and the second block to the first module (Figure 4). These are the result streams in table 4. (Figure 4).

IV. CONCLUSION

This manuscript's main purpose is to purify methane following methanation. Gas grid distribution requires natural gas enrichment. An efficient water removal strategy was detailed as well as strategies to achieve minuscule percentages of carbon dioxide and carbon monoxide in the methanation process's exit. Firstly, water was removed from the product stream using a flash separation. Following this phase, the need for H2 and CO2 removal revealed the requirement of membrane gas separation. There was no built-in model for gas permeation in Aspen Plus V8.6®. Unusual FORTRAN user model for inter gas permeability asymmetric hollow fiber system. This model, like the others in the Aspen Plus® V8.6 library, may be used to build, optimize, and analyze sensitivity of single and multiphase pervaporation systems. Comparison of different designs and arrangements revealed that the two-stage separation system without recycling lost the most value output. The two-stage with recycle initial permeate stream had a high quantity of CO2, which may be fed into the methanation process. Due to the high CH4 content, the subsequent module permeate stream may be built before the first permeator. Finally, a complete methanation and purification flowsheet was built.

V. ACKNOWLEDGEMENT

I thank co-authors for their expertise and assistance throughout all aspects of this research work.

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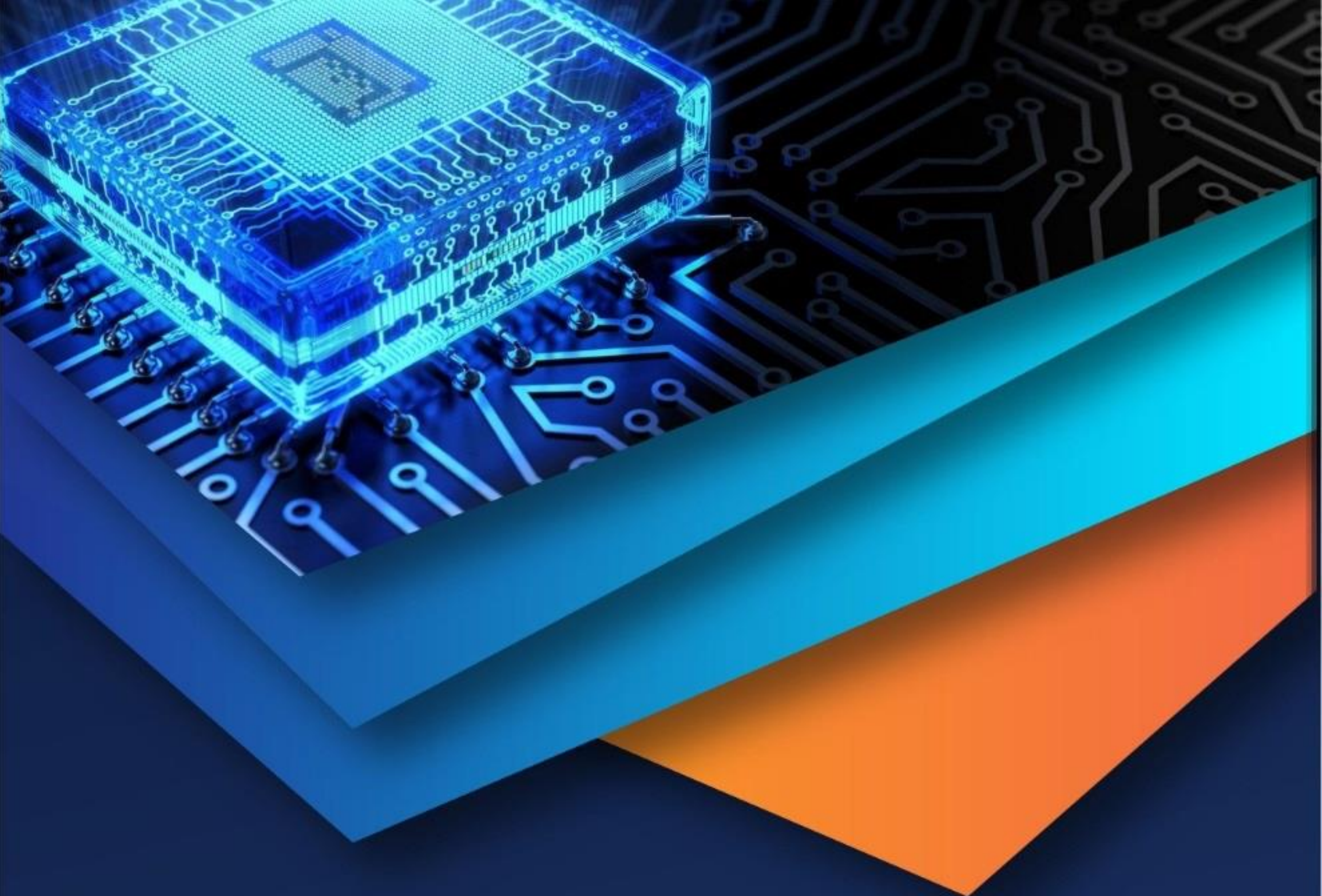

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