Studying the Effect of Carbon Dioxide on the Hydrate Formation of Natural Gas Mixtures Using Simulation Packages

by

Maryam Farzanah Mohd Fauzi

Dissertation submitted in partial fulfilment of
the requirements for the
Bachelor of Engineering (Hons)
(Chemical Engineering)

SEPTEMBER 2012

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CERTIFICATION OF APPROVAL

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Approved by,

_____

(AP Dr Khashayar Nasrifar)

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
September 2012

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

_____

MARYAM FARZANAH MOHD FAUZI

ACKNOWLEDGEMENT

My utmost gratitude goes to the Almighty God whom without His help by giving good health and time, I am unable to finish my project successfully.

This project would not be completed successfully without the assistance and guidance from individuals. Therefore, I owe my deepest gratitude to my supervisor, AP Dr Khashayar Nasrifar for his useful guidance, complete trust, and strong encouragement given. Thank you for the knowledge accommodated and the continuous support throughout the project.

Sincerest gratitude goes to Mr Behzad for his valuable input and guidance in HYSYS training. To the Final Year Research Paper and Project Coodinators, Dr Anis Suhaila bt Shuib (FYP I) and Dr Norhayati Mellon (FYP II), thank you for coordinating the series of trainings and talks, useful information, and quick respond towards the project completion. I thank all staffs of Chemical Engineering Department intentionally and unintentionally for any guidance and information regarding this course.

Last but not least, my warmest thanks to my dear family and friends who always give me undivided support and wonderful motivations I most certainly need to keep me driven.

ABSTRACT

Hydrate is a crystalline structure that is composed of water and small gas molecules. In natural gas processing field, the presence of hydrate may cause blockage to natural gas pipeline, which can contribute to huge economic loss. A previous experimental work reported that natural gas with high CO_2 content has a higher tendency of hydrate formation (Yu, Huen, and Ji, 2001). Unlike hydrocarbon, CO_2 is highly soluble in water. The objective of this project is to look into models that can best predict interaction of CO_2 and water to form hydrate. In this project, Aspen HYSYS software and CSMHyd hydrate program are used as simulation tools for hydrate phenomena. Hydrate formation condition is investigated at different composition of CO_2-containing gases. As a result, it is found that a higher CO_2 content corresponds to a higher tendency of hydrate formation. This is in agreement with the theory and previous experimental results. HYSYS and CSMHyd simulation results in this project can both accurately predict hydrate formation pressure of high CO_2 content gases. The presence of N_2, glycerol or salts, however, may decrease the accuracy of the prediction.

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LIST OF ABBREVIATIONS

NG	Natural gas
CO_2	Carbon dioxide
AADP	Average Absolute Deviation in Pressure
%E	Percentage error
PR	Peng-Robinson

CHAPTER 1
INTRODUCTION

1.1 BACKGROUND OF STUDY

Natural gas is a combustible mixture of gases that primarily comprises of hydrocarbons (Overview of Natural Gas, 2011). Common elements in natural gas include methane, ethane, propane, butane, carbon dioxide, oxygen, nitrogen, and hydrogen sulphide. Depending on location, natural gas varies in terms of its composition. Natural gas with high carbon dioxide (CO_2) composition is called acidic gas, while a high hydrogen sulphide (H_2S) content natural gas is called sour gas (Sour Gas, 2012).

Hydrate is a crystalline compound containing physically-combined water molecules. Water traps other light gas molecules, like carbon dioxide and methane to form hydrate. Water molecules form a cage with large cavities using hydrogen bonding, which can be occupied by selected light gas molecules, or commonly called guest molecules (Ganji et al., 2007). Hydrate forms at a high pressure and low temperature condition.

There are three types of hydrate structures, namely structure I, structure II and structure H (Sloan, 1997). Structure I forms with small guest molecules like carbon dioxide, methane, and ethane (Nasrifar and Moshfeghian, 2000). Larger molecules such as propane and iso-butane will form structure II (Nasrifar and Moshfeghian, 2000). On the other hand, structure H forms when two guest molecules are encaged (Nasrifar and Moshfeghian, 2000).

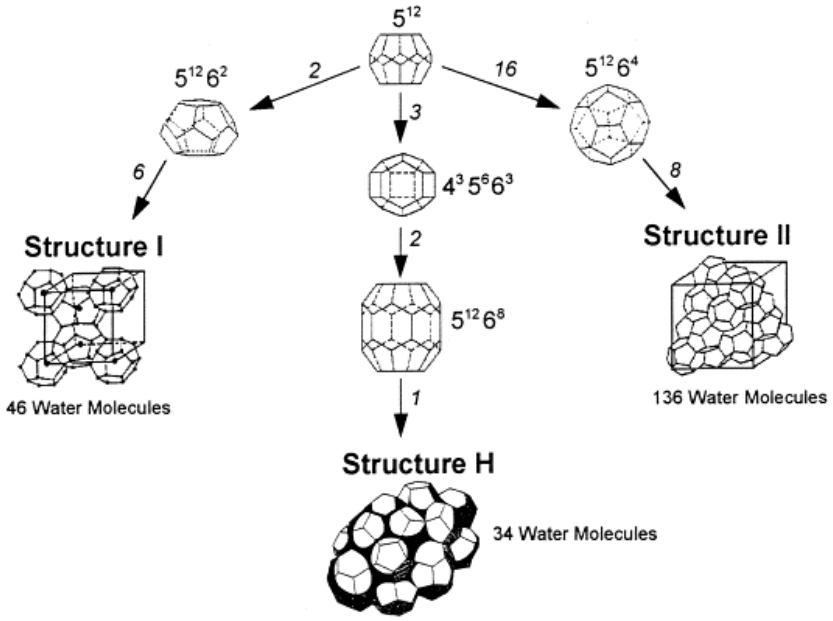


Figure 1: Three Structures of Hydrates
Source: Khokhar, Gudmundsson, and Sloan (1998)

In natural gas pipeline, formation of hydrate is disadvantageous. Formation of hydrate during natural gas transportation may cause plugging in the gas pipeline and equipment, which can contribute to safety hazards and economic loss (Wu, Wang, and Liu, 2007). Many wells around the world contained high CO_2 content natural gas, with CO_2 taking up to 80% of the overall composition (Azmi, Mukhtar, and M Sabil, 2010). It is believed that a high content of CO_2 in natural gas enhances hydrate formation. This hypothesis can be proven with the experiment results obtained in previous researches such as research by Fan et al. (2000), Sloan (1997), Yu et al. (2001), and Servio et al. (1999).

In a study conducted by Yu, Huen, and Ji (2001), it is discovered that at lower pressure, selectivity of CO_2 over methane (a hydrocarbon gas) as a guest molecule in hydrate phase is higher. When the concentration of CO_2 in vapour phase increases, then its concentration in hydrate phase will also increases (Yu, Huen, and Ji, 2001). One approach to prevent hydrate formation is by the addition of hydrate inhibitors to the natural gas. Inhibitors shift the condition of hydrate formation to be at lower temperature and higher pressure. The effect of inhibitors on a pressure-temperature graph can be shown in Figure 2.

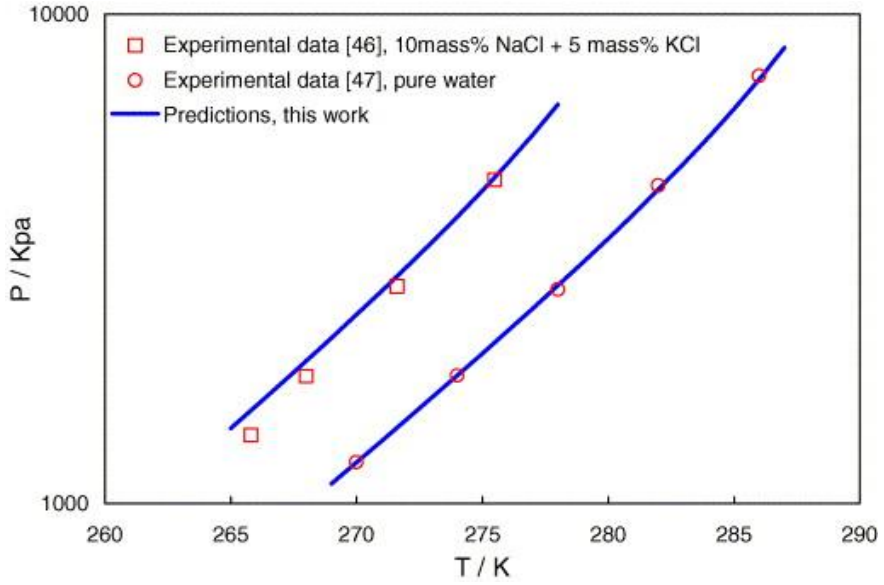


Figure 2: Effect of addition of inhibitors (NaCl & KCl)
Source: Rahim Masoudi (2004)

1.2 PROBLEM STATEMENT

In Malaysia, the natural gas (NG) commonly has high composition of CO_2. The composition of CO_2 can reach as high as 80% in certain NG wells (Azmi, Mukhtar, and M Sabil, 2010). Experimentally, a natural gas with high CO_2 content is reported to have a higher tendency of hydrate formation, compared to a typical natural gas (Yu, Huen, and Ji, 2001). The inhibiting effects of various inhibitors on hydrate formation have also been determined from conducted past experiments.

Since CO_2 is highly water-soluble in nature, its interaction with water may differ with other hydrocarbon components in natural gas. Thus, looking into correlation that can best predict interaction of CO_2 and water to form hydrate would assist in prevention of hydrate formation in pipeline.

1.3 OBJECTIVE AND SCOPE OF STUDY

This project aims to determine whether the models used in simulation software can accurately predict the effect of CO_2 in hydrate formation phenomena.

The scope of this project includes:

- To simulate the hydrate formation pressure for CO_2-containing gases with/ without the presence of inhibitors.

- To compare, using experimental results, the accuracy of hydrate formation prediction of the selected simulation approach.

1.4 PROJECT RELEVANCY

Natural gas with high CO_2 content is massively encountered in South China Sea, Gulf of Thailand, Central European Pannonian basin, Australian Cooper-Eromanga basin, New Zealand, etc. (Azmi, Mukhtar, and M Sabil, 2010). Therefore, it is very important to study on the effect of high CO_2 content to hydrate formation in natural gas. The project's aim is relevant to many natural gas processing plants since the condition for hydrate formation and its potential inhibitors are studied. In terms of course relevancy, the project involves hands-on experience using simulation programmes, which are very useful in simulating plant design. The project also comprises of study in thermodynamics of hydrate formation that closely related to chemical engineering course.

1.5 PROJECT FEASIBILITY

In terms of the scope, this project can be considered feasible as it involves a simulation studies with clearly defined goals. Whereas in terms of the time frame, the time allocated to complete the project is two semesters (8 months). This project is feasible to be done within the scope and time frame allocated with a proper planning. The planning of the project flow can be illustrated in Gantt chart (See Table 3).

CHAPTER 2
LITERATURE REVIEW

Previously, there are plenty of researches conducted in the field of natural gas hydrate. Some focuses on the prevention of hydrate formation as it causes blockage to pipeline or equipment. On the other hand, some others find opportunities in its formation, such as in environmental protection, transportation or storage.

Fan et al. (2000) investigated the conditions which causes hydrate formation in pure CO_2 and CO_2-rich gas mixture. The purpose of the study is to explore the hydrate formation of CO_2 and CO_2-rich gas mixture in the presence of an inhibitor, ethylene glycol (EG). In their studies, experiments were conducted using a sapphire cell installed in an air bath. Hydrate will be rapidly formed/dissociated inside the cell with the presence of magnetic stirrer. The experiment adapted isothermal-pressure search method to determine hydrate formation conditions. In this method, temperature is kept constant while pressure change is imposed. This method takes shorter time towards thermal equilibrium compared to enforcing temperature change (Servio and Englezos). A total of 8 systems have been studied, with 3 systems involving pure CO_2 and 5 systems involving CO_2-rich gas mixture.

Figure 3 and Figure 4 illustrate the results of the experiment conducted by Fan et al. (2000). Based on the result in Figure 3, addition of methanol or EG to a pure CO_2 system are observed to inhibit formation of hydrate, as it shift the P-T curve towards a lower temperature and higher pressure condition. Figure 4 is consistent with the hypothesis, whereby tendency of hydrate formation is higher in a system with higher concentration of CO_2.

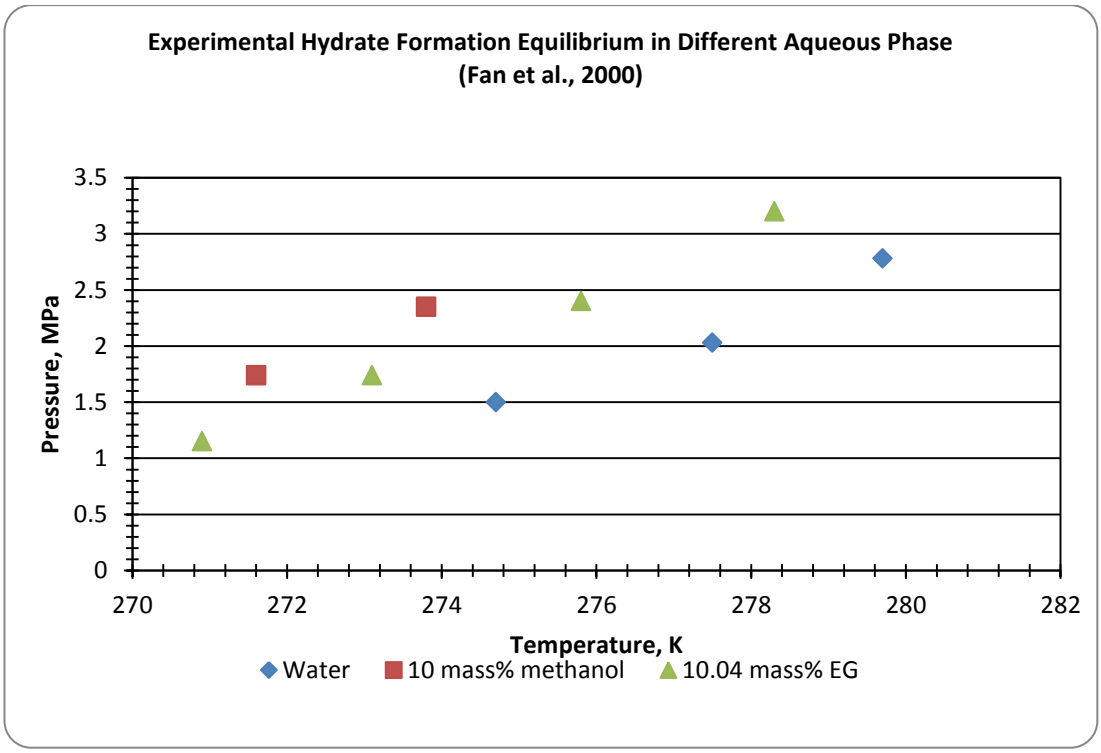


Figure 3: Experimental Hydrate Formation Data in Different Aqueous Phase (Fan et al., 2000)

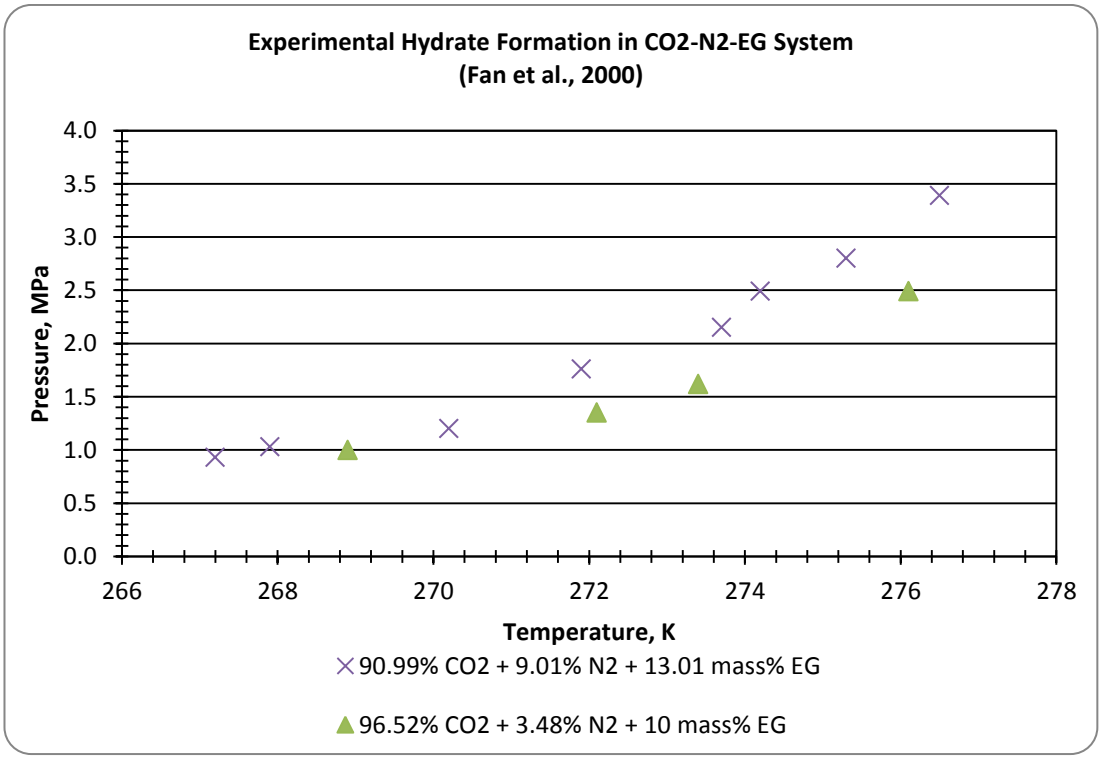


Figure 4: Experimental Hydrate Formation Data in CO2-N2-EG System (Fan et al., 2000)

Servio et al., (1999) conducted a study with an objective to investigate the formation of structure H hydrate in methane-CO_2 gas mixture with either pure water or neohexane solution in aqeouous phase. This experimental study also applied the isothermal-pressure search method. 80-20% and 50-50% methane-CO_2-neohexane mixture are tested against methane-CO_2-water mixture for any proof of structure H hydrate formation. As a result, it is believed that the presence of neohexane enhance the formation of structure H hydrate, assuming neohexane does not participate in the crystal structure. Comparing the formation condition for 80-20% and 50-50% methane-CO_2-water system, it is found that a higher content of CO_2 (50%) have higher tendency of hydrate formation. The comparison can be illustrated in Figure 5.

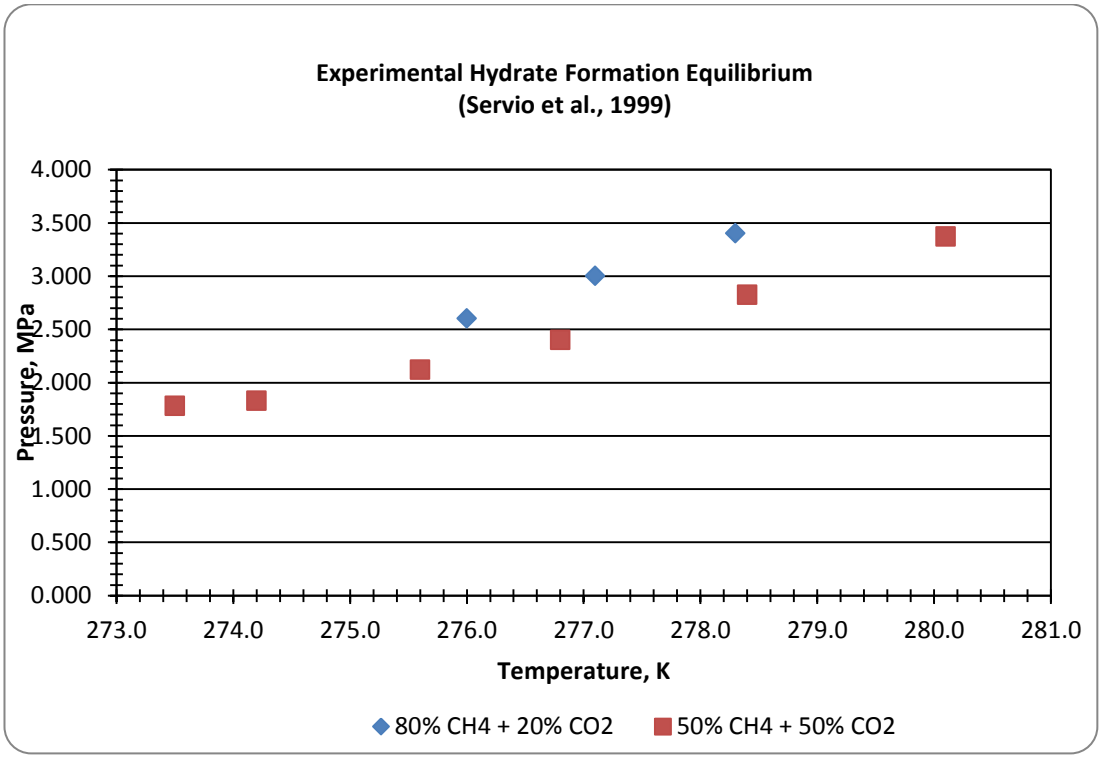


Figure 5: Experimental Hydrate Formation Data in CH4-CO2 System (Servio et al., 1999)

According to a compilation of experimental results in Sloan (1997) book, Adisasmito and Sloan (1992) examined the hydrate formation condition in natural gases containing different composition of CO_2. This work measured the equilibrium of a three-phase system (vapor-hydrate-aqueous liquid) in natural gas with high CO_2 content. The result of thie experimental work can be summarized in Figure 6.

Refering to Figure 6, it can be observed that at a higher CO_2 composition (83% and 90%), the tendency of hydrate formation increases with increasing CO_2 content. On

the other hand, at a lower CO_2 composition (0%, 31% and 67%), the results show contradiction to the hypothesis made for this project, since the tendency of hydrate formation decreases when CO_2 content increases.

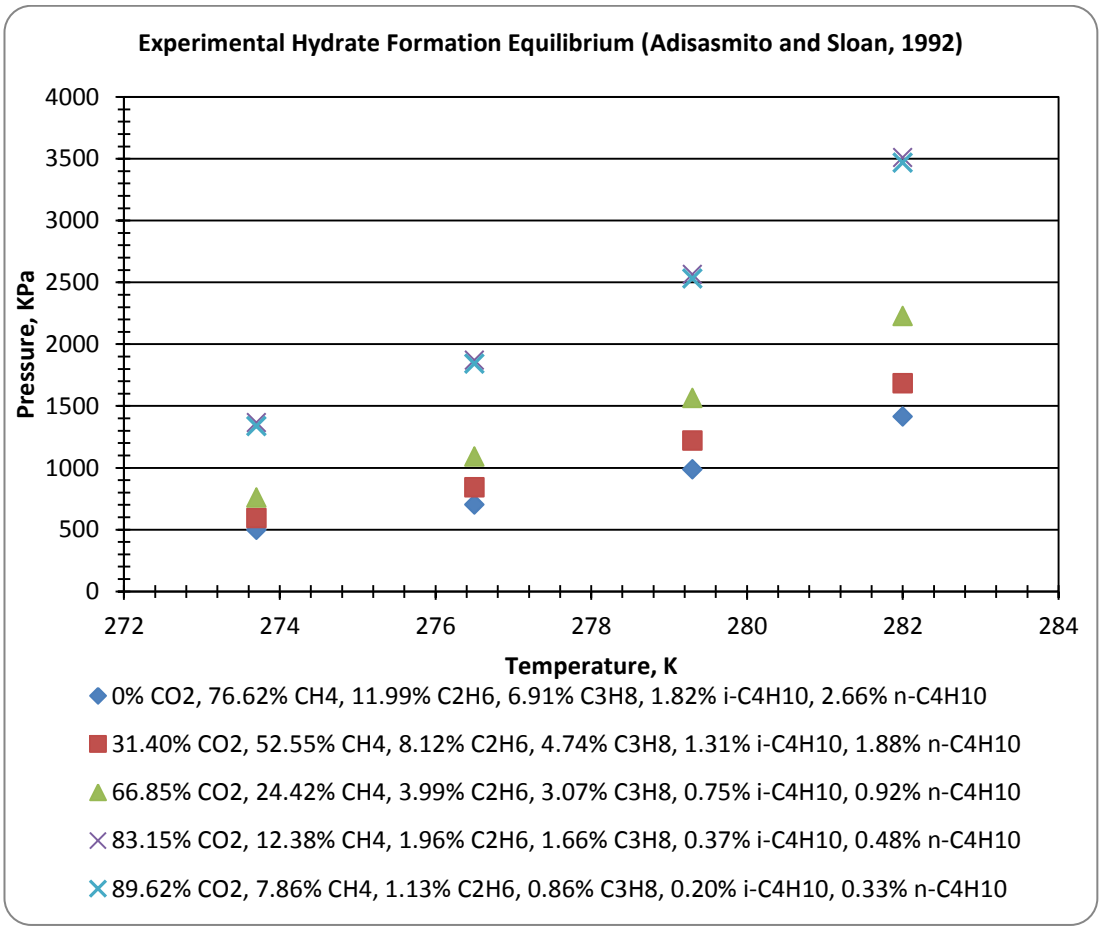


Figure 6: Experimental Hydrate Formation Equilibrium Data (Adisasmito and Sloan, 1992)

An experiment conducted by Yu, Huen, and Ji (2001) analyse the selectivity of CO_2 over methane in occupying the hydrate cage. This research use similar approach of experimental method with Fan et al. (2000) and Servio et al. (1999). According to Yu, Huen, and Ji (2001), in any composition fraction of CO2, occupancy of CO_2 in hydrate is preferred over methane when the equilibrium pressure is low. As observed in Figure 7, the curve shifted to a higher T and lower P condition as CO_2 composition increases.

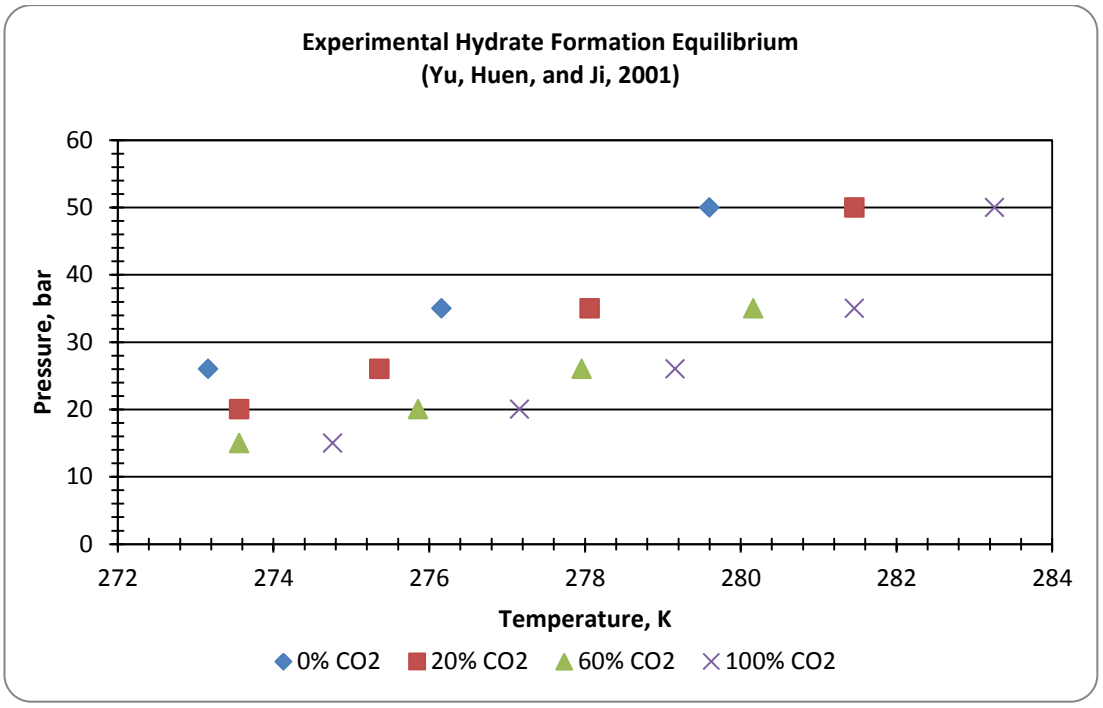


Figure 7: Experimental Hydrate Formation Data in CO2-CH4 System (Yu, Huen, and Ji, 2001)

Currently, hydrate formation can be prevented by addition of two types of inhibitors: thermodynamic inhibitors and kinetic inhibitors (Wu, Wang, and Liu, 2007). Thermodynamic inhibitors prevent hydrate formation by changing the chemical potential of hydration, thus shifting the phase equilibrium curves to a lower temperature and higher pressure (Wu, Wang, and Liu, 2007). Methanol and diethylene glycol are example of thermodynamic inhibitors (Baharudin, 2012). Whereas for the kinetic inhibitors, hydrate formation is prevented by delaying its nucleation and growth (Baharudin, 2012). The time for hydrate nucleation is longer with the presence of kinetic inhibitors like polymers and copolymers (Baharudin, 2012).

Compared to thermodynamic inhibitor, a kinetic inhibitor requires less concentration to control hydrate formation (Baharudin, 2012). In other words, a kinetic inhibitor has higher efficiency than a thermodynamic inhibitor (Wu, Wang, and Liu, 2007). However, one drawback of kinetic inhibitors is that it can only be applied in moderate sub-cooling of temperature less than 13°C (Baharudin, 2012). In practice, it is advantageous to use both thermodynamic inhibitor and kinetic inhibitor together (Wu, Wang, and Liu, 2007). A new type of inhibitors has been researched to cope with the drawbacks of both inhibitor types. This type is called thermo-kinetic

inhibitors, which not only shift the phase equilibrium, but also delay the hydrate nucleation time (Baharudin, 2012). Ionic liquids have been recognized to exhibit such potential due to their strong electrostatic charge and hydrogen bond with water (Hafiz).

For this study, 11 experimental studies of hydrate formation in CO_2-containing gas have been compiled and compared to. The following table summarizes the referred studies. Uninhibited data points refer to systems without inhibitors, while inhibited data points refer to systems with the presence of inhibitors.

Table 1: List of Experimental Studies References

Ref.	Experimental studies references	Data points		
		Uninhibited	Inhibited	**Total**
a	Fan et al. (2000)	3	33	36
b	Servio et al. (1999)	18	0	18
c	Yu, Huen and Ji (2001)	13	0	13
d	Adisasmito and Sloan (1992)	16	0	16
e	Dholabhai, Parent and Bishnoi (1996)	2	40	42
f	Breland and Englezos (1996)	3	19	22
g	Herri et. al. (2011)	21	0	21
h	Robinson and Mehta (1971)	44	0	44
i	Sabil, Witkamp and Peters (2010)	10	0	10
j	Bishnoi and Dholabhai (1999)	7	44	51
k	Dholabhai, Parent and Bishnoi (1997)	4	64	68
TOTAL		141	200	**341**

CHAPTER 3
METHODOLOGY

3.1 RESEARCH METHODOLOGY

In this work, two simulation tools, Aspen HYSYS and CSMHyd will be used to determine the hydrate formation pressure in gases containing CO_2, and with an addition of various inhibitor types. From the result, the effect of CO_2 and the effectiveness of inhibitors will be analysed. Comparison of the simulation result with previous experimental results will also be made to evaluate the accuracy of the results.

Basically in the study of natural gas hydrate formation, the equilibrium relation between three phases – vapour, liquid water, and solid hydrate (VL_WH) – is studied. The basic equations for this three-phase (VL_WH) equilibrium are (Karamoddin and Varaminian, 2011):

$$f_{H_2O}^{V} = f_{H_2O}^{L} = f_{H_2O}^{H}$$

Where $f = fugacity$. Thermodynamically, formation of gas hydrate can be expressed using van der Waals-Platteeuw model using the following chemical potential equation:

$$\Delta\mu_w{}^{H} = -RT \sum_m v_m \ln\left(1 - \sum_j \theta_{mj}\right)$$

Where v_m is the number of cavities of type m per water molecule in the hydrate lattice, and θ_{mj} is the fraction of cavities of type m that are occupied by the guest j. The prediction of hydrate formation utilizes the Equation of State (EOS) to determine the two-phase equilibrium. EOS enables calculation of the fugacity of components in gas and liquid phases. Mixing rule is then used to complement EOS in order to determine the equilibrium between three phases. In HYSYS, Peng-Robinson EOS is utilized for this work. The PR (Peng-Robinson) EOS is as follows (Karamoddin & Varaminian, 2011):

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

Where the coefficients a and b are obtained using equations in mixing rule.

3.2 PROJECT ACTIVITIES

The project activities can be divided into the following:

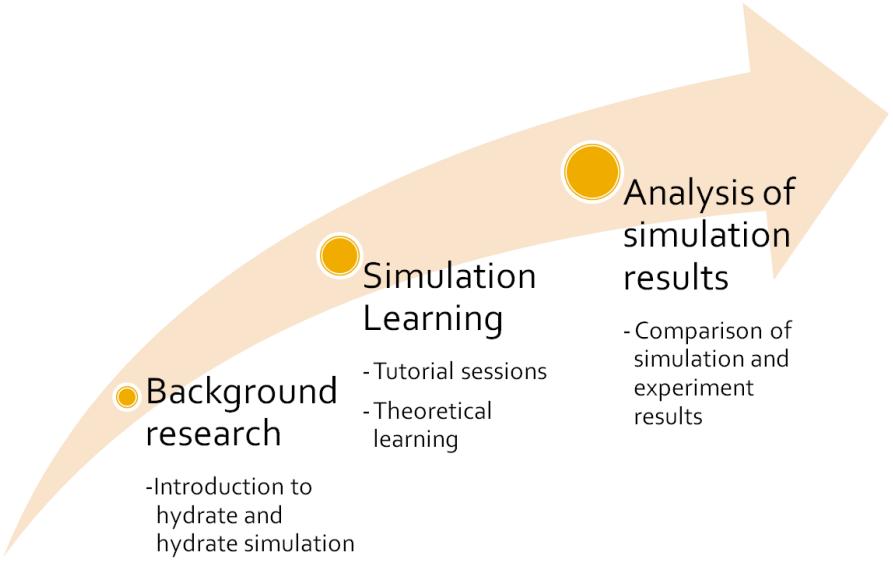


Figure 8: Planning of Project Activities

Background research work

- Understand of previous researches, obtain suitable experimental data from previous researches, and understand the thermodynamic and kinetic properties of hydrate formation

Simulation learning

- Learn using hydrate simulation softwares, understand the theories related to simulation, and define hydrate formation using software predictions.

Analysis of simulation results

- Compare simulation results with experimental results and calculate accuracy from results' deviation.

3.3 TOOLS

Software required : *Aspen HYSYS simulation tool*
CSMHyd hydrate program

3.4 SIMULATION FLOW

The flow of the simulation can be illustrated using the following algorithm:

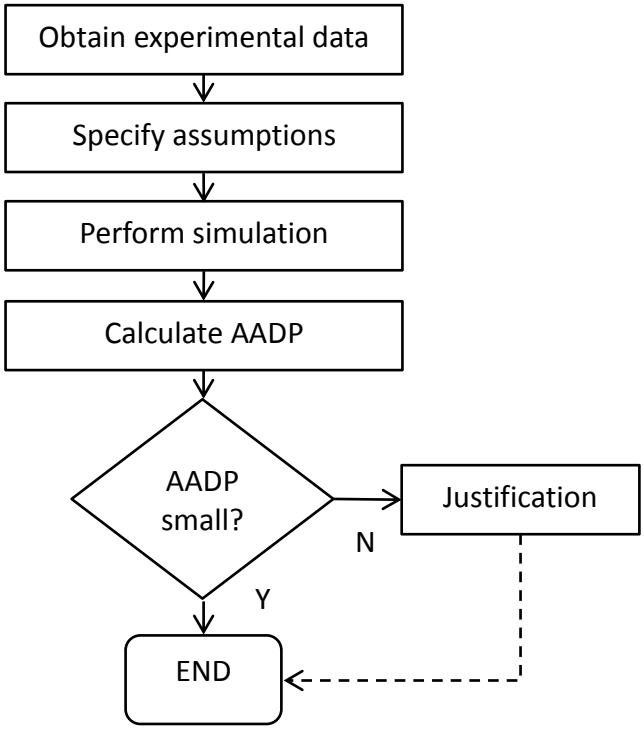


Figure 9: Simulation Algorithm

3.5 KEY MILESTONES

The milestones for FYP 2 can be summarized into the overleaf table:

Table 2: Key Milestones for FYP 2

Week	Events/ Milestones
1	Project's planning
2	Begin simulation activity
4	Begin analysis of simulation results
8	**Nov, 5**: Submission of progress report
11	**Nov, 26**: Pre-EDX presentation
12	**Dec, 3**: Submission of draft report
13	**Dec, 10**: Submission of soft bound dissertation and technical paper
14	Oral presentation
-	**Jan, 11**: Submission of hardbound dissertation

3.6 GANTT CHART

Table 3: Gantt Chart for Project

Week / Work Activity	FYP 1														FYP 2													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Identification of problem • Topic discussion																												
Planning phase • Prelim. research work • Extended proposal • Proposal defence																												
Development phase • Research work • Interim/progress report • Simulation development																												
Analysis phase • Discussion																												
Evaluation phase • Improvement/suggestion for continuation • Final report																												

CHAPTER 4
RESULT AND DISCUSSION

For this study, 129 systems consisting of 341 experimental data points have been studied. These data points are assumed to correctly represent the actual hydrate formation condition. Comparisons are made by using two means; HYSYS prediction and CSMHyd prediction. The corresponding value of hydrate formation pressure for CO_2-containing gas is simulated for a specified temperature. The simulation is done according to systems' category, and the simulation values obtained will then be compared to the experiment results.

For HYSYS simulation, Peng-Robinson property-package is selected as the basis environment. There are two approaches used for HYSYS simulation, which are based on two comparable assumptions.

The second means of comparison is made by using CSMHyd. For this simulation software, mol% of each gas component and mass% of inhibitors is specified to obtain hydrate formation pressure at a specified temperature.

The approaches used for simulation in this work can be summarized using the overleaf table.

Table 4: Summary of Simulation Approaches

Approach	HYSYS[A]	HYSYS[B]	CSMHyd
Gas composition specified?	Yes	Yes	Yes
Inhibitor composition specified?	Yes (if any)	Yes (if any)	Yes (if any)
Water composition specified?	**Yes**	**No**	**No**
Assumptions	Peng-Robinson property package	Peng-Robinson property package	Nil
	Gas flow rate = 100 kmol/h	Gas flow rate = 100 kmol/h	
	Solution flow rate = **1000 kmol/h** of **water and inhibitor** (if any)	Solution flow rate = **mass%** of **inhibitor** (if any) [kg/h]	

Two approaches used for HYSYS simulation are method A and method B. In HYSYS method A, water composition are specified in the simulation, whereas in HYSYS method B, water composition is not specified. The assumption in HYSYS method A is made to represent the actual condition of an experimental procedure, whereby the flow of solution is continuous. Therefore in this assumption, a ratio of 1:10 molar flow rate of gas-to-solution is used to reflect a free flow of solution.

On the other hand, HYSYS method B neglects the composition of water in the system. In thermodynamic models for hydrate calculation, water component is omitted from the equation. In other words, thermodynamically, calculation of hydrate formation does not require water component to be included. Hence, HYSYS method B is made to depict the thermodynamic models in calculating hydrate formation.

Values predicted by HYSYS method A, HYSYS method B, and CSMHyd are compared with the compiled experimental data. The results are evaluated based on the percentage deviation of hydrate formation pressures. The average absolute deviation in pressure (AADP) is calculated as:

$$AADP = \frac{\sum_n (|P_{predicted} - P_{experimental}|)/P_{experimental}}{n} \times 100\%$$

Where n = number of data points. A simulation approach with the smallest AADP indicates that it is the most accurate approach.

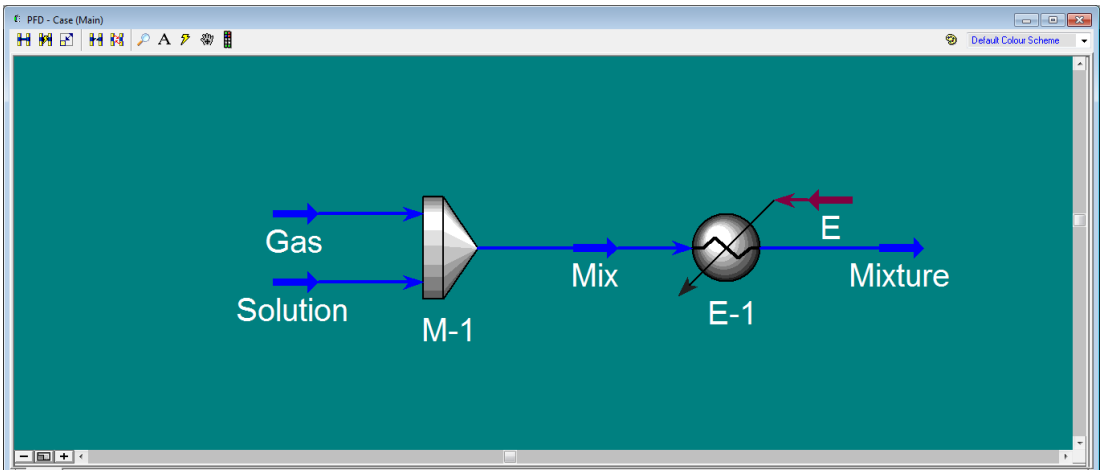


Figure 10: Simulation using HYSYS

```
   THREE-PHASE (Lw-H-V) EQUILIBRIUM CONDITION WITH INHIBITOR(S)
 Inhibitor :10.000 wt% Methanol

 Temperature :    278.000 K
 Equilibrium PRESSURE :    5845.078  kPa


Press RETURN to Continue . . .


          Equilibrium Hydrate : STRUCTURE I

       Composition of Phases at Equilibrium (moles)

                          FEED     WATER     VAPOR     HYDRATE
Methane                 0.8000    0.0024    0.8000    0.6771
Carbon Dioxide          0.2000    0.0117    0.2000    0.3229

Press RETURN to Continue . . .
```

Figure 11: Simulation using CSMHyd

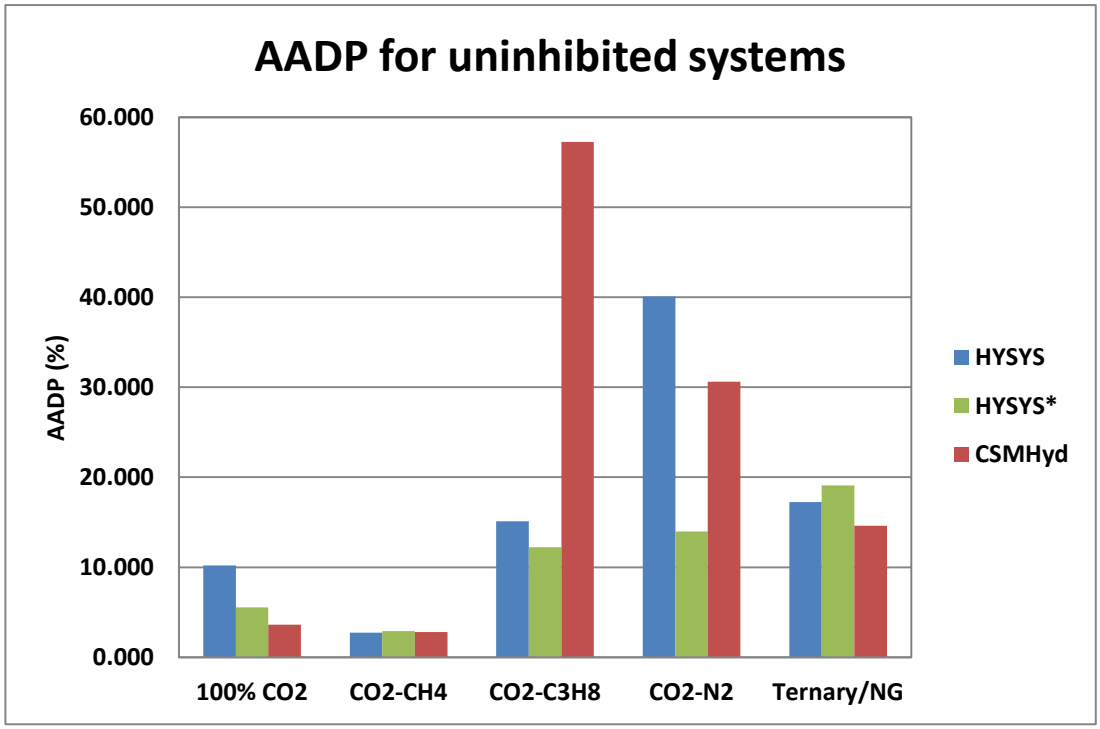
4.1 HYDRATE FORMATION PRESSURES FOR UNINHIBITED SYSTEMS

The results of simulation for uninhibited systems are arranged according to categories. They are classified into the following categories; single system (pure CO_2), binary mixture (CO_2-CH_4, CO_2-C_3H_8, CO_2-N_2), and ternary/natural gas mixture. In general, based on the uninhibited systems studied in this work, HYSYS method B gives a more accurate overall result (AADP = 9.87%).

Table 5 and Figure 12 summarize the results obtained for all uninhibited systems. In general, based on the uninhibited systems studied in this work, HYSYS method B gives a more accurate overall result (AADP = 9.87%).

Table 5: Average Absolute Deviation in Pressure (AADP) for uninhibited systems

Uninhibited systems	AADP		
	HYSYS[A]	HYSYS[B]	CSMHyd
Single (100% CO2)	10.193	5.538	3.620
Binary (CO2-CH4)	2.744	2.922	2.800
Binary (CO2-C3H8)	15.120	12.229	57.233
Binary (CO2-N2)	40.074	13.956	30.601
Ternary/ Natural gas	17.256	19.084	14.596
Overall	**14.368**	**9.865**	**22.354**



HYSYS = HYSYS[A]; HYSYS*= HYSYS[B]

Figure 12: Average Absolute Deviation in Pressure (AADP) for uninhibited systems

Table 6: Experimental Data and Comparison to Simulations for uninhibited, 100% CO_2 System

Experiment			HYSYS[A]		HYSYS[B]		CSMHyd	
Ref	T (K)	P (kPa)	P (kPa)	%E	P (kPa)	%E	P (kPa)	%E
h	270.54	1758.23	<empty>	-	1007.86	42.677	1033.39	41.225
h	273.93	1379.00	1357.22	1.579	1356.28	1.648	1380.67	0.121
a	274.70	1500.00	1483.08	1.128	1482.04	1.198	1503.02	0.201
c	274.76	1500.00	1493.42	0.439	1492.37	0.509	1513.05	0.870
e	275.11	1560.00	1555.41	0.294	1554.32	0.364	1573.06	0.837
i	275.12	1510.00	1557.23	3.127	1556.13	3.055	1574.82	4.293
h	275.21	1558.27	1573.66	0.987	1572.55	0.916	1590.70	2.081
f	275.50	1651.00	1627.96	1.395	1626.81	1.465	1643.13	0.477
k	275.72	1682.00	1670.60	0.678	1669.41	0.748	1684.21	0.132
f	276.80	1936.00	1899.67	1.876	1898.29	1.948	1903.80	1.663
i	276.88	1810.00	1918.06	5.970	1916.67	5.893	1921.35	6.152
g	277.15	2040.00	1981.72	2.857	1980.27	2.928	1981.98	2.844
c	277.16	2000.00	1984.13	0.794	1982.67	0.866	1984.27	0.787
a	277.50	2030.00	2068.05	1.874	2066.52	1.799	2063.98	1.674
i	277.83	2110.00	2153.66	2.069	2152.04	1.993	2145.00	1.659
k	278.70	2393.00	2401.23	0.344	2399.36	0.266	2377.78	0.636
h	278.93	2420.15	2472.58	2.167	2470.64	2.086	2444.41	1.003
i	278.99	2400.00	2491.64	3.818	2489.68	3.736	2462.17	2.591
c	279.16	2600.00	2546.67	2.051	2544.65	2.129	2513.82	3.315
e	279.49	2620.00	2658.09	1.454	2655.93	1.371	2616.69	0.126
a	279.70	2780.00	2732.33	1.715	2730.08	1.796	2685.25	3.408
i	279.94	2700.00	2820.61	4.467	2818.24	4.379	2766.43	2.460
f	280.20	3021.00	2920.64	3.322	2918.14	3.405	2858.01	5.395
h	280.71	3130.33	3131.57	0.040	3128.76	0.050	3049.53	2.581
i	280.71	3000.00	3131.57	4.386	3128.76	4.292	3049.53	1.651
i	281.42	3300.00	3463.41	4.952	3460.02	4.849	3351.08	1.548
c	281.46	3500.00	3483.64	0.467	3480.21	0.565	3369.14	3.739
h	282.04	3840.52	3798.94	1.083	3794.82	1.190	3647.67	5.021
i	282.06	3600.00	3810.62	5.851	3806.47	5.735	3657.85	1.607
i	282.41	3900.00	4025.21	3.210	4020.48	3.089	3843.96	1.437
i	282.90	4300.00	5888.07	36.932	4358.23	1.354	4131.30	3.923
c	283.26	5000.00	9672.09	93.442	6209.15	24.183	4366.63	12.667
h	283.32	4467.96	10339.84	131.42	6714.61	50.284	4408.26	1.336
			AADP	10.193	AADP	5.538	AADP	3.620

Ref according to Table 1

Table 6 shows the average pressure deviation of uninhibited, pure CO_2 systems. For single systems (100% CO_2), HYSYS simulation of method A and method B gives a great prediction for temperature range of 271K – 282K. However, the software is observed could not simulate the hydrate formation pressure at temperature less than

271K. While for temperature higher than 282K, HYSYS often over-predict the hydrate formation pressure of a system.

For all temperature range, AADP for 100% CO_2 systems simulated by HYSYS method A is 10.193%. On the other hand, simulation on HYSYS method B gives an overall AADP of 5.538% for the mentioned system. Meanwhile, CSMHyd simulation for 100% CO_2 systems gives the lowest AADP, which is 3.62%. Therefore, in this system, HYSYS method B is preferred over HYSYS method A, as it gives smaller AADP. Figure 13 - Figure 19 illustrate comparison between experiment results, HYSYS method B and CSMHyd simulations for various systems.

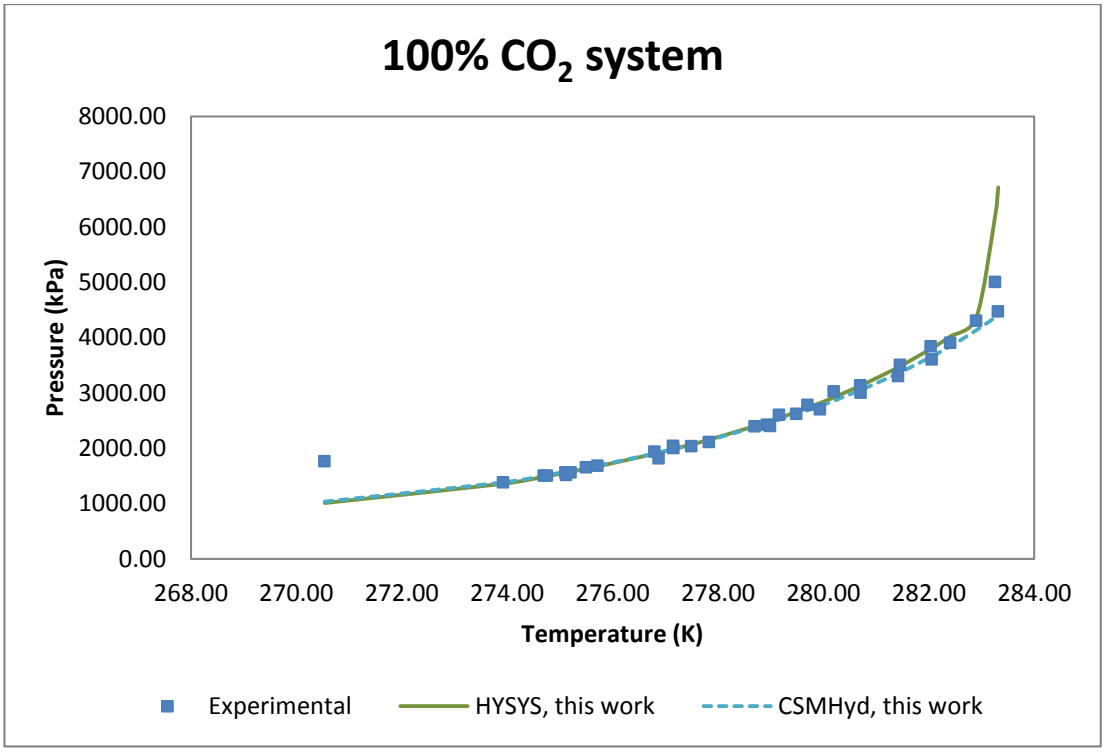


Figure 13: Hydrate Formation Curve for Pure CO_2 System

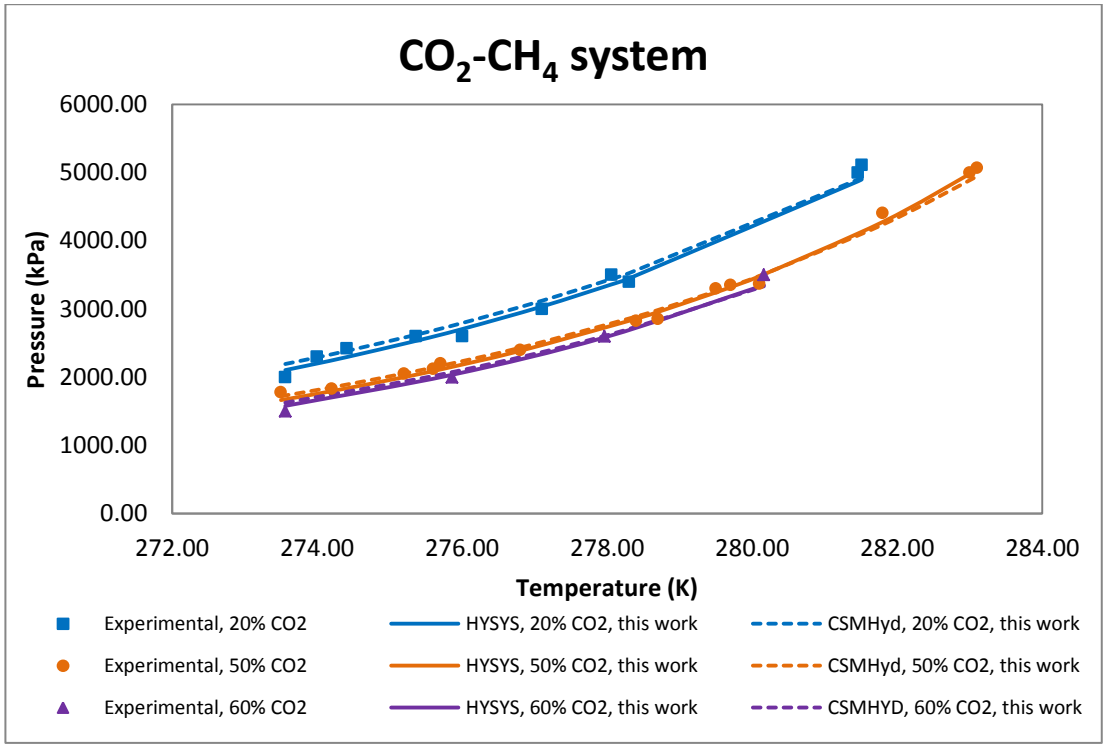


Figure 14: Hydrate Formation Curve for CO_2-CH_4 System

For binary CO_2-CH_4 systems, both HYSYS method B and CSMHyd give a relatively low deviation compared to other systems. Both simulation models are in great agreement with the experimental values. It is observed that CSMHyd offers slightly better result for CO_2-C_3H_8 systems, as compared to HYSYS ($AADP_{CSMHyd}$ = 2.800%, $AADP_{HYSYS}^{B}$ = 2.922%).

Whereas for CO_2-N_2 system, switching between simulation method A and B makes a huge difference in the AADP values ($AADP_{HYSYS}^{A}$ = 40.074%, $AADP_{HYSYS}^{B}$ = 13.956%). Based on the hydrate formation curve in Figure 15, deviation from CSMHyd is relatively huge compared to deviation from HYSYS method B. The large deviation may be caused by unsuitability of nitrogen, a non-hydrocarbon component, to be simulated using CSMHyd model. HYSYS shows acceptable agreement with the experimental data for this system (refer the following Figure 15).

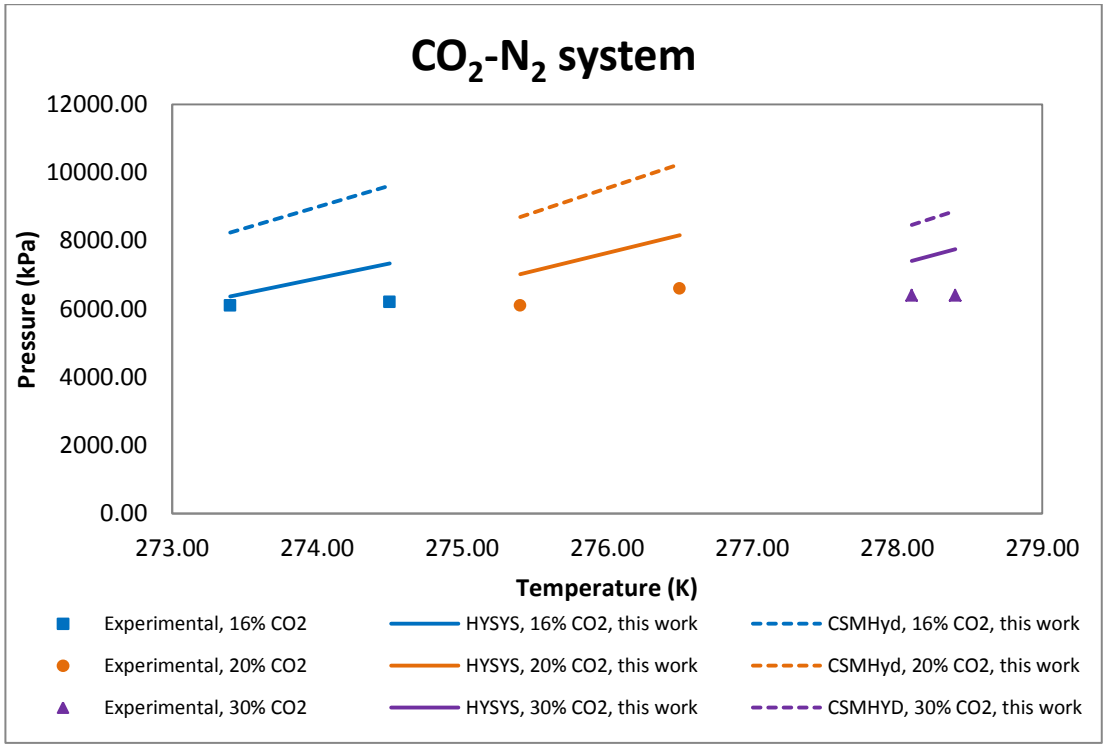


Figure 15: Hydrate Formation Curve for CO_2-N_2 System

Figure 16 and Figure 17 below illustrate hydrate formation curve for binary CO_2-C_3H_8 system. Based on the graph, prediction of HYSYS shows better accuracy compared to CSMHyd for all temperature range. CSMHyd gives observable deviation at temperature above 280K. On the other hand, HYSYS formation curve portrays good agreement with the experimental data for CO_2-C_3H_8 system.

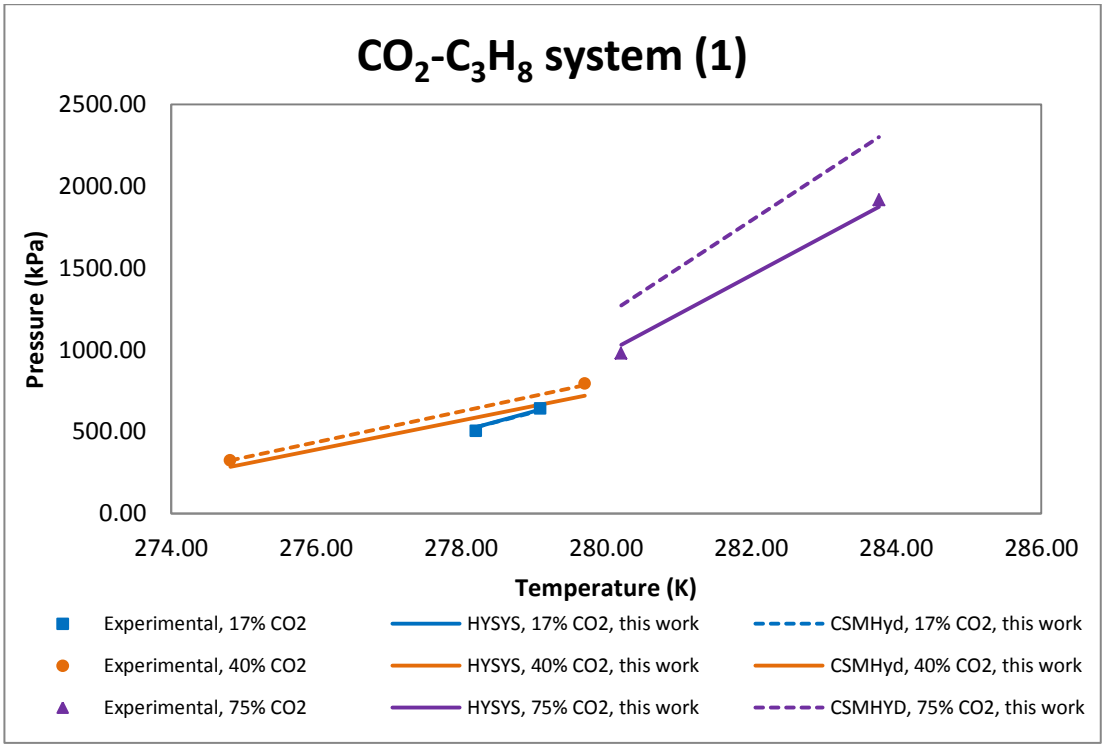


Figure 16: Hydrate Formation Curve for CO_2-C_3H_8 System (1)

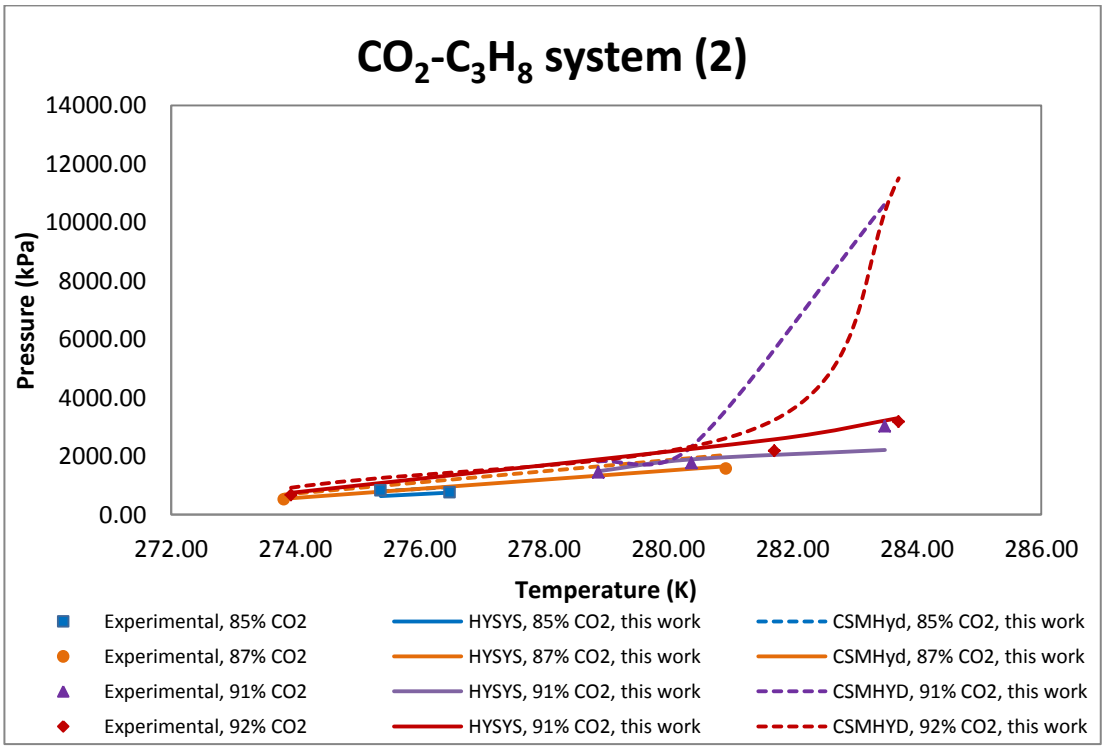


Figure 17: Hydrate Formation Curve for CO_2-C_3H_8 System (2)

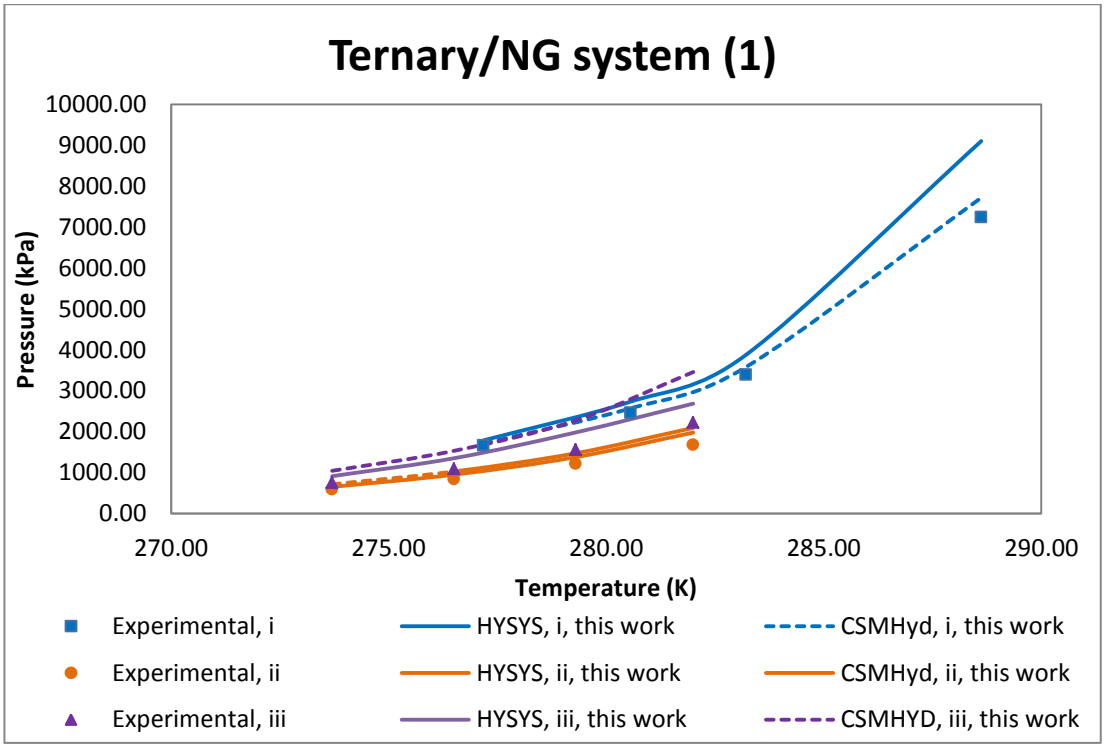


Figure 18: Hydrate Formation Curve for Ternary/NG System (1)

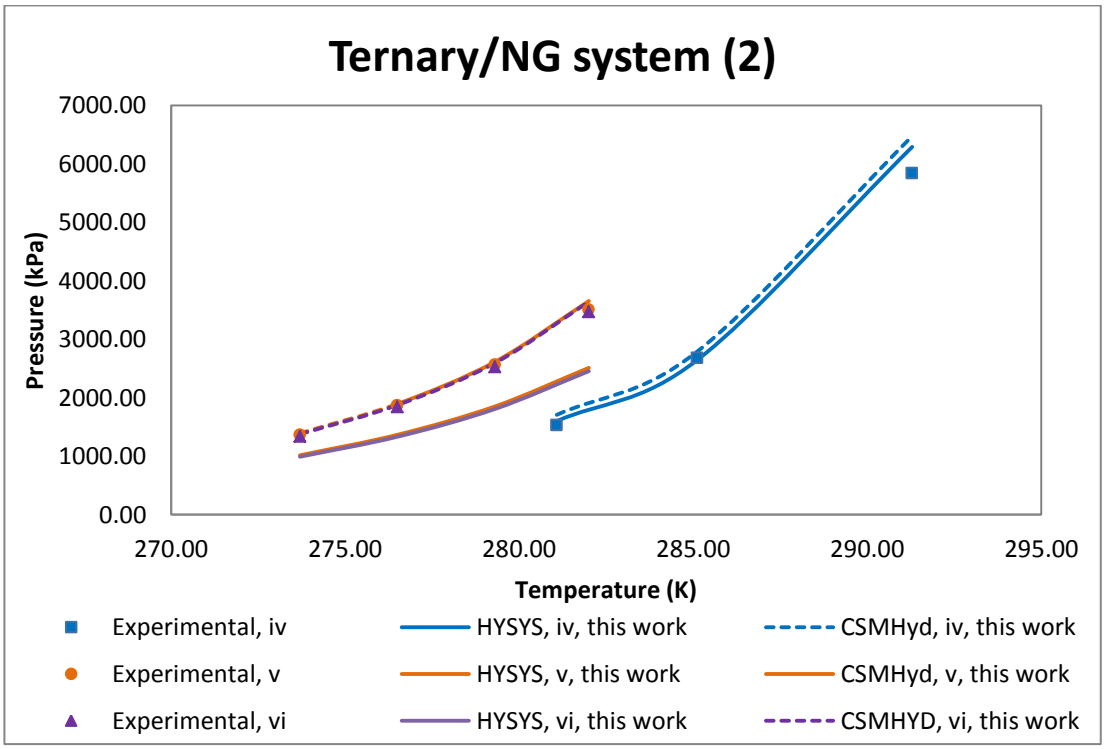


Figure 19: Hydrate Formation Curve for Ternary/NG System (2)

Table 7: Composition of Ternary Mixture/ Natural Gas

Gas	Molar composition	Ref
i	20.00% CO_2, 78% CH_4, 2% C_3H_8	j
ii	31.40% CO_2, 52.55% CH_4, 8.12% C_2H_6, 4.74% C_3H_8, 1.31% i-C_4H_{10}, 1.88% n-C_4H_{10}	d
iii	66.85% CO_2, 24.42% CH_4, 3.99% C_2H_6, 3.07% C_3H_8, 0.75% i-C_4H_{10}, 0.92% n-C_4H_{10}	d
iv	82.00% CH_4, 0.5% CO_2, 11.3% C_2H_6, 4.2% C_3H_8, 0.9 i-C_4H_{10}, 0.6 n-C_4H_{10}, 0.1 i-C_5H_{12}, 0.2 n-C_5H_{12}, 0.2 n-C_6H_{14}	j
v	83.15% CO_2, 12.38% CH_4, 1.96% C_2H_6, 1.66% C_3H_8, 0.37% i-C_4H_{10}, 0.48% n-C_4H_{10}	d
vi	89.62% CO_2, 7.86% CH_4, 1.13% C_2H_6, 0.86% C_3H_8, 0.20% i-C_4H_{10}, 0.33% n-C_4H_{10}	d

Ref according to Table 1

In ternary/ natural gas system, all models – HYSYS method A, HYSYS method B and CSMHyd – exhibit moderate deviation, even when the CO_2 content is high. The AADP for all models does not differ greatly. This proves that all models could predict typical components of natural gas with acceptable accuracy (AADP less than 20%).

4.2 HYDRATE FORMATION PRESSURES FOR INHIBITED SYSTEMS

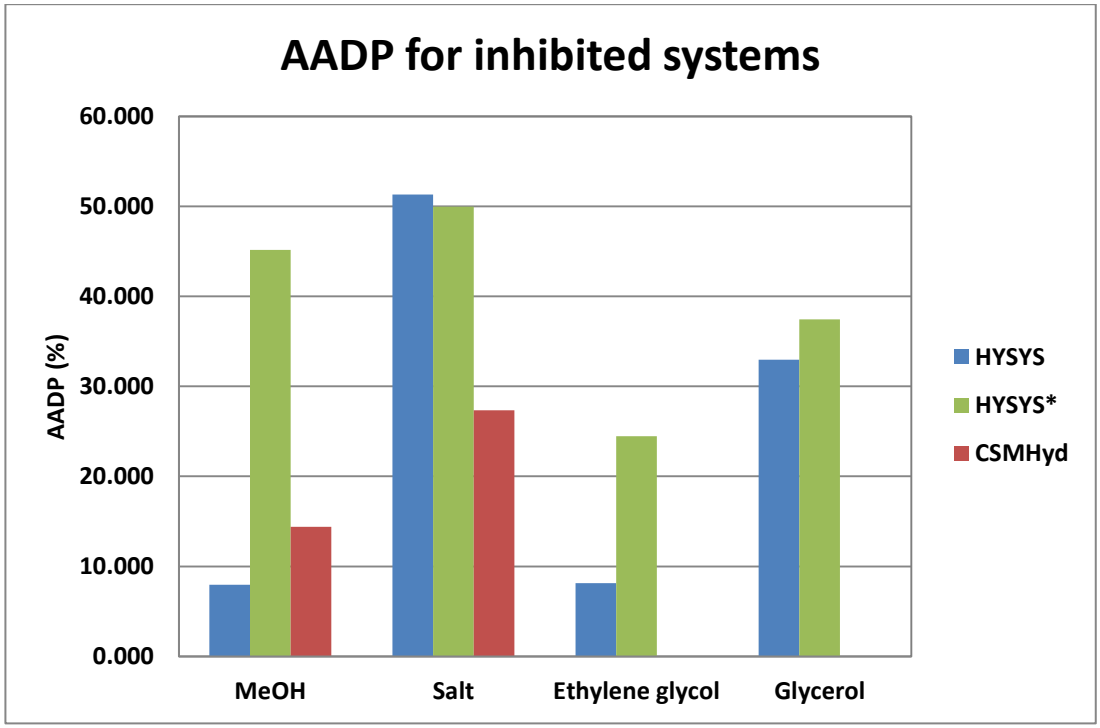
The addition of inhibitors in a system theoretically will increase the actual hydrate formation pressure of the system, given it is evaluated at the same temperature.

4.2.1 Single Inhibitor

Simulation results of the inhibited systems are presented in Table 8 and Figure 20. Simulations using HYSYS and CSMHyd are performed for systems containing methanol and salt. For systems with ethylene glycol (EG) or glycerol inhibitors, only HYSYS simulation is performed since CSMHyd do not offer the mentioned compounds in its database.

Table 8: Average Absolute Deviation in Pressure (AADP) for Single-inhibitor Systems

Inhibited systems	AADP		
	HYSYS[A]	HYSYS[B]	CSMHyd
MeOH	7.968	45.153	14.389
Salt	51.312	49.964	27.339
Ethylene glycol	8.154	24.454	-
Glycerol	32.975	37.445	-
Overall	**16.479**	**36.890**	**17.357**



HYSYS = HYSYS[A]; HYSYS*= HYSYS[B]

Figure 20: Average Absolute Deviation in Pressure (AADP) for Inhibited Systems

Based on the result, HYSYS method A generally offers the smallest AADP, followed by CSMHyd and HYSYS method B. There are obvious AADP difference between method A and B for a few inhibited systems (i.e. methanol inhibitor and EG inhibitor). Since HYSYS method A is more accurate over HYSYS method B for inhibited systems, the following graphs are plotted for hydrate formation curve using experimental data points, HYSYS method A predictions and CSMHyd predictions.

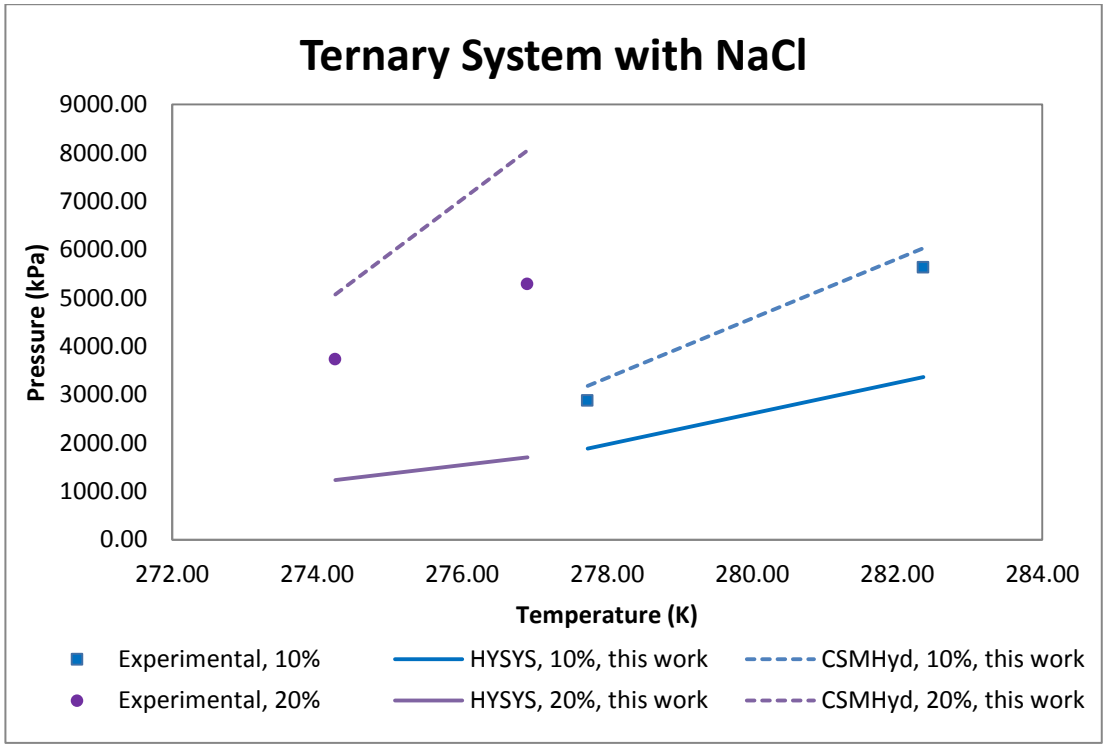


Figure 21: Hydrate Formation Curve for 20% CO_2 - 78% CH_4 - 2% C_3H_8 System with NaCl

In salt inhibition systems, AADP for HYSYS method A is two times the AADP for CSMHyd. The reason behind this large deviation in might probably be due to salts unavailability as components in Peng-Robinson property package. As a result, salts are added as hypothetical components, and their properties are predicted based on specified parameters. Minimum parameters need to be specified to define a hypothetical component are molecular weight and ideal liquid density/normal boiling point (Olutosin and Oluwaseun, 2007).

Furthermore, many models assume that for different gases having the same values of critical temperature (Tc), critical pressure (Pc) and ω, their dipole moments are equal. This assumption is not accurate considering the difference in type of compounds (ionic, organic, etc.). Thus, the properties and parameters predicted for any salts in HYSYS and CSMHyd might be different with the actual value.

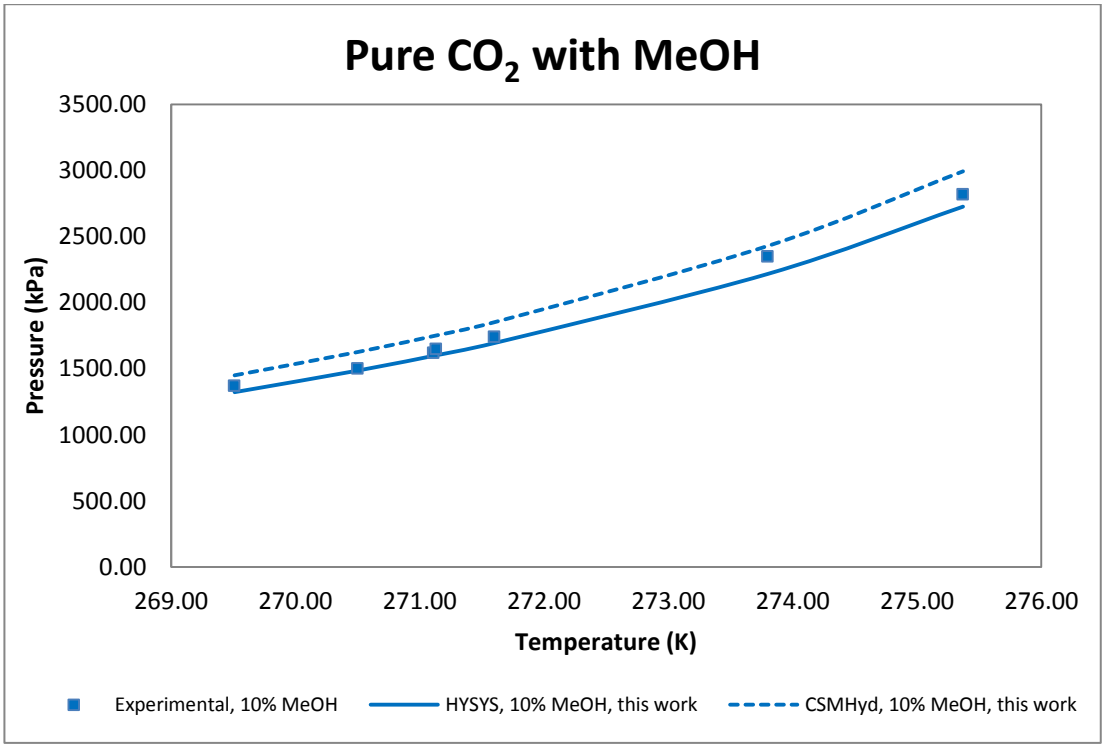


Figure 22: Hydrate Formation Curve for 100% CO_2 with Methanol

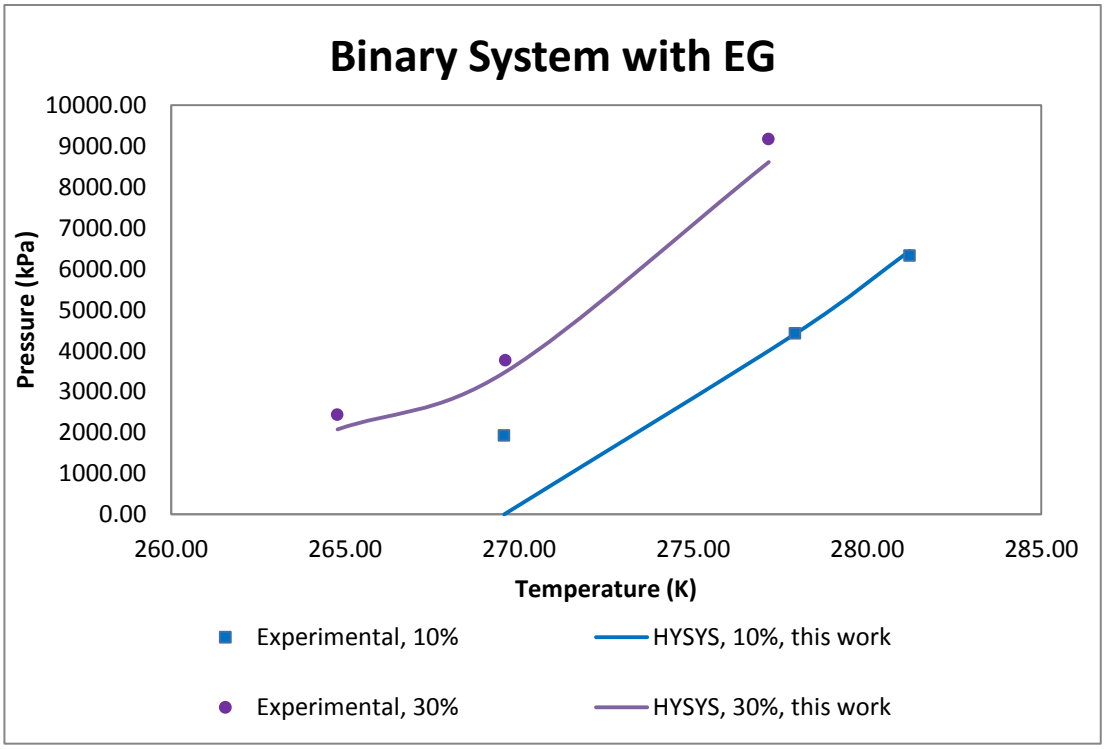


Figure 23: Hydrate Formation Curve for 20% CO_2 - 80% CH_4 with Ethylene Glycol

With reference to Figure 22 above, for pure CO_2 systems with MeOH inhibitor, both HYSYS method A and CSMHyd shows good agreement with the experimental values. Meanwhile, HYSYS method A in overall shows small deviation for systems with EG inhibitor, as observed in Figure 23.

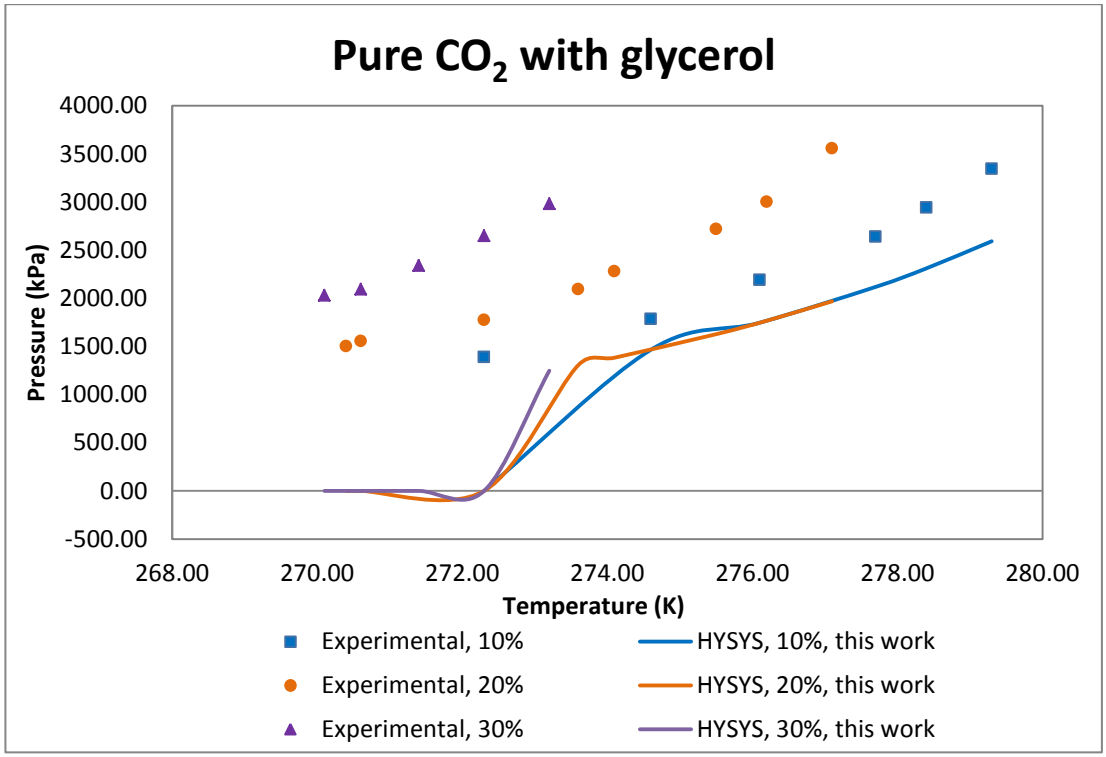


Figure 24: Hydrate Formation Curve for 100% CO_2 with Glycerol

On the other hand, for systems containing glycerol as inhibitor, HYSYS predictions deviate far from experimental values. This happens because glycerol is not accurately predicted by using Peng-Robinson equation of state, thus is not recommended to be used in that package.

4.2.2 Mixed inhibitors

Mixed inhibitor systems are systems that have more than one inhibitor. Within all of the experimental data compiled in this study, only two systems consist of EG and salt(s) mixture. The rest of the systems consist of mixture between methanol and salt(s). In section 4.2.1, which consists of inhibited systems, HYSYS method A gives better accuracy over HYSYS method B. Therefore, in this section, the mixed inhibitor systems are simulated by using HYSYS method A and CSMHyd. The results of the simulation are as follows:

Table 9: Average Absolute Deviation in Pressure (AADP) for Systems with Mixed Inhibitors

Inhibited systems	AADP	
	HYSYS[A]	CSMHyd
Mixture of alcohol and salt(s)	49.017	2480.881

Table 9 expresses the AADP values of two simulation approaches; HYSYS method A and CSMHyd. It can be observed that the AADP of CSMHyd prediction for mixed inhibitors systems is greater than 2000%, which is extremely high. Predictions using HYSYS method A also exhibit poor accuracy when compared to experimental results (AADP = 49.017%). The huge deviation can be justified due to the presence of salt in the system, which could not be accurately simulated by both models, as discussed in Section 4.2.1.

Based on the results for all uninhibited and inhibited systems, HYSYS simulation shows lesser deviation from experimental values compared to CSMHyd when appropriate assumption is made. HYSYS method A, which reflects free flow of water, gives great accuracy in simulation for inhibited systems. HYSYS method B on the other hand, shows better accuracy in simulating uninhibited system. The reason behind the difference lies in the different calculation method used by each approach. HYSYS method B assumes free water, since the equation for hydrate calculation does not include water as a component. Thus it is more suitable to simulate system with no inhibitor solution. In HYSYS method A, the calculation includes water in the equation to predict hydrate formation pressure. Therefore, it is more suitable in predicting hydrate for system containing inhibitor solution.

CHAPTER 5
CONCLUSION AND RECOMMENDATION

All three approaches of prediction show different accuracy for different systems. HYSYS software, using two comparable assumptions, results in different simulation values. HYSYS method A is more accurate in prediction of inhibited system, while HYSYS method B is more accurate in prediction of uninhibited system. As an overall, HYSYS could give greater accuracy compared to CSMHyd when proper assumption is made based on the system's type.

On the other hand, CSMHyd reported slightly better accuracy compared to HYSYS method B when simulating uninhibited CO_2 system, binary CO_2-CH_4, ternary/ natural gas mixture. Also, it shows smaller deviation in system with NaCl inhibitor, compared to HYSYS method A. While for mixed inhibitors' systems, CSMHyd predict the hydrate formation condition far beyond acceptable deviation.

As a conclusion, all approaches used in this work can reasonably predict hydrate formation pressure of a system with high CO_2 content. According to simulation results, higher CO_2 content corresponds to higher tendency of hydrate formation. This is in agreement with the theory and experimental results. For CO_2-CH_4 system, all approaches are in great agreement with the experimental data. This particular system is the benchmark in simulation of real natural gas in Malaysia, since Malaysia's natural gas consists mainly of carbon dioxide and methane. However, natural gas with N_2, glycerol or salt inhibitor may not be accurately predicted by the approaches used in this work.

As a continuation of this project, it is suggested that the common units in natural gas processing plant is simulated in HYSYS, and hydrate formation pressure is evaluated at the outlet of flash vessel (that separates natural gas and water). This simulation approach might produce more accurate simulation results as compared to the approaches done in this work, as it imitates the actual scenario.

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APPENDIX

Table 10: Compiled Results for Uninhibited Systems

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	P_{exp} (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
h	100% CO2	-	270.54	1758.23	<empty>	-	1007.86	42.677	1033.39	41.225
h	100% CO2	-	273.93	1379.00	1357.22	1.579	1356.28	1.648	1380.67	0.121
a	100% CO2	-	274.70	1500.00	1483.08	1.128	1482.04	1.198	1503.02	0.201
c	100% CO2	-	274.76	1500.00	1493.42	0.439	1492.37	0.509	1513.05	0.870
e	100% CO2	-	275.11	1560.00	1555.41	0.294	1554.32	0.364	1573.06	0.837
i	100% CO2	-	275.12	1510.00	1557.23	3.127	1556.13	3.055	1574.82	4.293
h	100% CO2	-	275.21	1558.27	1573.66	0.987	1572.55	0.916	1590.70	2.081
f	100% CO2	-	275.50	1651.00	1627.96	1.395	1626.81	1.465	1643.13	0.477
k	100% CO2	-	275.72	1682.00	1670.60	0.678	1669.41	0.748	1684.21	0.132
f	100% CO2	-	276.80	1936.00	1899.67	1.876	1898.29	1.948	1903.80	1.663
i	100% CO2	-	276.88	1810.00	1918.06	5.970	1916.67	5.893	1921.35	6.152
g	100% CO2	-	277.15	2040.00	1981.72	2.857	1980.27	2.928	1981.98	2.844
c	100% CO2	-	277.16	2000.00	1984.13	0.794	1982.67	0.866	1984.27	0.787
a	100% CO2	-	277.50	2030.00	2068.05	1.874	2066.52	1.799	2063.98	1.674
i	100% CO2	-	277.83	2110.00	2153.66	2.069	2152.04	1.993	2145.00	1.659
k	100% CO2	-	278.70	2393.00	2401.23	0.344	2399.36	0.266	2377.78	0.636
h	100% CO2	-	278.93	2420.15	2472.58	2.167	2470.64	2.086	2444.41	1.003
i	100% CO2	-	278.99	2400.00	2491.64	3.818	2489.68	3.736	2462.17	2.591

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	P_{exp} (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
c	100% CO2	-	279.16	2600.00	2546.67	2.051	2544.65	2.129	2513.82	3.315
e	100% CO2	-	279.49	2620.00	2658.09	1.454	2655.93	1.371	2616.69	0.126
a	100% CO2	-	279.70	2780.00	2732.33	1.715	2730.08	1.796	2685.25	3.408
i	100% CO2	-	279.94	2700.00	2820.61	4.467	2818.24	4.379	2766.43	2.460
f	100% CO2	-	280.20	3021.00	2920.64	3.322	2918.14	3.405	2858.01	5.395
h	100% CO2	-	280.71	3130.33	3131.57	0.040	3128.76	0.050	3049.53	2.581
i	100% CO2	-	280.71	3000.00	3131.57	4.386	3128.76	4.292	3049.53	1.651
i	100% CO2	-	281.42	3300.00	3463.41	4.952	3460.02	4.849	3351.08	1.548
c	100% CO2	-	281.46	3500.00	3483.64	0.467	3480.21	0.565	3369.14	3.739
h	100% CO2	-	282.04	3840.52	3798.94	1.083	3794.82	1.190	3647.67	5.021
i	100% CO2	-	282.06	3600.00	3810.62	5.851	3806.47	5.735	3657.85	1.607
i	100% CO2	-	282.41	3900.00	4025.21	3.210	4020.48	3.089	3843.96	1.437
i	100% CO2	-	282.90	4300.00	5888.07	36.932	4358.23	1.354	4131.30	3.923
c	100% CO2	-	283.26	5000.00	9672.09	93.442	6209.15	24.183	4366.63	12.667
h	100% CO2	-	283.32	4467.96	10339.84	131.422	6714.61	50.284	4408.26	1.336
h	14.0% CO2 + 86.0% C3H8	-	275.98	337.86	330.31	2.234	329.84	2.372	332.36	1.627
h	16.0% CO2 + 84.0% C3H8	-	277.76	475.76	481.35	1.176	480.72	1.043	480.23	0.940
h	17.0% CO2 + 83.0% C3H8	-	278.21	503.34	529.65	5.228	528.88	5.074	527.78	4.856
h	17.0% CO2 + 83.0% C3H8	-	279.09	641.24	637.97	0.509	636.75	0.699	629.60	1.815
h	18.0% CO2 + 82.0% C3H8	-	279.04	592.97	631.14	6.437	629.92	6.231	625.28	5.449
h	28.0% CO2 + 72.0% C3H8	-	275.21	303.38	294.70	2.861	294.34	2.979	314.85	3.781
h	35.0% CO2 + 65.0% C3H8	-	278.26	579.18	542.79	6.283	542.36	6.358	584.98	1.001
h	37.0% CO2 + 63.0% C3H8	-	279.59	751.56	702.27	6.558	701.32	6.685	753.98	0.322
h	39.0% CO2 + 61.0% C3H8	-	276.37	434.39	382.10	12.036	382.13	12.031	427.10	1.677
h	40.0% CO2 + 60.0% C3H8	-	274.82	324.07	286.02	11.741	285.96	11.757	325.54	0.455
h	40.0% CO2 + 60.0% C3H8	-	279.71	792.93	719.80	9.222	719.27	9.289	784.25	1.095
h	52.0% CO2 + 48.0% C3H8	-	281.09	1068.73	947.40	11.353	950.81	11.033	1085.87	1.604
h	52.5% CO2 + 47.5% C3H8	-	278.59	689.50	607.07	11.955	609.67	11.578	713.19	3.436
h	57.8% CO2 + 42.2% C3H8	-	275.65	413.70	374.96	9.364	376.85	8.907	460.99	11.431
h	58.0% CO2 + 42.0% C3H8	-	283.71	1654.80	1563.46	5.520	1563.37	5.525	2052.96	24.061
h	74.0% CO2 + 26.0% C3H8	-	281.82	1303.16	1282.25	1.604	1319.97	1.290	1616.38	24.036
h	75.0% CO2 + 25.0% C3H8	-	280.21	979.09	1004.27	2.571	1030.64	5.265	1271.97	29.914
h	75.0% CO2 + 25.0% C3H8	-	283.76	1916.81	1802.64	5.956	1874.14	2.226	2301.62	20.076
h	76.0% CO2 + 24.0% C3H8	-	277.37	655.03	649.80	0.798	663.09	1.231	832.34	27.071
h	77.0% CO2 + 23.0% C3H8	-	278.04	710.19	738.92	4.046	756.14	6.471	945.08	33.075
h	79.0% CO2 + 21.0% C3H8	-	273.98	358.54	405.15	13.000	411.77	14.847	529.49	47.678
h	84.0% CO2 + 16.0% C3H8	-	286.15	3378.55	14310.47	323.569	9683.23	186.609	27169.00	704.162
h	85.0% CO2 + 15.0% C3H8	-	275.37	827.40	615.25	25.641	632.25	23.586	796.65	3.716

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	P_{exp} (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
h	85.0% CO2 + 15.0% C3H8	-	276.48	758.45	729.81	3.776	752.67	0.763	942.09	24.212
h	86.0% CO2 + 14.0% C3H8	-	279.43	1206.63	1189.05	1.457	1245.11	3.190	1539.21	27.564
h	87.0% CO2 + 13.0% C3H8	-	273.82	517.13	527.41	1.990	541.34	4.682	684.58	32.381
h	87.0% CO2 + 13.0% C3H8	-	280.93	1572.06	1558.34	0.873	1654.55	5.247	2043.25	29.972
h	90.0% CO2 + 10.0% C3H8	-	278.32	1254.89	1210.03	3.575	1276.96	1.758	1567.62	24.921
h	91.0% CO2 + 9.0% C3H8	-	278.87	1454.85	1393.51	4.216	1483.88	1.996	1816.26	24.842
h	91.0% CO2 + 9.0% C3H8	-	280.37	1772.02	1749.41	1.276	1890.34	6.678	2323.09	31.098
h	91.0% CO2 + 9.0% C3H8	-	283.48	3033.80	2915.92	3.885	2211.35	27.109	10632.92	250.482
h	92.0% CO2 + 8.0% C3H8	-	273.93	675.71	717.43	6.175	745.43	10.318	918.92	35.993
h	92.0% CO2 + 8.0% C3H8	-	281.71	2185.72	2310.84	5.725	2575.45	17.831	3241.70	48.313
h	92.0% CO2 + 8.0% C3H8	-	283.71	3178.60	2351.90	26.008	3308.42	4.084	11512.58	262.191
h	93.0% CO2 + 7.0% C3H8	-	273.82	813.61	763.47	6.163	795.73	2.198	974.87	19.821
h	94.0% CO2 + 6.0% C3H8	-	276.26	1151.47	1190.68	3.406	1265.28	9.884	1531.19	32.977
h	94.5% CO2 + 5.5% C3H8	-	284.82	4268.01	3787.14	11.267	3685.62	13.645	17906.78	319.559
g	11% CO2 + 89% CH4	-	277.15	3550.00	3388.62	4.546	3320.89	6.454	3412.18	3.882
c	20% CO2 + 80% CH4	-	273.56	2000.00	2159.01	7.951	2104.77	5.239	2194.16	9.708
b	20% CO2 + 80% CH4	-	274.00	2300.00	2259.28	1.770	2201.77	4.271	2291.53	0.368
k	20% CO2 + 80% CH4	-	274.41	2419.00	2357.16	2.557	2296.44	5.066	2386.38	1.348
c	20% CO2 + 80% CH4	-	275.36	2600.00	2601.73	0.067	2532.94	2.579	2622.48	0.865
b	20% CO2 + 80% CH4	-	276.00	2600.00	2781.76	6.991	2706.99	4.115	2795.53	7.520
b	20% CO2 + 80% CH4	-	277.10	3000.00	3123.51	4.117	3037.36	1.245	3122.32	4.077
c	20% CO2 + 80% CH4	-	278.06	3500.00	3459.53	1.156	3362.26	3.936	3441.63	1.668
b	20% CO2 + 80% CH4	-	278.30	3400.00	3549.65	4.401	3449.41	1.453	3526.91	3.733
c	20% CO2 + 80% CH4	-	281.46	5000.00	5020.95	0.419	4874.92	2.502	4901.35	1.973
k	20% CO2 + 80% CH4	-	281.51	5112.00	5049.31	1.226	4902.46	4.099	4927.55	3.608
g	36% CO2 + 64% CH4	-	277.15	2800.00	2789.53	0.374	2703.61	3.443	2768.18	1.136
b	50% CO2 + 50% CH4	-	273.50	1780.00	1706.62	4.122	1665.10	6.455	1721.75	3.272
b	50% CO2 + 50% CH4	-	274.20	1830.00	1841.56	0.632	1795.47	1.887	1851.25	1.161
b	50% CO2 + 50% CH4	-	275.20	2050.00	2054.74	0.231	2001.28	2.377	2054.75	0.232
b	50% CO2 + 50% CH4	-	275.60	2120.00	2147.42	1.293	2090.72	1.381	2142.85	1.078
b	50% CO2 + 50% CH4	-	275.70	2200.00	2171.30	1.304	2113.76	3.920	2165.51	1.568
b	50% CO2 + 50% CH4	-	276.80	2400.00	2454.29	2.262	2386.77	0.551	2432.98	1.374
b	50% CO2 + 50% CH4	-	278.40	2825.00	2942.67	4.165	2858.00	1.168	2890.29	2.311
b	50% CO2 + 50% CH4	-	278.70	2851.00	3046.08	6.842	2957.84	3.747	2986.47	4.752
b	50% CO2 + 50% CH4	-	279.50	3301.00	3343.02	1.273	3244.76	1.704	3261.51	1.196
b	50% CO2 + 50% CH4	-	279.70	3351.00	3422.44	2.132	3321.57	0.878	3334.79	0.484

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	P_{exp} (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
b	50% CO2 + 50% CH4	-	280.10	3370.00	3588.04	6.470	3481.84	3.319	3487.18	3.477
b	50% CO2 + 50% CH4	-	281.80	4410.00	4407.99	0.046	4278.41	2.984	4238.73	3.884
b	50% CO2 + 50% CH4	-	283.00	5001.00	5127.87	2.537	4983.51	0.350	4890.21	2.215
b	50% CO2 + 50% CH4	-	283.10	5070.00	5194.32	2.452	5048.94	0.415	4950.06	2.366
g	52% CO2 + 48% CH4	-	277.15	2550.00	2523.01	1.058	2454.54	3.743	2495.45	2.139
c	60% CO2 + 40% CH4	-	273.56	1500.00	1613.73	7.582	1580.12	5.341	1626.52	8.435
c	60% CO2 + 40% CH4	-	275.86	2000.00	2083.62	4.181	2035.86	1.793	2074.43	3.721
c	60% CO2 + 40% CH4	-	277.96	2600.00	2648.50	1.865	2583.31	0.642	2604.85	0.187
c	60% CO2 + 40% CH4	-	280.16	3500.00	3438.89	1.746	3350.75	4.264	3334.66	4.724
g	64% CO2 + 36% CH4	-	277.15	2360.00	2361.25	0.053	2308.74	2.172	2333.19	1.136
g	16% CO2 + 84% N2	-	273.40	6100.00	7987.37	30.940	6370.68	4.437	8244.75	35.160
g	16% CO2 + 84% N2	-	274.50	6200.00	9261.19	49.374	7338.20	18.358	9619.23	55.149
g	19% CO2 + 82% N2	-	275.40	6400.00	9381.50	46.586	7355.70	14.933	9277.44	44.960
g	20% CO2 + 80% N2	-	275.40	6100.00	8963.92	46.949	7022.80	15.128	8700.88	42.637
g	20% CO2 + 80% N2	-	276.50	6600.00	10500.93	59.105	8166.52	23.735	10251.86	55.331
g	22% CO2 + 78% N2	-	276.00	6200.00	9069.94	46.289	7072.84	14.078	8583.91	38.450
g	25% CO2 + 75% N2	-	273.90	5900.00	6021.44	2.058	4838.03	17.999	5633.03	4.525
g	26% CO2 + 74% N2	-	276.00	5900.00	7861.59	33.247	6169.98	4.576	7181.14	21.714
g	26% CO2 + 75% N2	-	274.70	5900.00	6565.51	11.280	5234.17	11.285	6072.40	2.922
g	27% CO2 + 74% N2	-	276.90	6000.00	8778.33	46.306	6827.60	13.793	7937.14	32.286
g	29% CO2 + 71% N2	-	277.80	6300.00	9363.72	48.630	7243.00	14.968	8305.65	31.836
g	30% CO2 + 70% N2	-	278.60	6500.00	10315.95	58.707	7925.55	21.932	9066.67	39.487
g	30% CO2 + 71% N2	-	278.10	6400.00	9601.95	50.030	7413.08	15.829	8468.74	32.324
g	30% CO2 + 71% N2	-	278.40	6400.00	10079.54	57.493	7755.83	21.185	8880.59	38.759
g	56% CO2 + 44% N2	-	280.10	5300.00	6494.95	22.546	5416.63	2.201	5527.73	4.297
g	59% CO2 + 42% N2	-	281.10	5600.00	7372.31	31.648	6095.60	8.850	6147.35	9.774
d	31.40% CO2, 52.55% CH4, 8.12% C2H6, 4.74% C3H8, 1.31% i-C4H10, 1.88% n-C4H10	-	273.70	593.10	645.54	8.842	652.50	10.015	715.83	20.693
d	31.40% CO2, 52.55% CH4, 8.12% C2H6, 4.74% C3H8, 1.31% i-C4H10, 1.88% n-C4H10	-	276.50	841.40	937.20	11.385	951.09	13.037	1028.84	22.277
d	31.40% CO2, 52.55% CH4, 8.12% C2H6, 4.74% C3H8, 1.31% i-C4H10, 1.88% n-C4H10	-	279.30	1220.70	1352.30	10.781	1379.81	13.034	1475.33	20.859
d	31.40% CO2, 52.55% CH4, 8.12% C2H6, 4.74% C3H8, 1.31% i-C4H10, 1.88% n-C4H10	-	282.00	1682.80	1926.97	14.510	1980.93	17.716	2095.20	24.507

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	P_{exp} (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
d	66.85% CO2, 24.42% CH4, 3.99% C2H6, 3.07% C3H8, 0.75% i-C4H10, 0.92% n-C4H10	-	273.70	758.60	884.66	16.617	914.15	20.505	1045.48	37.817
d	66.85% CO2, 24.42% CH4, 3.99% C2H6, 3.07% C3H8, 0.75% i-C4H10, 0.92% n-C4H10	-	276.50	1089.70	1293.25	18.680	1352.58	24.124	1533.48	40.725
d	66.85% CO2, 24.42% CH4, 3.99% C2H6, 3.07% C3H8, 0.75% i-C4H10, 0.92% n-C4H10	-	279.30	1565.50	1895.17	21.058	1983.87	26.724	2277.12	45.456
d	66.85% CO2, 24.42% CH4, 3.99% C2H6, 3.07% C3H8, 0.75% i-C4H10, 0.92% n-C4H10	-	282.00	2227.60	2747.49	23.339	2687.70	20.654	3460.65	55.353
j	78% CH4 + 20% CO2 + 2% C3H8	-	277.18	1660.00	1762.49	6.174	1791.24	7.906	1714.57	3.287
j	78% CH4 + 20% CO2 + 2% C3H8	-	280.56	2461.00	2673.93	8.652	2736.43	11.192	2573.34	4.565
j	78% CH4 + 20% CO2 + 2% C3H8	-	283.21	3397.00	3757.95	10.626	3878.52	14.175	3581.53	5.432
j	78% CH4 + 20% CO2 + 2% C3H8	-	288.62	7241.00	8448.39	16.674	9107.60	25.778	7721.79	6.640
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	-	281.08	1530.00	1601.31	4.661	1600.62	4.616	1707.60	11.608
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	-	285.12	2684.00	2648.86	1.309	2648.61	1.319	2793.11	4.065
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	-	291.29	5841.00	6287.23	7.640	6292.76	7.734	6476.39	10.878
d	83.15% CO2, 12.38% CH4, 1.96% C2H6, 1.66% C3H8, 0.37% i-C4H10, 0.48% n-C4H10	-	273.70	1365.50	1022.05	25.152	1014.84	25.680	1392.65	1.989
d	83.15% CO2, 12.38% CH4, 1.96% C2H6, 1.66% C3H8, 0.37% i-C4H10, 0.48% n-C4H10	-	276.50	1869.00	1376.99	26.325	1365.41	26.945	1894.78	1.380
d	83.15% CO2, 12.38% CH4, 1.96% C2H6, 1.66% C3H8, 0.37% i-C4H10, 0.48% n-C4H10	-	279.30	2565.50	1869.56	27.127	1850.64	27.864	2614.07	1.893

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	P_{exp} (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
d	83.15% CO2, 12.38% CH4, 1.96% C2H6, 1.66% C3H8, 0.37% i-C4H10, 0.48% n-C4H10	-	282.00	3510.30	2542.49	27.571	2511.65	28.449	3655.50	4.136
d	89.62% CO2, 7.86% CH4, 1.13% C2H6, 0.86% C3H8, 0.20% i-C4H10, 0.33% n-C4H10	-	273.70	1337.90	994.55	25.663	990.04	26.000	1375.96	2.845
d	89.62% CO2, 7.86% CH4, 1.13% C2H6, 0.86% C3H8, 0.20% i-C4H10, 0.33% n-C4H10	-	276.50	1841.40	1339.62	27.250	1332.51	27.636	1874.85	1.817
d	89.62% CO2, 7.86% CH4, 1.13% C2H6, 0.86% C3H8, 0.20% i-C4H10, 0.33% n-C4H10	-	279.30	2531.00	1818.50	28.151	1807.13	28.600	2593.05	2.452
d	89.62% CO2, 7.86% CH4, 1.13% C2H6, 0.86% C3H8, 0.20% i-C4H10, 0.33% n-C4H10	-	282.00	3469.00	2473.18	28.706	2455.07	29.228	3643.55	5.032

Ref according to Table 1

Table 11: Compiled Results for Single Inhibitor Systems

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	Pexp (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
f	100% CO2	10% glycerol	272.30	1391.00	<empty>	-	1076.52	22.608	-	-
f	100% CO2	10% glycerol	274.60	1786.00	1465.99	17.917	1464.99	17.974	-	-
f	100% CO2	10% glycerol	276.10	2191.00	1747.29	20.251	1746.07	20.307	-	-
f	100% CO2	10% glycerol	277.70	2640.00	2119.40	19.720	2117.85	19.779	-	-
f	100% CO2	10% glycerol	278.40	2942.00	2312.00	21.414	2310.26	21.473	-	-
f	100% CO2	10% glycerol	279.30	3345.00	2593.14	22.477	2591.10	22.538	-	-
e	100% CO2	10.00% MeOH	269.51	1370.00	1323.54	3.391	972.38	29.024	1451.13	5.922
e	100% CO2	10.00% MeOH	270.50	1500.00	1486.58	0.895	1009.53	32.698	1627.16	8.477
e	100% CO2	10.00% MeOH	271.11	1620.00	1598.37	1.335	1033.01	36.234	1748.00	7.901
e	100% CO2	10.00% MeOH	271.13	1650.00	1602.20	2.897	1033.79	37.346	1752.16	6.191
a	100% CO2	10.00% MeOH	271.60	1740.00	1695.24	2.572	1052.22	39.528	1852.85	6.486
a	100% CO2	10.00% MeOH	273.80	2350.00	2218.56	5.593	1340.57	42.954	2430.22	3.414
e	100% CO2	10.00% MeOH	275.37	2820.00	2727.37	3.285	1607.34	43.002	2994.67	6.194
a	100% CO2	10.04% EG	270.90	1150.00	1239.33	7.768	1021.59	11.166	-	-
a	100% CO2	10.04% EG	273.10	1740.00	1601.45	7.962	1109.02	36.263	-	-
a	100% CO2	10.04% EG	275.80	2400.00	2210.95	7.877	1685.23	29.782	-	-
a	100% CO2	10.04% EG	278.30	3200.00	3075.74	3.883	2281.49	28.703	-	-
e	100% CO2	10.04% MeOH	272.36	1870.00	1863.54	0.345	1082.60	42.107	2035.68	8.860
e	100% CO2	10.06% MeOH	269.83	1400.00	1378.21	1.557	984.25	29.696	1510.59	7.899
e	100% CO2	10.06% MeOH	269.90	1380.00	1389.55	0.692	986.87	28.488	1522.84	10.350
e	100% CO2	10.06% MeOH	271.31	1610.00	1642.38	2.011	1040.81	35.353	1796.14	11.561
f	100% CO2	20% glycerol	270.40	1502.00	<empty>	-	1002.56	33.252	-	-
f	100% CO2	20% glycerol	270.60	1556.00	<empty>	-	1010.14	35.081	-	-

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	Pexp (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
f	100% CO2	20% glycerol	272.30	1776.00	<empty>	-	1076.52	39.385	-	-
f	100% CO2	20% glycerol	273.60	2096.00	1306.93	37.646	1306.06	37.688	-	-
f	100% CO2	20% glycerol	274.10	2281.00	1383.91	39.329	1382.98	39.370	-	-
f	100% CO2	20% glycerol	275.50	2721.00	1627.92	40.172	1626.81	40.213	-	-
f	100% CO2	20% glycerol	276.20	3001.00	1768.13	41.082	1766.91	41.123	-	-
f	100% CO2	20% glycerol	277.10	3556.00	1969.69	44.609	1968.30	44.648	-	-
f	100% CO2	30% glycerol	270.10	2030.00	<empty>	-	991.29	51.168	-	-
f	100% CO2	30% glycerol	270.60	2096.00	<empty>	-	1010.14	51.806	-	-
f	100% CO2	30% glycerol	271.40	2340.00	<empty>	-	1040.93	55.516	-	-
f	100% CO2	30% glycerol	272.30	2651.00	<empty>	-	1076.52	59.392	-	-
f	100% CO2	30% glycerol	273.20	2981.00	1248.74	58.110	1247.92	58.137	-	-
k	100% CO2	9.99% MeOH	269.74	1460.00	1358.83	6.929	980.90	32.815	1489.14	1.996
k	100% CO2	9.99% MeOH	276.67	3530.00	3274.14	7.248	1874.82	46.889	3611.83	2.318
a	94.69% CO2 + 5.31% C2H6	10.06% EG	269.10	850.00	<empty>	-	981.52	15.473	-	-
a	94.69% CO2 + 5.31% C2H6	10.06% EG	271.00	1030.00	1103.92	7.177	1054.25	2.355	-	-
a	94.69% CO2 + 5.31% C2H6	10.06% EG	272.90	1310.00	1369.59	4.549	1131.49	13.626	-	-
a	94.69% CO2 + 5.31% C2H6	10.06% EG	274.90	1820.00	1714.26	5.810	1552.21	14.714	-	-
a	94.69% CO2 + 5.31% C2H6	10.06% EG	276.40	2310.00	2048.01	11.342	1849.60	19.931	-	-
k	20% CO2 + 80% CH4	10.00% EG	269.57	1920.00	<empty>	-	1707.85	11.049	-	-
k	20% CO2 + 80% CH4	10.00% EG	277.93	4417.00	4413.36	0.082	3316.36	24.918	-	-
k	20% CO2 + 80% CH4	10.00% EG	281.22	6318.00	6441.65	1.957	4745.67	24.886	-	-
k	20% CO2 + 80% CH4	10.00% MeOH	268.79	2211.00	2048.02	7.371	1666.08	24.646	2202.21	0.397
k	20% CO2 + 80% CH4	10.00% MeOH	270.41	2627.00	2426.53	7.631	1761.97	32.929	2594.51	1.237
k	20% CO2 + 80% CH4	10.00% MeOH	276.95	5104.00	4975.46	2.518	2998.79	41.246	5190.12	1.687
k	20% CO2 + 80% CH4	10.00% MeOH	277.17	5198.00	5103.12	1.825	3069.11	40.956	5319.70	2.341
k	20% CO2 + 80% CH4	10.00% MeOH	277.18	5235.00	5109.02	2.407	3072.35	41.311	5325.65	1.732
k	20% CO2 + 80% CH4	10.00% MeOH	280.85	7900.00	7959.30	0.751	4570.27	42.149	8213.87	3.973
k	20% CO2 + 80% CH4	10.00% MeOH	280.90	8022.00	8010.18	0.147	4595.84	42.710	8265.45	3.035
k	20% CO2 + 80% CH4	19.98% MeOH	264.28	2376.00	2134.41	10.168	1421.46	40.174	2514.07	5.811
k	20% CO2 + 80% CH4	19.98% MeOH	269.15	3841.00	3615.88	5.861	1687.21	56.074	4234.96	10.257
k	20% CO2 + 80% CH4	19.98% MeOH	277.26	9676.00	9911.88	2.438	3098.83	67.974	11803.47	21.987
k	20% CO2 + 80% CH4	20.06% MeOH	264.34	2416.00	2157.78	10.688	1424.51	41.038	2543.14	5.262
k	20% CO2 + 80% CH4	20.06% MeOH	268.98	3845.00	3565.46	7.270	1677.29	56.377	4179.81	8.708
k	20% CO2 + 80% CH4	30.00% EG	264.78	2428.00	2076.27	14.486	1444.51	40.506	-	-
k	20% CO2 + 80% CH4	30.00% EG	269.61	3760.00	3484.95	7.315	1710.45	54.509	-	-
k	20% CO2 + 80% CH4	30.00% EG	277.17	9167.00	8611.36	6.061	3060.58	66.613	-	-
k	50% CO2 + 50% CH4	19.99% MeOH	264.64	1877.00	1767.46	5.836	1094.05	41.713	2081.22	10.880
k	50% CO2 + 50% CH4	19.99% MeOH	270.42	3379.00	3482.88	3.074	1354.04	59.928	4125.09	22.080
k	50% CO2 + 50% CH4	19.99% MeOH	275.80	6731.00	7265.49	7.941	2143.98	68.148	9303.64	38.221
a	96.52% CO2 + 3.48% CH4	10.00% EG	268.70	1140.00	<empty>	-	957.44	16.014	-	-
a	96.52% CO2 + 3.48% CH4	10.00% EG	271.30	1600.00	1321.19	17.426	1055.97	34.002	-	-
a	96.52% CO2 + 3.48% CH4	10.00% EG	274.20	2260.00	1847.69	18.244	1420.68	37.138	-	-

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	Pexp (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
a	96.52% CO2 + 3.48% CH4	10.00% EG	278.00	3220.00	2995.24	6.980	2227.33	30.828	-	-
a	90.99% CO2 + 9.01% N2	13.01% EG	267.20	930.00	<empty>	-	931.44	0.154	-	-
a	90.99% CO2 + 9.01% N2	13.01% EG	267.90	1030.00	<empty>	-	956.61	7.126	-	-
a	90.99% CO2 + 9.01% N2	13.01% EG	270.20	1200.00	1396.23	16.352	1043.39	13.051	-	-
a	90.99% CO2 + 9.01% N2	13.01% EG	271.90	1760.00	1713.55	2.639	1111.73	36.834	-	-
a	90.99% CO2 + 9.01% N2	13.01% EG	273.70	2150.00	2139.66	0.481	1375.84	36.008	-	-
a	90.99% CO2 + 9.01% N2	13.01% EG	274.20	2490.00	2283.39	8.298	1456.19	41.518	-	-
a	90.99% CO2 + 9.01% N2	13.01% EG	275.30	2800.00	2646.89	5.468	1652.04	40.999	-	-
a	90.99% CO2 + 9.01% N2	13.01% EG	276.50	3390.00	3140.25	7.367	1900.60	43.935	-	-
a	96.52% CO2 + 3.48% N2	10.00% EG	268.90	1000.00	<empty>	-	980.60	1.940	-	-
a	96.52% CO2 + 3.48% N2	10.00% EG	272.10	1350.00	1486.43	10.106	1106.26	18.054	-	-
a	96.52% CO2 + 3.48% N2	10.00% EG	273.40	1620.00	1726.34	6.564	1322.10	18.389	-	-
a	96.52% CO2 + 3.48% N2	10.00% EG	276.10	2490.00	2418.53	2.870	1810.23	27.300	-	-
j	78% CH4 + 20% CO2 + 2% C3H8	10.00% NaCl	277.73	2876.00	1885.90	34.426	1917.43	33.330	3182.36	10.652
j	78% CH4 + 20% CO2 + 2% C3H8	10.00% NaCl	282.36	5633.00	3365.23	40.259	3459.44	38.586	6030.44	7.056
j	78% CH4 + 20% CO2 + 2% C3H8	20.00% MeOH	274.16	3189.00	3690.88	15.738	1240.79	61.091	4298.56	34.793
j	78% CH4 + 20% CO2 + 2% C3H8	20.00% MeOH	277.15	4895.00	5696.51	16.374	1792.89	63.373	6950.49	41.992
j	78% CH4 + 20% CO2 + 2% C3H8	20.00% MeOH	280.73	8942.00	11446.84	28.012	2811.32	68.561	16033.76	79.308
j	78% CH4 + 20% CO2 + 2% C3H8	20.00% NaCl	274.25	3728.00	1234.95	66.874	1248.90	66.499	5073.02	36.079
j	78% CH4 + 20% CO2 + 2% C3H8	20.00% NaCl	276.90	5286.00	1705.18	67.742	1730.35	67.265	8051.44	52.316
j	78% CH4 + 20% CO2 + 2% C3H8	20.01% NaCl	279.97	8874.00	2487.45	71.969	2538.31	71.396	16801.85	89.338
j	78% CH4 + 20% CO2 + 2% C3H8	5.00% NaCl	280.78	3269.00	2749.79	15.883	2814.72	13.897	3432.99	5.016
j	78% CH4 + 20% CO2 + 2% C3H8	5.00% NaCl	285.19	6025.00	4927.82	18.210	5132.88	14.807	6314.80	4.810
j	78% CH4 + 20% CO2 + 2% C3H8	5.00% NaCl	288.03	9849.00	7629.43	22.536	8150.07	17.250	10342.13	5.007
j	78% CH4 + 20% CO2 + 2% C3H8	9.99% MeOH	277.09	2567.00	2912.33	13.453	1779.27	30.687	2994.71	16.662
j	78% CH4 + 20% CO2 + 2% C3H8	9.99% MeOH	283.18	5635.00	6911.03	22.645	3885.42	31.048	7156.56	27.002
j	78% CH4 + 20% CO2 + 2% C3H8	9.99% MeOH	285.73	8846.00	11301.58	27.759	5607.66	36.608	11847.56	33.931
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	20.01% MeOH	277.65	3198.00	3389.79	5.997	1055.44	66.997	3471.34	8.547
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	20.01% MeOH	281.10	4878.00	5686.14	16.567	1615.22	66.888	5878.82	20.517
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	20.01% MeOH	284.26	8515.00	11376.05	33.600	2392.49	71.903	12301.31	44.466
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	20.20% NaCl	276.89	3223.00	954.64	70.380	953.92	70.403	4355.91	35.151

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	Pexp (kPa)	P_{HYS}^{A} (kPa)	%Dev	P_{HYS}^{B} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	20.20% NaCl	280.03	5723.00	1407.24	75.411	1406.48	75.424	7353.59	28.492
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	20.20% NaCl	281.98	9289.00	1789.28	80.738	1788.57	80.745	11779.35	26.810
a	88.53% CO2 + 6.83% CH4 + 0.38% C2H6 + 4.26% N2	10.00% EG	268.80	800.00	<empty>	-	1013.70	26.712	-	-
a	88.53% CO2 + 6.83% CH4 + 0.38% C2H6 + 4.26% N2	10.00% EG	270.70	1160.00	1308.48	12.800	1089.07	6.114	-	-
a	88.53% CO2 + 6.83% CH4 + 0.38% C2H6 + 4.26% N2	10.00% EG	274.40	1820.00	2016.00	10.769	1527.85	16.052	-	-
a	88.53% CO2 + 6.83% CH4 + 0.38% C2H6 + 4.26% N2	10.00% EG	276.40	2410.00	2590.92	7.507	1928.86	19.964	-	-
a	88.53% CO2 + 6.83% CH4 + 0.38% C2H6 + 4.26% N2	10.00% EG	278.10	2850.00	3251.97	14.104	2368.95	16.879	-	-
a	88.53% CO2 + 6.83% CH4 + 0.38% C2H6 + 4.26% N2	10.00% EG	279.30	3500.00	3863.56	10.387	2755.06	21.284	-	-

Ref according to Table 1

Table 12: Compiled Results for Mixed Inhibitors Systems

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	Pexp (kPa)	P_{HYS}^{A} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
e	100% CO2	10% MeOH + 10.01% KCl	265.58	1248.00	<empty>	-	868.56	30.404
e	100% CO2	10% MeOH + 10.01% KCl	268.90	1828.00	1304.44	28.641	2238.04	22.431
e	100% CO2	10% MeOH + 10.01% KCl	271.85	2767.00	1854.02	32.995	3188.40	15.230
e	100% CO2	15.03% MeOH + 5.02% CaCl2	264.72	1160.00	631.69	45.544	106370.11	9069.837
e	100% CO2	15.03% MeOH + 5.02% CaCl2	267.77	1658.00	637.41	61.555	138491.08	8252.900
e	100% CO2	15.03% MeOH + 5.02% CaCl2	270.76	2456.00	643.15	73.813	172918.92	6940.673
e	100% CO2	15.14% MeOH + 5% NaCl	264.76	1243.00	1048.40	15.656	1262.31	1.554
e	100% CO2	15.14% MeOH + 5% NaCl	267.77	1807.00	1490.61	17.509	1726.12	4.476
e	100% CO2	15.14% MeOH + 5% NaCl	270.83	2730.00	2174.46	20.349	2419.58	11.371
e	100% CO2	4.96% MeOH + 10.00% CaCl2	265.94	985.00	<empty>	-	879.75	10.685
e	100% CO2	4.96% MeOH + 10.00% CaCl2	271.04	1807.00	643.63	64.381	640109.69	35323.890
e	100% CO2	4.96% MeOH + 10.00% CaCl2	274.19	2809.00	649.78	76.868	677337.13	24013.105
e	100% CO2	5% MeOH + 10.01% KCl	265.53	910.00	<empty>	-	867.02	4.724
e	100% CO2	5% MeOH + 10.01% KCl	268.79	1381.00	<empty>	-	1925.07	39.397
e	100% CO2	5% MeOH + 10.01% KCl	272.36	2103.00	1476.44	29.794	3016.57	43.441
e	100% CO2	5% MeOH + 10.01% KCl	274.71	2900.00	1944.01	32.965	12535.44	332.257
e	100% CO2	5% MeOH + 15% NaCl	263.39	1271.00	<empty>	-	25467.55	1903.741
e	100% CO2	5% MeOH + 15% NaCl	265.94	1736.00	<empty>	-	48248.70	2679.303

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	Pexp (kPa)	P_{HYS}^{A} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
e	100% CO2	5% MeOH + 15% NaCl	269.20	2707.00	<empty>	-	81935.13	2926.787
e	100% CO2	5% MeOH + 5% NaCl	270.63	1480.00	1192.25	19.442	1621.57	9.566
e	100% CO2	5% MeOH + 5% NaCl	273.53	2139.00	1662.18	22.292	2290.61	7.088
e	100% CO2	5% MeOH + 5% NaCl	276.23	3038.00	2315.49	23.782	3282.84	8.059
e	100% CO2	5.00% MeOH + 15.00% CaCl2	265.23	1328.00	<empty>	-	-	-
e	100% CO2	5.00% MeOH + 15.00% CaCl2	267.84	1827.00	<empty>	-	-	-
e	100% CO2	5.00% MeOH + 15.00% CaCl2	270.74	2715.00	643.01	76.316	-	-
e	100% CO2	9.95% MeOH + 9.93% CaCl2	264.72	1137.00	<empty>	-	842.30	25.919
e	100% CO2	9.95% MeOH + 9.93% CaCl2	267.28	1543.00	636.45	58.752	522460.69	33760.058
e	100% CO2	9.95% MeOH + 9.93% CaCl2	270.93	2552.00	643.44	74.787	577706.63	22537.407
e	100% CO2	9.96% MeOH + 9.96% NaCl	264.00	1184.00	<empty>	-	820.81	30.675
e	100% CO2	9.96% MeOH + 9.96% NaCl	267.37	1818.00	1091.85	39.942	2506.92	37.895
e	100% CO2	9.96% MeOH + 9.96% NaCl	270.83	2872.00	1636.46	43.020	13452.21	368.392
k	20% CO2 + 80% CH4	10.00% MeOH + 9.96% CaCl2	262.25	2030.00	<empty>	-	1420.38	30.030
k	20% CO2 + 80% CH4	10.00% MeOH + 9.96% CaCl2	268.38	3717.00	1300.88	65.002	168887.72	4443.657
k	20% CO2 + 80% CH4	10.00% MeOH + 9.96% CaCl2	276.10	9361.00	1329.90	85.793	246422.39	2532.437
k	20% CO2 + 80% CH4	15.00% EG + 5.02% NaCl + 4.98% CaCl2	264.95	2359.00	<empty>	-	-	-
k	20% CO2 + 80% CH4	15.00% EG + 5.02% NaCl + 4.98% CaCl2	269.69	3959.00	1272.66	67.854	-	-
k	20% CO2 + 80% CH4	15.00% EG + 5.02% NaCl + 4.98% CaCl2	276.96	9253.00	1304.66	85.900	-	-
k	20% CO2 + 80% CH4	20.00% EG + 5.02% CaCl2	265.78	2102.00	1305.92	37.872	-	-
k	20% CO2 + 80% CH4	20.00% EG + 5.02% CaCl2	269.89	3375.00	1319.14	60.915	-	-
k	20% CO2 + 80% CH4	20.00% EG + 5.02% CaCl2	276.79	7656.00	1342.98	82.458	-	-
k	20% CO2 + 80% CH4	4.96% MeOH + 14.98% CaCl2	262.24	2156.00	<empty>	-	425231.56	19623.171
k	20% CO2 + 80% CH4	4.96% MeOH + 14.98% CaCl2	267.98	3966.00	<empty>	-	503894.06	12605.347
k	20% CO2 + 80% CH4	4.96% MeOH + 14.98% CaCl2	274.80	9244.00	1327.29	85.642	-	-
k	20% CO2 + 80% CH4	5.00% EG + 15.03% CaCl2	264.77	2274.00	<empty>	-	-	-
k	20% CO2 + 80% CH4	5.00% EG + 15.03% CaCl2	269.79	3708.00	<empty>	-	-	-
k	20% CO2 + 80% CH4	5.00% EG + 15.03% CaCl2	276.89	8870.00	1337.39	84.922	-	-
k	20% CO2 + 80% CH4	5.00% MeOH + 15.00% NaCl	262.37	2151.00	<empty>	-	4171.45	93.931
k	20% CO2 + 80% CH4	5.00% MeOH + 15.00% NaCl	268.06	4061.00	<empty>	-	7497.29	84.617
k	20% CO2 + 80% CH4	5.00% MeOH + 15.00% NaCl	274.85	9371.00	3196.78	65.886	17729.19	89.192
k	20% CO2 + 80% CH4	5.00% MeOH + 4.93% NaCl + 4.96% KCl + 5.00% CaCl2	263.58	2136.00	<empty>	-	1528.56	28.438
k	20% CO2 + 80% CH4	5.00% MeOH + 4.93% NaCl + 4.96% KCl + 5.00% CaCl2	269.13	3901.00	<empty>	-	2574.58	34.002
k	20% CO2 + 80% CH4	5.00% MeOH + 4.93% NaCl + 4.96% KCl + 5.00% CaCl2	276.09	9048.00	2122.57	76.541	5184.08	42.705

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	Pexp (kPa)	P_{HYS}^{A} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
k	20% CO2 + 80% CH4	5.00% MeOH + 5.00% NaCl	268.29	2140.00	<empty>	-	1726.68	19.314
k	20% CO2 + 80% CH4	5.00% MeOH + 5.00% NaCl	277.32	5552.00	4063.76	26.805	4960.57	10.653
k	20% CO2 + 80% CH4	5.00% MeOH + 5.00% NaCl	281.91	9682.00	6893.99	28.796	8290.38	14.373
k	20% CO2 + 80% CH4	5.00% MeOH + 9.97% CaCl2	266.51	2211.00	<empty>	-	149009.63	6639.467
k	20% CO2 + 80% CH4	5.00% MeOH + 9.97% CaCl2	273.72	4727.00	1317.06	72.137	217411.48	4499.354
k	20% CO2 + 80% CH4	5.00% MeOH + 9.97% CaCl2	280.35	10348.00	1343.05	87.021	295813.78	2758.657
k	20% CO2 + 80% CH4	5.00% MeOH + 9.97% KCl	267.58	2172.00	<empty>	-	1688.24	22.273
k	20% CO2 + 80% CH4	5.00% MeOH + 9.97% KCl	276.52	5752.00	3877.22	32.594	6379.24	10.905
k	20% CO2 + 80% CH4	5.00% MeOH + 9.97% KCl	280.42	9705.00	5394.30	44.417	10085.81	3.924
k	20% CO2 + 80% CH4	9.99% MeOH + 9.98% NaCl	262.15	2063.00	<empty>	-	1415.69	31.377
k	20% CO2 + 80% CH4	9.99% MeOH + 9.98% NaCl	268.09	3822.00	2004.18	47.562	4161.49	8.882
k	20% CO2 + 80% CH4	9.99% MeOH + 9.98% NaCl	275.19	8754.00	4317.73	50.677	8773.09	0.218
k	50% CO2 + 50% CH4	10.02% MeOH + 10.07% NaCl	264.46	2153.00	<empty>	-	1148.81	46.641
k	50% CO2 + 50% CH4	10.02% MeOH + 10.07% NaCl	270.44	4163.00	2067.23	50.343	4443.51	6.738
k	50% CO2 + 50% CH4	10.02% MeOH + 10.07% NaCl	274.00	6785.00	3120.97	54.002	6855.58	1.040
k	50% CO2 + 50% CH4	14.99% MeOH + 5.00% NaCl	266.08	2564.00	1628.71	36.478	1879.08	26.713
k	50% CO2 + 50% CH4	14.99% MeOH + 5.00% NaCl	270.17	4049.00	2593.56	35.946	2829.79	30.111
k	50% CO2 + 50% CH4	14.99% MeOH + 5.00% NaCl	274.12	6888.00	4212.30	38.846	4334.79	37.067
k	50% CO2 + 50% CH4	5.00% MeOH + 4.93% NaCl + 4.96% KCl + 5.00% CaCl2	264.52	1960.00	<empty>	-	1314.30	32.944
k	50% CO2 + 50% CH4	5.00% MeOH + 4.93% NaCl + 4.96% KCl + 5.00% CaCl2	270.14	3846.00	1526.82	60.301	2318.45	39.718
j	78% CH4 + 20% CO2 + 2% C3H8	10.00% MeOH + 10.00% NaCl	278.90	8161.00	3948.56	51.617	9249.33	13.336
j	78% CH4 + 20% CO2 + 2% C3H8	10.00% MeOH + 10.00% NaCl	279.66	8590.00	4384.34	48.960	10828.68	26.062
j	78% CH4 + 20% CO2 + 2% C3H8	10.00% MeOH + 10.00% NaCl	279.88	9452.00	4521.95	52.159	11358.88	20.174
j	78% CH4 + 20% CO2 + 2% C3H8	10.00% MeOH + 4.99% NaCl + 5.01% CaCl2	274.09	3164.00	1273.88	59.738	2683.67	15.181
j	78% CH4 + 20% CO2 + 2% C3H8	10.00% MeOH + 4.99% NaCl + 5.01% CaCl2	277.08	4691.00	1286.21	72.581	3842.96	18.078
j	78% CH4 + 20% CO2 + 2% C3H8	10.00% MeOH + 4.99% NaCl + 5.01% CaCl2	280.12	8057.00	1299.00	83.877	5757.28	28.543
j	78% CH4 + 20% CO2 + 2% C3H8	10.01% MeOH + 9.99% NaCl	274.78	3853.00	2322.56	39.721	4829.32	25.339
j	78% CH4 + 20% CO2 + 2% C3H8	10.01% MeOH + 9.99% NaCl	277.30	5767.00	3195.83	44.584	6959.18	20.672
j	78% CH4 + 20% CO2 + 2% C3H8	10.01% MeOH + 9.99% NaCl	280.09	9744.00	4661.61	52.159	11872.80	21.847
j	78% CH4 + 20% CO2 + 2% C3H8	14.97% MeOH + 4.98% NaCl	273.81	3443.00	2687.39	21.946	2820.65	18.076
j	78% CH4 + 20% CO2 + 2% C3H8	14.97% MeOH + 4.98% NaCl	277.50	5632.00	4384.73	22.146	4429.31	21.355

Ref	Mixture composition (mol%)	Inhibitor composition (mass%)	T (K)	Pexp (kPa)	P_{HYS}^{A} (kPa)	%Dev	PCSMHyd (kPa)	%Dev
j	78% CH4 + 20% CO2 + 2% C3H8	14.97% MeOH + 4.98% NaCl	279.96	8250.00	6362.77	22.876	6228.65	24.501
j	78% CH4 + 20% CO2 + 2% C3H8	4.99% MeOH + 4.97% CaCl2	277.31	2518.00	1305.81	48.141	30666.43	1117.889
j	78% CH4 + 20% CO2 + 2% C3H8	4.99% MeOH + 4.97% CaCl2	283.29	5685.00	1328.16	76.637	61169.84	975.987
j	78% CH4 + 20% CO2 + 2% C3H8	4.99% MeOH + 4.97% CaCl2	285.94	8881.00	7757.07	12.655	77630.09	774.114
j	78% CH4 + 20% CO2 + 2% C3H8	5.00% MeOH + 5.00% NaCl	277.50	2672.00	2378.39	10.989	2855.57	6.870
j	78% CH4 + 20% CO2 + 2% C3H8	5.00% MeOH + 5.00% NaCl	283.13	5961.00	4989.32	16.301	6021.60	1.017
j	78% CH4 + 20% CO2 + 2% C3H8	5.00% MeOH + 5.00% NaCl	285.65	8490.00	7382.44	13.045	9210.23	8.483
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	15.00% MeOH + 5.02% NaCl	277.19	3473.00	2397.30	30.973	2661.60	23.363
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	15.00% MeOH + 5.02% NaCl	281.12	6012.00	4046.80	32.688	4288.10	28.674
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	15.00% MeOH + 5.02% NaCl	283.75	10088.00	6092.48	39.607	6196.90	38.572
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	5.01% MeOH + 14.98% NaCl	277.13	3779.00	1339.66	64.550	7838.48	107.422
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	5.01% MeOH + 14.98% NaCl	281.07	7046.00	2178.06	69.088	18542.21	163.159
j	82% CH4 + 0.5% CO2 + 11.3% C2H6 + 4.2% C3H8 + 0.9 i-C4 + 0.6 n-C4 + 0.1 i-C5 + 0.2 n-C5 + 0.2 n-C6	5.01% MeOH + 14.98% NaCl	282.87	9782.00	2734.47	72.046	24971.77	155.283

Ref according to Table 1