

Simulation Analysis and Design Modelling of Raw Natural Gas Dehydration and Sweetening Preliminary to Liquefaction Stage

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ABSTRACT

Natural gas (NG) purification prior to liquefaction, such as sweetening and dehydration, is the subject of the present study. There are a variety of impurities that must be removed from the NG in order to meet LNG criteria since they may cause corrosion, clogging, and other issues. Utilizing molecular sieves, gPROMS® was utilized to duplicate the sweetening of NG with diethanolamine (DEA), as well as its dehydration with glycol solvent absorption (adsorption). Both of the first two approaches rely on absorption columns with equilibrium phases to keep the solvent and pollutants in close contact. After that, in distillation columns, both solvents are regenerated in trays by heating them to a high temperature. NG was dehydrated using Zeolite 5A adsorption and custom models were created. In this case, water adsorption was simulated using an isothermal adsorption bed. Chemicals such as dimethylaminoethylamine (DEA) were used to sweeten natural gas (NG) with CO₂ values of 1.33x10⁻⁴ mole percent and H₂S of 5.22x10⁻⁴ mole percent, respectively. With triethylene glycol (TEG), a dry gas was produced with 41ppmv of water absorption at an energy consumption rate (EER) of 5.54 GJ/ton water absorption and a solvent concentration of 99.9 per cent. Zeolite-induced dehydration of NG was simulated, and the breakthrough time was 1336 minutes.

Keywords: Simulation, Natural Gas, Liquefaction Stage, Modelling, Analysis

I. INTRODUCTION

NG is a manufacturing fuel and raw ingredient. It's in furnaces, heaters, and stoves. It's used in brick, concrete, and porcelain kilns and boilers to create steam. NG is used in the petrochemical sector to generate hydrogen, sulphur, carbon black, ammonia, and nitric acid and urea. NG is used to create the petrochemical ethylene.

Conventional energy sources, NG has less emissions of sulphur dioxide, nitrous oxide, and carbon dioxide. This reduces acid rain, ozone layer depletion, and GHG emissions. In the previous 20 years, conventional NG reserves grew by 36% and production by 61%. Between 2010 and 2013, proved NG reserves grew 3% and production grew 15%.

NG consumption climbed faster than coal for the very first time in years in 2012. Natural gas will surpass coal as second most used fuel by 2025. Despite economic concerns, the global gas sector is expected to reach 4,700 billion cubic meters by 2030. This rise is supported by rising gas production potential and an increase in LNG facilities and high-pressure pipelines.

II. BACKGROUND

NG is found beneath pressures in rock formations down within the Earth's crust, either alone or dissolved with heavy hydrocarbons and water. Decomposing organic detritus over millions of years produces NG.

The main component of NG is methane. Paraffinic hydrocarbons include ethane, propane, and butane. NGs contain nitrogen, carbon dioxide, hydrogen

sulfide, and water. NG's makeup varies with location. "Dry gas" is methane-rich gas. It's called "wet gas" otherwise.

Due to storage difficulties, produced gas must be delivered immediately. Getting NG from oil and gas fields to the market requires a range of options. Pipelines are a convenient means of transport, but not versatile. A pipeline shutdown typically necessitates shutting production down and collecting facilities as well.

LNG has been proven useful since the mid-1970s. LNG is natural gas cooled to -162°C and compressed to 1/600 volume. The cost of developing an LNG plant has reduced since the mid-1980s, making LNG a significant gas export technique globally. LNG is generated at moderate temperatures, therefore impurity levels are lower than in pipeline gas (Table 1).

Table 1: LNG and pipeline gas composition[1]

Impurity	Feed to LNG plant	Pipeline gas
H ₂ O	<0.1 ppmv	150 ppmv
H ₂ S	<4 ppmv	5.7-22.9 mg/Sm ³
CO ₂	<50 ppmv	3-4 mol %
N ₂	<1 mol %	3 mol %
C ₄ H ₁₀	<2 mol %	-
C ₅ +	<0.1 mol %	-

Purification, separation, and liquefaction are the three major reasons for processing the raw NG. A typical NG processing procedure includes the following steps: removal of condensate and water, sweetening, dehydration, removal of mercury, rejection of nitrogen, recovery of natural gas liquids, and fractionation.

1.1. Sweetening

Sulfur-containing chemicals such as CO₂, H₂S, and others are common in natural gas, and they must be removed entirely or partially since they may produce acids when exposed to water. This has led to the term "acid gases" being used to describe them. Solvent absorption (chemical, physical, or hybrid) is the most common way of eliminating them, followed by solid adsorption and membrane separation.

To sweeten NG, the most popular chemical solvent is amine, which is readily available and affordable. Amines are synthesized by attaching OH groups to hydrocarbon groups that have one or more hydrogen atoms removed from ammonia (NH₃). Chemically, amines remove acid gases by first dissolving the gas in the liquid (physical absorption), and then reacting with the dissolved gas.

1.2. Dehydration

Plants are almost always equipped with a dehydration stage since water-laden gas exits the sweetening unit. Furthermore, the cryogenic component of the facility cannot accept most gas streams because of the excessive water content. Standard compliance, reduced corrosion, and the avoidance of hydrate formation need dehydration.

One of the most pressing issues in the oil and gas business has been the formation of gas hydrates. Absorption and adsorption are the most common methods of achieving the necessary level of dehydration.

When the gas is handled with a fluid that preferentially takes water vapour, water levels may be reduced to the 10-ppmv range by physical absorption. NG dehydration uses TEG as the most common liquid desiccant for many reasons.

Adsorbent may also be used to dehydrate NG streams. First, the component touches the particle's surface; subsequently, the adsorbate moves through the adsorbent's channels to complete the process. Due to a rigorous water standard for LNG generation, adsorption operations are much superior to the more common absorption processes, since water is removed from the NG stream considerably more forcefully than any other component. Commercial desiccants most often used in this purpose include silica gel, molecular sieves, and activated alumina. The most adaptable desiccants are molecular sieves, which may be tailored to a certain pore size and dehydrated to less than 0.1 ppm water content.

III. MATERIALS AND METHODS

Process Systems Enterprise Ltd. (PSE) created gPROMS®, a process simulator application, to produce the flowsheets. gPROMS® ModelBuilder and gPROMS® ProcessBuilder were used to develop, verify, execute, and deploy steady-state and dynamic process models.

1.3. gPROMS[®] as Model Builder

It is described as a collection of numbers and mathematical equations that, when paired with a set of requirements, describe a system's behavior. The equations, variables, and parameters that make up a model may be summarized as follows: Parameters and variables may be assigned or computed in the SET and ASSIGN sections of the model, respectively. Variables are classified according to their kind and their upper and lower bounds. The model's TOPOLOGY section contains information on the relationships among its many objects. To create these links, just drag & drop objects from the Project Tree into the desired locations and click "Join." Because of this, the TOPOLOGY tab of the model in gPROMS[®] may be used to create models visually.

A collection of equations called a component model describes the physical and chemical behavior of a unit. These models are often taken from a preexisting repository. As a result, a flowsheet is a composite model, or one that includes other entities as sub-models, and depicts a process made of interrelated unit activities. Each component model's specifications are defined using dialogs that equal to providing parameters and allocating variables.

1.4. Physical Properties Package

In most gPROMS[®] process models, physical factors such as density, enthalpy, and fugacity, which are generally consequences of temperature, pressure, and composition, are employed. Therefore, it is important to establish a suitable model for predicting these characteristics while using separation equipment.

GSAFT[®] was employed in the amine sweetening flowsheet whereas MultiflashTM (with the Peng-Robinson (PR) equation of state) was used to predict NG dehydration physical parameters.

1.4.1. MultiflashTM

One of the most advanced software packages available today is MultiflashTM. This package's most essential thermodynamic calculation is phase equilibrium. At equilibrium, a product's humidity and low in all stages is equal.

When calculated from extrapolation of experimental vapour-liquid equilibrium data,

binary interaction parameters (BIPs) define systems more accurately. BIPs may be used to alter a model's predictions until they match experimental data. The closer a binary system is approaching ideality, when the BIP is zero [9], the smaller it is. Because most BIPs in MultiflashTM were zero, which doesn't match reality, BIPs were estimated using experimental VLE data for dehydrating NG with glycol for a more accurate prediction. MultiflashTM and Excel[®] were utilized.

1.4.2. gSAFT[®]

An advanced molecular thermodynamic method, the Statistical Associating Fluid Theory (SAFT), may predict mixture thermodynamic characteristics. Physically precise models of molecules and their relationships with one another are the foundation of this technique. As a result, SAFT can account for non-spherical molecules, strong directional connections, and other types of interactions that aren't always spherical, including attraction and repulsion. This is the major benefit of SAFT. In this way, SAFT is able to anticipate characteristics that are beyond the experimental data's range of possible states of affairs. SAFT is a great tool for modelling the behavior of complex materials including polar solvents, hydrogen-bonded fluids, and polymers in this technique.

The gSAFT[®] Physical Properties Package is an efficient implementation of the SAFT-VR SW (SAFT-VR SW) and SAFT-Mie equations of state. SAFT-VR SW is used to model the sweetening process. In addition to the basic SAFT technique, this equation of state expands the range of systems that may alter their polarity. This equation is used to describe molecules as chains of spherical sections with varying attractive interactions.

IV. MODELLING OF NATURAL GAS PURIFICATION

1.5. Sweetening

Using data from Abdulrahman et al., gPROMS[®] Process Builder constructed a simulation for sweetening NG using DEA as a solvent. Figure 1 depicts the flowsheet.

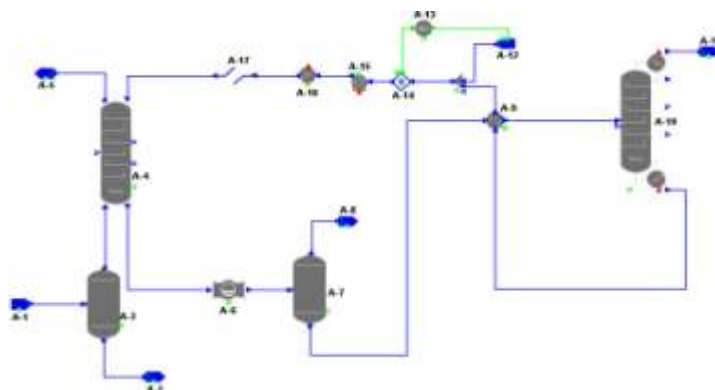


Figure 1: Assembled NG sweetening flowsheet

Entering the sweetening unit (A-1) at 38 oC and 35.5 bar, the NG feed (A-1) contains the following:

Table 2: NG feed Composition

Component	Molar composition (%)	Component	Molar composition (%)
H ₂ S	5.37	C3H8	6.02
CO ₂	4.47	i-C4H10	1.36
N ₂	0.11	n-C4H10	2.44
H ₂ O	0.13	i-C5H12	1.03
CH ₄	63.27	n-C5H12	0.73
C2H6	13.88	C6H14	1.19

A knock out drum (A-3) removes stray liquids from gas (A-2). The solvent is a 35% DEA solution that enters the column at 400 m³/h at 40 oC and 35.5 bar. The absorber has 20 equilibrium stages, and the pressure (35.5 bar).

Rich amine is lowered to 620 kPa by an A-6 valve before being flashed in a flash tank (A-7). The flash tank's rich amine solution is heated to 95 oC in heat exchanger A-9 with a 70 kPa pressure drop.

Before returning to the absorber, the rich solvent must be regenerated using a distillation column (A-10) at 1.9 bar, a kettle reboiler, and a partial condenser at full reflux. At the fourth of 23 equilibrium phases, rich amine is supplied. The

reflux ratio was 1.5 mol/mol and the boilup ratio was 0.12 mol/mol to produce the desired DEA concentration in the regenerated solvent stream.

The cooled regenerated amine is introduced to the solvent solution in the amine-amine heat exchanger (A-9). The lean solvent is pumped (A-16) and refrigerated before recycling (A-15).

1.5.1. Main Results

According to Abdulrahman et al., the acid gas concentrations in the sweet gas are shown in Table 3.

Table 3: Sweet stream outcomes compared

	Abdulrahman et al. gPROMS® [10]	
CO ₂ in sweet gas (mol. %)	3.74x10 ⁻²	1.34x10 ⁻⁴
H ₂ S in sweet gas (mol. %)	3.42x10 ⁻⁴	5.24

The sweet gas nevertheless contains a lot of H₂S, indicating a low absorption efficiency (4.8

wt. percent). This is because gSAFT® has not validated data for H₂S removal with amines.

Sweet gas contains 1.3 ppmv of CO₂, less than the 50 ppmv needed for liquefaction. DEA reduces CO₂ to 50 ppmv. Because amine CO₂ absorption is viable, a higher CO₂ removal rate is expected. Because H₂S is not absorbed well in

DEA, there is no challenging absorption seen between acid gases, exacerbating CO₂ to have almost removed completely from the NG feed. Table 4 displays regeneration results (A-10).

Table 4:Regeneration simulation results (A-10)

	Top (acid gases, A-11)	Bottom (lean solvent)
Temperature (°C)	83.7	122.3
Pressure (bar)	1.9	1.9
Mass flowrate (kg/s)	3.4	111.2
Condenser heat duty (kW)	6134	
Reboiler heat duty (kW)	21451	
	Mass composition (%)	
H ₂ S	3.3	0
CO ₂	82.3	0.2
H ₂ O	14.3	64.4
DEA	0	35.4

Since some water is removed during the simulation, a water show is necessary to keep the absorber supplied with 400 m³/h of DEA solution. The mixer loses around 0.516 kg/s of water, requiring water make-up (A-12).

1.6. Glycol Dehydration

A flowsheet for dehydrating NG using triethylene glycol (TEG) as a solvent was designed. Figure 2 shows a flowchart generated using Ghati data in gPROMS® ModelBuilder.

70 MMSCFD of NG feed was selected at 30 oC and 81.7 psi (B-1). Table 5 displays the NG feed composition.

Table 5:NG feed Composition

Component	Molar composition (%)	Component	Molar composition (%)
CH ₄	97.00	C6H14	0.03
C2H6	1.03	C7H16	0.11
C3H8	0.31	C8H18	0.05
i-C4H10	0.07	C9+	0.02
n- C ₄ H ₁₀	0.09	H ₂ O	0.13
i-C5H12	0.03	CO ₂	0.37
n-C5H12	0.03	N ₂	0.72

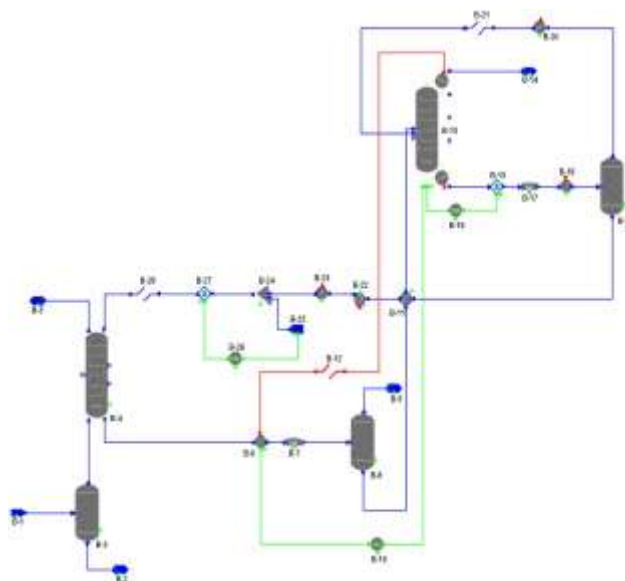


Figure 2:Process flowsheet of NG dehydration

Inlet scrubber (B-3) removes liquids from NG feed (B-2). The B-4 absorber operates at 81.7 bar and in counter-current flow. The gas passes the column at 30°C, whereas the solvent (TEG) at 35°C and comprises 98% glycol. The glycol flow rate should be around 1250 kg/h in the absorber column.

Rich glycol cools the regenerator condenser (B-13). In gPROMS®, the solvent stream cannot be linked directly to the condenser.

Rich solvent reaches a heater (B-6) including an outer power connection (red line B-12). The heater's heat job is like the regenerator's condenser. The adj spec model (B-10) is used to allocate the heater's outlet temperature. This model adjusts the regeneration column's reflux ratio to achieve a desired heater outlet temperature.

After being heated by a valve's pressure drop to 3.013 bar, the rich solvent flashes (B-8) (B-7). Rich solvent is heated to 165 oC in glycol-glycol heat exchanger before entering regeneration column (B-11). The rich solvent is regenerated in a distillation column (B-13) with incomplete condenser (at full reflux) and kettle reboiler. Solvent enters the third equilibrium stage of this five-step column. 1.2 bar is column pressure. Due to solvent breakdown, the reboiler's maximum temperature is 204°C. To achieve this temperature,

an adj spec model (B-16) changes the distillation column's boilup ratio.

The vapour at the top of the vacuum drum (B-19) is likewise transferred to the regeneration column. Bottom-flowing stream.

At 204 oC, the lean solvent leaves the regenerator and the water vapour rises. Before being transferred to a vacuum drum, the lean solvent's pressure is reduced to 0.8 bar (B-17) and warmed to 204 oC (B-18) (B-19). The top vapour is cooled to 165°C before being recycled into the regenerator.

The desired-concentration liquid in B-19 is chilled in B-11, pumped (B-22), and cooled again (B-23). The lean solvent is then combined with a solvent make-up (B-25) of equal content (B-24).

1.6.1. Main Results

A 44 ppm (41 ppmv) measured water content in the dry gas means that 94.2 wt% water is eliminated in the absorber. The gas's water content meets pipeline requirements but not those of LNG facilities. In NG dehydration, glycol dehydration is utilized for bulk water removal and molecular sieves for final purification.

Table 6 compares Ghati absorber findings to gPROMS® absorber results.

Table 6: Analyses based on simulations vs observations from Ghati

	Ghati[11]	gPROMS®	Deviation (%)
Dry gas temperature (°C)	30.73	30.66	0.4
Dry gas mass flowrate (kg/h)	58500	58528	0.05
Rich glycol temperature (°C)	30.55	30.50	0.2
Rich glycol mass flowrate (kg/h)	1299	1292	0.6
Absorption capacity (%)	98.2	94.2	4.1

Other than Ghati's simulations having a higher absorption capacity, there aren't any significant differences. Ghati's physical characteristics package is most likely to blame for this: Because it employs the Twu-SimTassone equation of state in

its glycol package, Aspen Hysys® may be able to account for the discrepancy in absorption capacity. Table 7 summarizes the regenerator's key findings (B-13).

Table 7: The main outcomes of the regenerator's simulations(B-13)

	Top (B-14, water vapour)	Bottom (lean solvent)
Temperature (°C)	105	204
Mass flowrate (kg/h)	42	1266
Condenser heat duty (kW)	11.0	
Reboiler heat duty (kW)	62.6	
Reflux ratio (mol/mol)	0.41	
Boilup ratio (mol/mol)	0.24	
	Mass composition (%)	
CH ₄	0.2	0
H ₂ O	99.0	1.6
CO ₂	0.8	0

TEG

0

98.4

Since some glycol is lost throughout the process, a solvent is needed. Only 0.0018% of the solvent flow entering the absorber is lost in glycol loss. Thus, a glycol make-up rate of 0.023 kg/h is needed.

1.7. Molecular Sieves Dehydration

Subsequently, a flowsheet for the dehydration of NG using molecular sieves, notably zeolite 5A, was put together, for which various unique models were developed. gPROMS® ProcessBuilder was used to dynamically model this process. There was no simulation of water adsorption in gPROMS®.

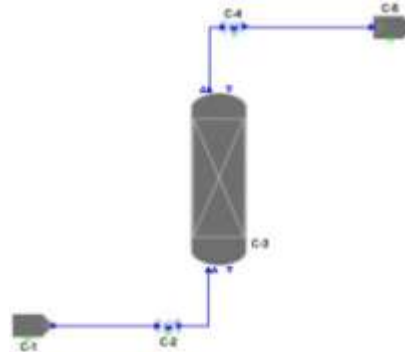


Figure 3: Adsorption flowchart

As part of their research, Gholami, Ruthven, and their colleagues developed custom models to calculate both the axial distribution factor and the adsorption isotherm. The model for mass transfer rate was also altered. The axial dispersion coefficient may be calculated using the equation below:

$$D_{axi} = \gamma_1 D_{mi} + \gamma_2 d_{pu} \quad (1)$$

where γ_2 is a standard unit of measure that is normally set at 0.5.

The constant γ_1 has the following implications in relation to bed voidage:

$$\gamma_1 = 0.45 + 0.55 \varepsilon_b \quad (2)$$

Multi-component Langmuir isotherms are used to calculate the equilibrium state of constituent I in the micropores:

$$q_{ci}^* = q_{si1} \frac{\beta_{i1} p_i}{1 + \sum_{j=1}^n \beta_{j1} p_j} + q_{si2} \frac{\beta_{i2} p_i}{1 + \sum_{j=1}^n \beta_{j2} p_j} \quad (3)$$

The constants β_{ij} and q_{sij} are method for calculating temperature-dependent constants.

$$\beta_{i1,2} = b_{0i,2} \exp\left(\frac{E_{i1,2}}{RT}\right) \quad (4)$$

$$q_{si1,2} = \frac{A_{i1,2}}{T} + A_{i1,2} \quad (5)$$

It is determined using the linear driving force (LDF) model, which is provided by the following equation:

$$\frac{\partial q_{ci}}{\partial t} = \frac{15 D_{ci}}{R_c^2} (q_{ci}^* - q_{ci}) \quad (6)$$

With the following formula, we compute the crystalline diffusivity

$$D_{ci} = D_{0i} \exp\left(-\frac{E_i}{RT}\right) \quad (7)$$

Gholami et al. supply all equation parameters. With 295.5 K and 64.8 pressure, NG feed (C-1) enters an adsorption bed at 23929 kmol/h. Table 8 lists the gas's chemicals.

Table 8: NG feed Molar composition

Component	Molar composition (%)
H ₂ O	0.184
CO ₂	0.998
CH ₄	95.300
N ₂	3.518

Adsorption bed (C-3) comprises one layer of zeolite 5A and the adsorbent parameters defined in gPROMS® may be found in Table 9.

Table 9: properties specified for Bed and adsorbent

Bed properties		Adsorbent particle properties	
Layer length (m)	5.5	Particle density (kg/m ³)	1812.5
Bed internal diameter (m)	3.5	Particle void (m ³ /m ³)	0.36
Bed void (m ³ /m ³)	0.34	Particle diameter (m)	0.0026
		Particle thermal conductivity (W/(m.K))	0.5
		Particle heat capacity (J/(kg.K))	1000

An isothermal process was chosen for heat transfer because of its simplicity and speed. That's how the temperature was set for the bed. We finally settled on 80 discretization points per layer, simplified momentum balancing, and unidirectional flow mode.

1.7.1. Main Results

As shown in Table 10, the gPROMS®-measured breakthrough time is less than the period reported by Gholami et al. A breakthrough was achieved when the water concentration at the end of the bed surpassed the maximum concentration allowed in LNG facilities (0.1 ppmv).

Table 10: Comparison of gPROMS® breakthrough time with Gholami et al. breakthrough time

Breakthrough time (min)	
gPROMS®	1336
Gholami et al. [13]	610
Deviation (%)	119

According to gPROMS®, it will take longer to break through than planned. One aspect that affects the time it takes for a breakthrough to occur is the concentrations and flow rates at which the reaction begins. gPROMS® incorporated all of this data from Gholami et al., so it was not expected that the breakthrough time would be different. The breakthrough time is most likely influenced by the adsorption isotherm parameters, hence these parameters were further examined.

gPROMS® and Ohlin's specific saturation capacities and affinity characteristics were compared. Ohlin used the dual-site Langmuir isotherm to study the removal of CO₂ and water

from NG using zeolite ZSM5 (pore size of about 5). The parameter values, especially for water, were found to be quite diverse. We have already suggested that the breakthrough time would be significantly affected by this fluctuation in factors. Adsorption capacity of the more strongly removed component rises with an increase in parameters, and this causes the breakthrough time to grow as well. Water, the most firmly adsorbent component, appears to be overestimated in the isotherm's parameters.

The Gholami et al. results were closely matched by the mean interstitial velocity between the two models.

Table 11: The comparison of the mean interstitial velocity findings

Mean interstitial velocity (m/s)	
gPROMS®	0.71
Gholami et al. [13]	0.71
Deviation (%)	0.69

Adsorption bed pressure drop was also compared, and the results were strikingly consistent.

Table 12: The comparison of the mean pressure drop findings

Mean pressure drop (bar)	
gPROMS®	1.81
Gholami et al. [13]	1.78
Deviation (%)	1.7

V. CONCLUSIONS

Depending on the extraction location, the NG generated might have a broad variety of components. In this procedure, it might be difficult to accurately analyze a property's physical properties. In contrast, the NG processing method provides a large range of diverse alternatives, which will be influenced by a variety of factors, such as composition.

The NG sweetening flowsheet was built using gSAFT®, a program that PSE just created (and is continuing developing) to implement the SAFT-VR SW equation of state.

In these solutions, gSAFT® does not have validation for H₂S absorption, and estimation of physical properties is crucial for modelling NG treatment, as previously indicated. To put it another way: The sweetened gas contains 7.8 wt. percent H₂S (4.8 wt. percent reduction in the absorber) and just 1.3 ppmv CO₂ (99% removal in the absorber)

at a cost of roughly 21.5 MW (7.3 GJ/ton acid gases absorbed).

NG dehydration is one of the most important procedures in LNG treatment due to tight requirements for NG water.

It is possible to dehydrate using either absorption or adsorption procedures, which are the two most often used techniques. Absorption and adsorption were used to remove the majority of the water before liquefaction, which is common in NG dehydration prior to liquefaction.

After creating and simulating the glycol-based NG dehydration flowsheet, the process was tested. Due to the reboiler's temperature restriction, a traditional atmospheric regenerator was unable to attain the required glycol purity of 99 weight percent. Instead, an improved stripping process was used.

Although there is a 4 percent discrepancy in the absorption capacity, the dehydration

flowsheet developed in gPROMS®, which utilizes Peng-Robinson (PR) equation of state, matches the simulated data from the literature well. It is possible to dry the natural gas to a water content of 41 parts per million by volume (ppmv) using 63 kW of power (5.4 GJ/ton water absorbed).

Lastly, water adsorption from NG was predicted and simulated using molecular sieves. The anticipated breakthrough time (1336 min) in the gPROMS® simulation is almost twice as lengthy as the published results. This is because gPROMS® predicts substantially greater adsorption capabilities. Comparing the gPROMS®

adsorption isotherm properties to industry standards was a must. There may be a disparity in breakthrough times stated since gPROMS® values are often much higher.

VI. ACKNOWLEDGEMENT

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Nomenclature

A_{ij}	Auxiliary adsorption equilibrium parameters	q_{ci}	Equilibrium concentration of component i in the micropores (mol/kg)
b_{0j}	Pre-exponential factor on site j (kPa^{-1})	q_{sij}	Specific saturation capacity of component i on site j (mol/kg)
D_{0i}	Diffusional pre-exponential factor of component i (m^2/s)	R	Ideal gas constant ($\text{J}/(\text{mol}\cdot\text{K})$)
D_{axi}	Axial dispersion coefficient of component i (m^2/s)	R_c	Sorbent crystal radius (m)
D_{ci}	Crystalline diffusivity of component i (m^2/s)	t	Time (s)
D_{ij}	Diffusivity coefficient (m^2/s)	T	Absolute temperature (K)
D_{mi}	Molecular diffusivity of component i (m^2/s)	u	Interstitial gas velocity (m/s)
d_p	Adsorbent particle diameter (m)	Y_i	Molar fraction of component i in the adsorbed phase (mol/mol)
E_i	Diffusional activation energy of component i (J/mol)	β_{ij}	Affinity parameter of gas i on site j (kPa^{-1})

E_{ij}	Adsorption energy of component i on site j (J/mol)	Auxiliary parameter for axial dispersion
p_i	Partial pressure of component i (kPa)	Auxiliary parameter for axial dispersion
q_{ci}	Mass of component i adsorbed into the micropore volume (mol/kg)	Bed voidage (m^3/m^3)

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