Comparison of CO₂ dehydration processes after CO₂ capture

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Kenneth Ikechukwu Okoli

Faculty of Technology, Natural sciences and Maritime Sciences
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Student: Kenneth Ikechukwu Okoli
Supervisor: Professor Lars Erik Øi
External partner: John Oscar Pande
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Summary:
This study compares two conventional methods of CO₂ dehydration processes after CO₂ capture and its suitability of use. The methods are Triethylene Glycol (TEG) absorption and 3A Molecular sieve adsorption. Chapter 1 and 2 covers an in-depth theoretical review of the processes and literature review, chapter 3 deals with the process description while chapters 4,5,6,7 and 8 analyzes the process simulation, dimension, cost estimation and its comparison. The results obtained shows that energy consumption in 3A Mol. Sieve adsorption is higher when compared with TEG absorption. The total installation cost of 1589.91 kNOK for absorber and desorber is higher when compared with 1115.99 kNOK for adsorption and regen/cooling tower. Thus TEG dehydration is recommended for large scale process unit as it has lower operating cost and lower energy consumption. In this report, TEG dehydration process was used to calculate the water content in dry CO₂ gas from 22ppm to 48.9 ppm. For small scale process unit capable of lower water removal in dehydrated dry CO₂ gas to as low as 0.1ppm, 3A Molecular sieve adsorption which has lower equipment cost is more preferable.
Preface

This project report is submitted to the Faculty of Technology, University College of Southeast Norway in partial fulfillment for the award of Master’s degree in Process Technology.

I want to express my deepest appreciation to my Supervisor, Lars Erik Øi for being a wonderful mentor to me. Without his guidance, this thesis report would have not been possible.

To Lars Andre Tokheim, Britt Moldestad, Knut Vågsæther, Nils Eldrup, I am highly grateful for instilling in me the technical competence which guided me in the course of this report. My special thanks goes to my best friends, Victor Igbokwe, Cornelius Agu and my Family for their constant support and encouragement.

Porsgrunn, 12th May 2017

Kenneth Ikechukwu Okoli
Nomenclature

\( A \)  Heat transfer area \([m^2]\) 
\( A_T \)  Total cross-sectional area \([m^2]\) 
\( C_i \)  Molar concentration of species \(i\) \([kmol/m^3]\) 
\( C_E \)  Equipment cost with capacity/size \(Q\) \([kNOK]\) 
\( C_B \)  Known base cost for equipment with capacity/size \(Q_B\) \([kNOK]\) 
\( d \)  Diameter \([m]\) 
\( F_g \)  Gravity force 
\( F_{LT} \)  LMTD correction factor \([-]\) 
\( lb_m \)  Pound-mass 
\( lb_f \)  Pound-force 
\( L \)  Length \([m]\) 
\( L_{MTZ} \)  Length of the Mass transfer zone \([ft, m]\) 
\( L_s \)  Length of the saturation zone \([ft, m]\) 
\( M_i \)  Molecular weight of species \(i\) \([kg/kmol, g/mol]\) 
\( p \)  Partial pressure of pollutant \([Pa]\) 
\( P \)  Pressure, \([Psi, kPa]\) 
\( q \)  Heat transfer per unit time \([J/s, W]\) 
\( Q_g \)  Gas flow rate \([MMscfd, kgmole/h]\) 
\( Q_{Reb} \)  Reboiler heat duty \([kW, MW]\) 
\( R_i \)  Gas constant for species \(i\) \([J/mol.K]\) 
\( t_w \)  Wall thickness \([m]\) 
\( T \)  Temperature \([^\circ C, K]\) 
\( \Delta T_{LM} \)  Logarithmic mean temperature difference \((LMTD)\) \([^\circ C, K]\) 
\( \Delta T_{min} \)  Minimum temperature difference \([^\circ C, K]\) 
\( U \)  Overall heat transfer coefficient \([W/m^2.K]\) 
\( v_f \)  Flooding velocity \([m/s]\) 
\( V \)  Effective volume \([m^3]\) 
\( V_g \)  Velocity of the gas \([m/s]\) 
\( V_s \)  Superficial Velocity \([ft/min]\) 
\( \dot{V} \)  Volumetric flow rate \([m^3/s, m^3/h]\) 
\( X \)  Amount of adsorbate actually adsorbed on the adsorbent \([kg/kg]\) 
\( X_m \)  Amount of adsorbate required to form a monolayer on the adsorbent \([kg/kg]\).
Nomenclature

\( Z \)  Compressibility factor \([\text{ - }]\)
\( Z \)  Packing Height \([m]\)

**Abbreviations**

BTEX  Benzene, Toluene, Ethylbenzene, and Xylene
CCUS  Carbon Capture, Utilization and Storage
GHG  Greenhouse gas
GPSA  Gas Processors Suppliers Association
\( MMscfd \)  Million standard cubic feet of gas per day
MTZ  Mass transfer zone
ppm  Parts per million
PSA  Pressure swing adsorption

**Greek Letters**

\( \varepsilon \)  External void fraction \([-]\)
\( \rho \)  Fluid density \([\text{kg/m}^3]\)
\( \tau \)  Hydraulic residence time (retention time) \([\text{s}, \text{min}, \text{h}]\)
\( \Delta \)  Difference operator
\( \mathcal{R} \)  Universal gas constant \([8.314 \text{ J/mol.K}]\)

**Subscripts/Superscripts**

\( i \)  Species or component
\( o \)  Denotes an initial value at source
\( sh \)  Denotes shell
\( g \)  Gas phase
\( v \)  Denotes vessel
\( vap \)  Vapour phase
\( op \)  Operation
List of Tables and Figures

Figure 1.2.2-1: Two-Film Concept for CO₂ Absorption 10
Figure 1.3.1-1a: Molecular sieve structure 13
Figure 1.3.1-1b: Enlargement of a Molecular Sieve Particle 13
Figure 2.1.1-1a: Schematic view of Mass Transfer Zone 14
Figure 2.1.1-1b: Vapour-phase concentration profile of an adsorbate in the three zones of an adsorption bed 15
Figure 2.2-1: Molecular Sieve Package at Dumbarton Field Development by FRAMES 19
Figure 3.1.1-1: TEG Absorption process with extra stripping column 20
Figure 3.1.2-1: Adsorption-Solid Desiccant Dehydrator Twin Tower System 21
Figure 4.1-1: Aspen HYSYS process flow diagram (PFD) for TEG dehydration process 28
Figure 4.2-1: Aspen HYSYS PFD for 3A Mol. Sieve dehydration process 29

Table 2.2-1: CO₂ dehydration in Industries and their Projects 17
Table 3.3-1: Specifications for the TEG dehydration of CO₂ wet gas, base case 24
Table 3.4-1: Specifications for 3A Molecular Sieve dehydration, base case 26
Table 5.1-1: Separator dimension specification 31
Table 5.1-2: Tube and Shell HX temperatures data calculated by Aspen HYSYS 32
Table 5.1-3: Shell and tube heat exchanger dimensioning 32
Table 5.1-4: Dimension of the Absorption column 33
Table 5.1-5: Dimension of the Desorption column 34
Table 5.1-6: Reboiler, Condenser, Glycol pump and Glycol cooler HYSYS output data 36
Table 5.2-1: Adsorption tower dimensions 38
Table 5.2-2: Regeneration and cooling tower dimensions 40
Table 6.2.1-1: Material factors 42
Table 6.2.2-1: C_B, known base cost with capacity, Q_B 43
Table 6.2.2-2: TEG dehydration _ Cost Estimation calculation results 45
Table 6.2.2-3: 3A Molecular Sieve dehydration _ Cost Estimation calculation results 47
Table 6.2.4-1: Example of NPV analysis of a new project installation 48
Table 7-1: Aspen HYSYS_TEG dehydration material streams simulation results 49
Table 7-2: Aspen HYSYS_TEG dehydration energy streams simulation results 49
Table 7-3: HRT of Absorption and Adsorption equipment 50
Contents

Nomenclature .................................................................................................................. 4

List of Tables and Figures .............................................................................................. 6

1. Introduction .................................................................................................................. 8

   1.1 Dehydration Methods ............................................................................................ 8
   1.2 Absorption theory .................................................................................................. 9
       1.2.1 Absorbents ..................................................................................................... 10
   1.2.2 Mass transfer concepts .................................................................................... 10
   1.3 Adsorption theory ................................................................................................. 13
       1.3.1 Adsorbents ................................................................................................... 14
       1.3.2 Mass Transfer Zone (MTZ) .......................................................................... 15

2. Literature review .......................................................................................................... 17

   2.1 Review of academic/published research work ...................................................... 17
   2.2 Review of industrial optimization in CO$_2$ dehydration ...................................... 18

3. Process description ..................................................................................................... 21

   3.1 Base case ................................................................................................................ 21
       3.1.1 CO$_2$ dehydration-Absorption Method ......................................................... 21
       3.1.2 CO$_2$ dehydration-Adsorption Method ......................................................... 22
   3.2 Concentration, Retention time, Water content and Glycol circulation rate analysis ... 23
       3.2.1 Concentration, Retention time and Water content ......................................... 23
       3.2.2 Glycol circulation rate .................................................................................. 24
   3.3 Specification for TEG dehydration process ........................................................... 25
   3.4 Specification for 3A Mol. Sieve dehydration process ............................................ 27

4. Process simulation ........................................................................................................ 29

   4.1 Base Case-Absorption simulation ......................................................................... 29
   4.2 Base Case-Adsorption simulation ......................................................................... 30

5. Process equipment dimensioning ............................................................................. 31

   5.1 Dimension of Absorption Equipment .................................................................. 31
   5.2 Dimension of Adsorption Equipment .................................................................. 38

6. Cost estimation methods ............................................................................................. 42

   6.1 Classification of cost ............................................................................................. 42
   6.2 Cost Estimation of Base Case (Absorption and Adsorption) processes ............... 43
       6.2.1 Installation factor .......................................................................................... 43
       6.2.2 Installation cost calculation for the base cases .............................................. 44
       6.2.3 Energy estimation method .......................................................................... 48
       6.2.4 Net present value calculation and Economic potential of a project ............. 49

7. Results/Base case simulation result ............................................................................ 50

8. Comparison of Absorption and Adsorption ............................................................ 52

9. Discussion of results .................................................................................................... 54

   9.1 General Uncertainties in the calculations ............................................................ 54
   9.2 Further work ......................................................................................................... 54

10. Conclusion ................................................................................................................... 55

References ......................................................................................................................... 56

Appendices ....................................................................................................................... 60
1 Introduction

Due to the strong dependence on fossil fuels within the current energy scenario, Carbon Capture, Utilization and Storage (CCUS) will play a crucial role to attain the required greenhouse gas (GHG) emissions reduction, in order to avoid permanent and irreversible damage to the Climate system [1, 2]

Natural gas usually contains significant amount of water vapour. Changes in temperature and pressure condense this water vapour, altering the physical state from gas to liquid and then to solid. [3, 4].

Depending on the reference power plant, the type of fuel and the capture method used, the CO₂ product stream contains several impurities which may have a negative impact on pipeline transportation, geological storage and/or Enhanced Oil Recovery (EOR) applications.

After CO₂ capture, water should be removed from the gas through a process called dehydration to ensure that the pipeline does not get clogged up by hydrate formation and to prevent corrosion [4] as well as meet the CO₂ product specification.

The CO₂ streams produced by the various combustion and capture processes are of different quality, containing different types and concentrations of inert and impurities. These differences can significantly affect the design and operation of a CO₂ dehydration unit. Furthermore, the dehydration unit is a critical process that provides moisture integrity for the downstream transportation and injection systems.

The most commonly used method for dehydration are absorption and adsorption [5-7]. Absorption is the process of dehydration using a liquid such as glycols; in adsorption solids like molecular sieves are used in the dehydration process.

A number of suitable technologies for CO₂ dehydration exist. This study focusses on a comparison of TEG absorption and 3A Molecular sieves adsorption processes.

1.1 Dehydration Methods

With the requirement to dehydrate the CO₂ stream from the majority of CO₂ capture processes prior to transportation in pipelines, low moisture content is critical in prevention or minimization of both corrosion and solid hydrates formation. Flue gas can be purified of pollutants (SO₂, CO₂, Dust, CO, NOx, N₂O, dioxins, HF, Hcl, Cl₂) with the following cleaning methods [8];

- Mechanical separation
- Absorption (+ Desorption/regeneration)
- Adsorption (+ Desorption/regeneration)
- Membrane separation
- Chemical conversion (without or with a catalyst)

But for CO₂ streams, the following different types of dehydration technologies, which are suitable for its dehydration exists [4, 5, 9, 10];

- Absorption (Continuous Liquid Circulation Systems): Several liquids are used as absorbents in this process
- Adsorption: Dehydration takes place by adsorption using adsorbents (solid desiccant).
- Membranes: Molecules can permeate membranes using a variety of different mechanisms ranging from size sieving to solution/diffusion properties to effect a separation. Membrane processes has been used on natural gas duty. The driving force for separation of gases is the partial pressure difference across the membrane. Though
research are ongoing in this area, membranes technology have not been used on CO₂ dehydration [4, 11, 12].

- **Joule Thomson Valve**: Saturated gas at pressure (typically from compressor) is cooled and expanded across a Joule Thompson valve. CO₂ is subjected to adiabatic (Joule Thomson) cooling that accompanies the expansion of a real gas.

- **Cooling**: Cooling of raw CO₂ gas streams using compressor inter-stage trains, will move the gas towards saturation due to the reduction in CO₂ water solubility with reduced temperature.

- **Refrigeration**: Saturated gas is cooled against product gas in a gas/gas heat exchanger, further cooled in a refrigerated exchanger and passes to a separator for water removal. Dried gas leaves the top the separator.

- **Turbo Expander**: CO₂ is subjected to isentropic cooling that accompanies the expansion of a real gas.

- **Supersonic Separators**: Gas expansion to supersonic velocity in a Laval nozzle resulting in low pressure and temperature, a liquid mist forms and this condensed droplets are removed from the gas using a cyclonic co-axial separator.

- **Supersonic Separators combined with Hydrate Separation technology**.

Among all the technologies, glycol dehydration absorption and molecular sieve adsorption is the most commonly used in industrial processes [6, 10, 13].

### 1.2 Absorption theory

In absorption, a gas mixture is contacted with a liquid solvent in which one or more components in the gas phase are transferred to (absorbed into) a liquid solvent. The fundamental principles underlying the process of gas absorption are, [9];

- Solubility of the absorbed gas
- Rate of mass transfer

Gas absorption is usually carried out in a vertical counter-current columns called absorption column. A large contact area between gas and liquid is created in the absorber by means of plates or packing elements. The solvent is fed at the top of the absorber, whereas the gas mixture enters from the bottom. The absorbed mixture is washed out by the solvent and leaves the absorber as a liquid solution. This solvent is often recovered in a subsequent stripping or desorption operation. This second step is the reverse of absorption. The purpose of absorption are as follows,

1. Gas purification and dehydration
2. Product recovery
3. Production of solutions of gases for various purposes
4. Gas separation

Absorption dehydration involves the use of a liquid desiccant to remove water vapour from the gas.
1.2.1 Absorbents

Absorbents are liquid desiccant used in the dehydration of natural gas. The most commonly available glycol absorbents are:

- Monoethylene glycol (MEG)
- Diethylene glycol (DEG)
- Triethylene glycol (TEG)
- Tetraethylene glycol (TREG)

TEG is by far the most common liquid desiccant used in natural gas dehydration. It exhibits most of the desirable criteria of commercial suitability as listed below.[5, 14, 15]:

i. TEG is regenerated more easily to a concentration of 98–99% in an atmospheric stripper because of its high boiling point and decomposition temperature.

ii. TEG has an initial theoretical decomposition temperature of 404°F (206.7°C) whereas that of diethylene glycol is only 328°F (164°C) (See Appendix D).

iii. Vaporization losses are lower than Mono-ethylene glycol or Diethylene glycol. Therefore, TEG can be regenerated easily to the high concentrations needed to meet pipeline water dew point specifications.

iv. Capital and operating costs are lower.

1.2.2 Mass transfer concepts

Mass transfer is mass in transit as the result of a species concentration difference in a mixture [16]. In order to determine the size of the equipment necessary to absorb a given amount of solvent per unit time, not only the equilibrium solubility of the solvent but also the rate at which the equilibrium is established must be known. One of the theoretical models describing the absorption process proposed an essentially stable gas-liquid interface, [6, 17, 18]. Large fluid motions are presumed to exist at a certain distance from this interface distributing all material rapidly and equally in the bulk of the fluid so that no concentration gradients are developed. Closer to this interface, however, the fluid motions are impaired and the slow process of molecular diffusion becomes more important as a mechanism of mass transfer [9].

Transfer of materials through the interface itself is normally presumed to take place instantaneously so that equilibrium exists between these two films precisely at the interface[19]. The rate governing step in gas absorption is therefore the transfer of solute through two thin gas and liquid phase interface. The resulting concentration profile is shown in Figure 1.2.2-1 below;
Figure 1.2.2-1: Two-Film Concept for CO₂ Absorption, [9, 18].

\[ y_A \] and \[ x_A \] = concentrations in the bulk of the phases.
\[ y_{Ai} \] and \[ x_{Ai} \] = Actual interfacial concentrations at equilibrium.
\[ y_A^* \] = Mole fraction of A (in the gas) that would be in equilibrium with \[ x_A \]
\[ x_A^* \] = Mole fraction of A (in the liquid) that would be in equilibrium with \[ y_A \]

In a flowing system, Figure 1.2.2-1 above represents conditions at some counter-current flow point e.g. at a certain height in an absorption tower, [9]. The experimentally rate of mass transfer are often proportional to the displacement from equilibrium, thus the rate equation for the gas and liquid film are defined as follows;

\[
N_A = k_y (y_A - y_{Ai}) \tag{1-1}
\]
\[
F_A = N_A A \tag{1-2}
\]
\[
F_{Ay} = k_y A (y_A - y_{Ai}) \tag{1-3}
\]
\[
F_{Ax} = k_x A (x_{Ai} - x_A) \tag{1-4}
\]

Thus, concentration difference between a bulk phase (o) and the gas/liquid interface (i) for CO₂ is;

\[
N_{CO_2} = k_x A (C_{CO_2,i} - C_{CO_2,o}) \tag{1-5}
\]

Where;
\[ N_A \] = Flux of A from gas to liquid [mol/s.m²]
\[ F_A \] = Rate of A from gas to liquid [mol/s]
\( A = \text{Interface Area} \ [m^2] \)

\( k_y = \text{Mass transfer coefficient for the gas film} \ [mol/s.m^2] \)

\( k_x = \text{Mass transfer coefficient for the liquid film} \ [mol/s.m^2] \)

Defining specific surface of the column:

\[ a \equiv \frac{A}{V} \quad (1-6) \]

\( V = \text{volume of the packed column.} \)

Kidnay et al., [20], stated that most commercially used synthetic zeolites (i.e. Molecular sieves) have surface-to-volume ratio, \( \frac{A}{V} \), in the range of 750 cm\(^2\)/cm\(^3\), with most of the surface for adsorption inside of the adsorbent.

Applying Henry’s law assuming that pollutant concentration is low;

\[ y_A^* = \frac{H}{P} X_A \quad (1-7) \]

Define \( m \equiv \frac{H}{P} ; \ y_A = mX_A \quad (1-8) \)

Where;

\( H = \text{Henry’s constant} \ [(pa)] \)

\( P = \text{Total pressure} \ [(pa)] \)

From further analysis,

\[ F_A = \kappa_y aV(y_A - y_A^*) \quad (1-9) \]

\[ \kappa_y \equiv \frac{1}{\frac{1}{k_y} + \frac{m}{k_x}} \]

\( \kappa_y = \text{Overall mass transfer coefficient.} \)

But for diffusion in a non-stationary medium;

\[ N_{Ax} = \left(-CD_{AB} \frac{dx_A}{dx}\right) + \left(X_A(N_{Ax} + N_{Bx})\right) \quad (1-10) \]

\( N_{Ax} = \text{Diffusion flux} + \text{Advection flux} \)

Diffusion flux = \( -CD_{AB} \frac{dx_A}{dx} \)

Advection Flux = \( X_A(N_{Ax} + N_{Bx}) \)

\( N_{Ax} = \text{flux of A in X-direction.} \)

Assuming, \( N_{Bx} \approx 0 \) and \( X_A \ll 1 \), then advection flux is negligible as there will be no advection in the system. Thus according to Øi, [17],

\[ N_{CO_2} (\text{by diffusion}) = -D_{CO_2} * \frac{dCO_2}{dx} \quad (1-11) \]
1.3 Adsorption theory

Solid desiccant dehydration systems work on the principle of adsorption. Adsorption is a phenomenon that occurs when molecules of a gas are brought into contact with a solid surface and some of them condense on the surface. Adsorption processes can be divided into two broad classes, [21]:

- Physical adsorption, in which physical bonds form between the adsorbent and the adsorbate (gas or a liquid).
- Chemical adsorption, in which chemical bonds form between the adsorbent and the adsorbate.

This report only considers physical adsorption. The adsorbate in the report is the wet CO₂ gas. Physical adsorption involves a form of adhesion between the surface of the solid desiccant and the water vapour in the gas. Water forms a thin film that is held to the desiccant surface by forces of attraction, not by chemical reaction. This force is called van der Waals forces, that is, the attractive and repulsive intermolecular forces that hold liquids and solids together and give them their structure. Redlich-Kwong (RK) improved the Van der Waals equation by including a temperature dependence on the attraction term while Peng-Robinson (PR) and Soave Redlich–Kwong (SRK) added the acentric factor, which describes the molecular behaviour of the specie.

Physical adsorption is an equilibrium process like vapour-liquid equilibria. To achieve equilibrium on a small surface: Some passing molecules will condense on the surface and after some finite time, the molecule may acquire sufficient energy to leave and be replaced by another. Finally, after sufficient time, a state of equilibrium will be reached wherein the number of molecules leaving the surface will equal the number arriving, [15]. The number of molecules on the surface is a function of:

- The nature of the adsorbent.
- The nature of the molecule being adsorbed (the adsorbate).
- The temperature of the system and adsorbate concentration over the adsorbent surface.

**Adsorption Isotherms:**

Adsorption process can also be described through isotherms, that is, the amount of adsorbate on the adsorbent as a function of its pressure (if gas) or concentration (if liquid) at constant temperature. From the adsorption isotherms graph, we can predict that after saturation pressure, Ps, adsorption does not occur anymore. Two Isotherms model are stated as follows:

- **Langmuir:**
  \[ X = X_m \left( \frac{p}{a+p} \right) \]  
  \[ (1-12) \]

- **Freundlich:**
  \[ X = C_F p^{n_F} \]  
  \[ (1-13) \]

\( X \) = amount of adsorbate actually adsorbed on the adsorbent [kg/kg]. In this study, \( X \) is the amount of water adsorbed on 3A molecular sieve.

\( X_m \) = amount of adsorbate required to form a monolayer on the adsorbent [kg/kg].

\( p \) = partial pressure of pollutant [Pa]

\( a \) = constant [Pa]; \( C_F \) = constant; \( n_F \) = constant
1.3.1 Adsorbents

Adsorbents used for removing water from a fluid stream are known as "solid desiccant". There are several solid desiccants which possess the physical characteristics to adsorb water from natural gas. These desiccants generally are used in dehydration systems consisting of two or more towers and associated regeneration equipment. They are:

- Silica gel, which is made of pure SiO$_2$,
- Activated carbon
- Activated alumina, which is made of Al$_2$O$_3$,
- Molecular sieves: Molecular sieves are synthetically produced zeolites.

Emphasis is on Molecular sieve as it was used in this report.

Molecular sieves are crystalline alkali metal (calcium, sodium, potassium) aluminosilicates comprising a three-dimensional interconnecting network of silica and alumina tetrahedral structure, Figure 1.3.1-1a. The enlargement of the Molecular sieve is shown in Figure 1.3.1-1b.

![Molecular sieve structure](image1.png)

**Figure 1.3.1-1a: Molecular sieve structure**

![Enlargement of a Molecular Sieve Particle](image2.png)

**Figure 1.3.1-1b: Enlargement of a Molecular Sieve Particle, [15]**

Molecular sieve can be altered to affect adsorption characteristics. They produce the lowest water dew points, thus they are capable of dehydration to less than 0.1 ppm water content. They
can also be used to simultaneously sweeten and dry gases and liquids. According to Campbell, [22], industries like ZEOCHEM, INTERRA Global, SIGMA Aldrich, [23, 24], the following molecular sieves with their chemical formula exist:

i. 3A: Potassium zeolite, $K_{12}[(A_1O_2)_{12}(S_iO_2)_{12}] * nH_2O$
ii. 4A: Sodium zeolite, $Na_{12}[(A_1O_2)_{12}(S_iO_2)_{12}] * nH_2O$
iii. 5A: Calcium zeolite, $Ca_{4.5}[(A_1O_2)_{12}(S_iO_2)_{12}] * nH_2O$
iv. 10X: Calcium zeolite
v. 13X: Sodium zeolite, $Na_{86}[(A_1O_2)_{86}(S_iO_2)_{106}] * nH_2O$

1.3.2 Mass Transfer Zone (MTZ)

At the inlet of the bed and for a certain distance into it, the adsorbent is saturated to equilibrium value with the absorbable component such as water in natural gas. In this, there is

- Equilibrium zone: it is the saturation zone. Here, no additional adsorption occurs.
- Mass transfer zone (MTZ)
- Active Zone: It is at the outlet of the bed. Here, the adsorbent is unsaturated and the water content of the gas is in equilibrium with the unsaturated activated adsorbent.

The MTZ is defined as the zone between these two zones where the concentration of the water in the natural gas is falling. It is the volume where mass transfer and adsorption take place. (Figure 1.3.2-1a and 1.3.2-1b).

![Figure 1.3.2-1a: Schematic view of Mass Transfer Zone, [15].](image-url)
Figure 1.3.2-1b: Vapour-phase concentration profile of an adsorbate in the three zones of an adsorption bed, [20].

Figure 1.3.2-1b shows the three zones in an adsorbent bed. In the mass transfer zone, the concentration drops from the inlet value, \( y_{in} \) to the outlet value, \( y_{out} \) in a smooth S-shaped curve. MTZ is a function of the following factors, [15]:

- Adsorbent used
- Adsorbent particle size
- Fluid velocity
- Fluid properties
- Temperature
- Pressure
- Adsorbate concentration in the entering fluid
- Adsorbate concentration in the adsorbent if it is not fully reactivated
- Past history of the system

MTZ lengths can be obtained experimentally for various materials and systems and used in graphical correlations for design purposes. GPSA, [14], stated that the length of the MTZ can be estimated with the following equation;

\[
L_{MTZ} (ft) = \left(\frac{V_{adjusted}}{35}\right)^{0.3} (Z)
\]  

(1-14)

While Trent, [25] suggested in Kidnay, [20], the following dimensioned equation for estimating the thickness of the MTZ, \( L_{MTZ} \) in feet of 4 × 8 (1/8-inch[3 mm] diameter) mesh beads:

\[
L_{MTZ} (ft) = 2.5 + 0.025 V_s
\]  

(1-15)

Where;

Factor, \( Z = 1.70\) ft for 1/8 inch (3 mm) sieve and 0.85 ft for 1/16 inch (1.5 mm) sieve

\( V_{adjusted} = V_s = \) Superficial Velocity (ft/min)

\( L_{MTZ} \) acceptable design range is 0.5 – 6 ft (0.2 – 1.8 m). Equation 1-15 is more preferable for calculation of \( L_{MTZ} \) because it is more conservative.
2 Literature review

In this Chapter, an evaluative report of scholarly paper and industrial implementation of CO\textsubscript{2} dehydration was carried out. Thus, the methodology and the results of the study in respect to the project task are presented below.

2.1 Review of academic/published research work

**Absorption publications Review:**

Several Glycol dehydration of CO\textsubscript{2} has been carried out as student thesis by Mirela, Rai and presented in a conference by Lars Erik, [26-28]. In this study, dehydration of CO\textsubscript{2} by absorption in TEG was chosen for simulation with Aspen HYSYS program. The absorption process was simulated for CO\textsubscript{2} dehydration down to a water level of 5 ppm.

The options for dehydrating and compressing CO\textsubscript{2} to achieve the optimum result while meeting all technical requirements was presented at Abu Dhabi conference [29]. Technical and economic aspects of CO\textsubscript{2} water content specification were analyzed and discussed along with current international practices in this paper.

A project was carried out by Hansen et al, [30], to design a TEG (Triethylene glycol) train model using the glycol property package in HYSYS. From their simulations, it was found that stripping gas can increase TEG purity to about 99.6% if it is injected at the right rates. The coldfinger setup can also give TEG purity of about 99.8%. It was realized that TEG could be used to remove approximately 99% of the water from the gas, thus it is recommended.

Using Aspen HYSYS simulation tool, Even Birkelund, [31], compared the standard absorption process, a vapour recompression and a lean split with vapour recompression. Kent Eisenberg was used as the thermodynamic model for the aqueous amine solution and Peng-Robinson for the vapour phase. In capital cost estimation, equipment, engineering and installation cost were considered. The standard absorption process was estimated to have the lowest capital cost by 514 MNOK. The two other modifications were more expensive. The biggest difference was due to the extra compressor.

Abbas et al, [32], made a comparison between the purification requirements of the three major applications (Absorption using EG, Adsorption using silica gel, Refrigeration and Condensation) and the CO\textsubscript{2} composition from post-combustion capture. The paper concluded that the two impurities that require deep removal are water (from 7.3% to 50 ppmv) and oxygen (from 300 ppmv to 10 ppmv). They also evaluated CO\textsubscript{2} purification requirements for the three major applications: pipeline transportation, EOR and geological storage.

**Adsorption publications Review:**

Hefti et al carried out a model-based process design of adsorption processes for CO\textsubscript{2} capture in the presence of moisture, [33]. In their work, the potential of two types of zeolites, 13X and ZSM-5, was investigated in regards to their use in a temperature swing adsorption process for a post combustion capture application. Additionally, the competition for adsorption sites between CO\textsubscript{2} and N\textsubscript{2} was investigated by applying the ideal adsorbed solution theory (IAST) to predict the binary adsorption equilibrium on both sorbents. These predictions indicate a very high selectivity of 13X for CO\textsubscript{2}, making this a very promising sorbent for temperature swing adsorption in a post-combustion capture environment, with the stipulation that it also strongly adsorbs water vapour. More work was done on the development of a pressure swing adsorption process for CO\textsubscript{2} capture from flue gas using solid amine sorbents in
Anahita Govar PhD, [34]. In the dissertation, the key results regarding the use of solid amines for post combustion CO$_2$ capture from flue gas by PSA were presented. The effects of different parameters on the performance of the PSA process in terms of recovery and purity of CO$_2$ and the required energy were also discussed.

Farag et al, [35] , carried out a study of natural gas dehydration using 3A molecular sieve. The scope of their work was to build up a pilot scale unit for natural gas dehydration as simulation of actual existing plant for Egyptian Western Desert Gas Company (WDGC). Mustafa et al, [36], presented at international conference on process engineering and advanced materials, a paper on the description of carbon dioxide adsorption and desorption onto Malaysian coals under subcritical condition. The evaluation of the equilibrium adsorption data were fitted using by Langmuir, Freundlich, Redlich-Peterson, Koble-Corrigan, Toth and Sips models. Toth model provided the best fit for all adsorption experimental data.

### 2.2 Review of industrial optimization in CO$_2$ dehydration

Some dehydration processes has been in existence for natural gas dehydration. Though some companies are in the pilot phase of CO$_2$ dehydration, some of these technology has been applied in water removal after CO$_2$ capture in industrial processes. Table 2.2-1 gives an overview of companies involved in industrial CO$_2$ dehydration and their projects.

**Table 2.2-1: CO$_2$ dehydration in Industries and their Projects**

<table>
<thead>
<tr>
<th>COMPANY</th>
<th>PROJECTS</th>
<th>Contact e-mail/Phone</th>
<th>Address</th>
</tr>
</thead>
<tbody>
<tr>
<td>Worley Parsons</td>
<td>Project: Mountaineer Plant Commercial Scale Carbon Capture and Storage (CCS)  <strong>Customer:</strong> American Electric Power, U.S.A  Project: ENDESA CCS project  <strong>Customer:</strong> Endesa, S.A, Spain  Project: Large Scale Integrated CCS Network.  <strong>Customer:</strong> State of Victoria, Australia and Commonwealth of Pennsylvania.  Project: Weyburn Field CO$_2$-EOR Program  <strong>Customer:</strong> Encana Resources, Canada</td>
<td><a href="mailto:carbonstorage@worleyparsons.com">carbonstorage@worleyparsons.com</a></td>
<td>Various offices, See link below: <a href="http://www.worleyparsons.com/Contact/Pages/OfficeListings.aspx">http://www.worleyparsons.com/Contact/Pages/OfficeListings.aspx</a></td>
</tr>
</tbody>
</table>
| FRAMES | ➤ Stublach Gas Storage UK – comprises gas dehydration trains, glycol regeneration units and hot water boiler system.  
➤ CA Litoral A project Gulf of Mexico  
➤ Dumbarton Field Development  
➤ Desiccant dehydration, Dolphin onshore gas plant project | info@frames-group.com  
+31 172 464 200  
Contact: Drazenka Gazibaric, Process Technical Expert.  
+31 172 504800 | Dr. A.D. Sacharovlaan 2, 2405 WB, Alphen aan den Rijn, The Netherlands. |
| HTC Purenergy | (306) 352-6132 | 2305 Victoria Avenue, Regina, Saskatchewan S4P 0S7, Canada. |
| AKER Solutions | | |
| Schlumberger | | |
| SHELL | ➤ **Quest, Canada:** It is part of the Athabasca Oil Sands Project, a joint venture with Shell (operator and 60% owner) Chevron Canada and Marathon Oil Canada Corp.  
➤ **Shell Cansolv CCS technology:** Shell Cansolv is now in use at the Boundary Dam power station in Saskatchewan, Canada. Boundary Dam is SaskPower’s largest coal-fired power station and a significant source of power for the region. | Tel. +31 70 377 9111 | Shell headquarters: Carel van Bylandtlaan 16, 2596 HR The Hague, The Netherlands  
Postal address: P.O.box 162, 2501 AN The Hague, The Netherlands |
| PROSERNAT | | |
| Siemens | Siemens has developed a proprietary absorption process for post-combustion carbon dioxide capture (called Siemens PostCap™) which is applicable to coal-fired power stations and natural gas-fired power plants. PostCap™ can be integrated in new power plants, but could also be retrofitted to existing power plants at small, medium or large scale. This technology has been used successfully in ADNOC project in Abu Dhabi of which its commissioning year was 2016. | support.energy@siemens.com  
Wittelsbacherplatz 2  
80333 Munich Germany  
Siemens AG  
Freyeslebenstrasse 1  
91058 Erlangen Germany.  
+49 (69) 797 6660 |

For the special case of dehydrating supercritical carbon dioxide, Shell Oil Company has developed the technology of using glycerol [37]. Detailed discussions of the process are given by [38]. At subcritical conditions the conventional glycols, DEG and TEG, are effective for dehydrating CO₂-rich gas streams; however, at supercritical conditions the CO₂-rich fluids can dissolve substantial amounts of the glycols. Under these conditions, glycerol is an attractive desiccant. The drying capability of glycerol is roughly similar to TEG.
Frames has implemented a molecular sieve adsorption-dehydration for Dumbarton field development in the UK sector of the North Sea which is located northeast of Aberdeen, Scotland, see Figure 2.2-1 below;

![Image of Molecular Sieve Package at Dumbarton Field Development by FRAMES.](image)

Figure 2.2-1: Molecular Sieve Package at Dumbarton Field Development by FRAMES.

IEAGHG commissioned AMEC to evaluate and analyse the performance of dehydration units. In this study, whilst several vendors (SPX Flow Technology, FRAMES Process Systems, Exterran (UK) Ltd, Zeochem AG, UOP Products Ltd and Grace Materials Technology) has assisted, most others have been unable or unwilling to do so. Their reasons being that vendors have provided many quotations for CCS projects without any orders being placed. The main dehydration processes AMEC examined based on vendor recommendations are TEG liquid absorbent and Molecular sieve adsorbent. Their analysis stated that the presence of inert and impurities can lead to significant changes in the CO$_2$ physical properties and rates of corrosion. They presented a chart summarising the applicability of the different dehydration technologies. Other analysis pertaining to their research are presented in IEA environmental projects [4].

According to [13] publication, ADNOC in alliance with Masdar and Siemens have completed a FEED study for capturing and dehydrating 1,800,000 tons of CO$_2$ annually from a natural gas fired power plant in Abu Dhabi. It was executed by application of Siemens PostCap™ technology. The solvent Siemens based its technology on is an aqueous amino acid salt solution. This simple flow diagram was integrated into the existing Abu Dhabi gas-fired power plant. This project which started in 2013 is on stream 2016 while the dehydration unit is on a pilot scale.
3 Process description

This chapter presents in detail, the process description for the removal of water from wet CO$_2$ feed stream after CO$_2$ capture.

3.1 Base case

For the base cases, the principal process diagrams (including Equipment) of dehydration processes of the model drawn with Microsoft Visio are shown in Figures 3.1.1-1 and 3.1.2-1. These figures are the processes I calculated and evaluated in this report.

3.1.1 CO$_2$ dehydration-Absorption Method

The process flow shows CO$_2$ dehydration using TEG. Arrow indicates the direction of the flow.

![Diagram of CO$_2$ dehydration-Absorption Method](image)

Figure 3.1.1-1: TEG Absorption process with extra stripping column [28, 39]

The gas to be dehydrated is fed into the absorption column from the bottom where it is counter-currently treated with a regenerated or lean glycol. The lean glycol solvent is fed at the top of the absorber. During absorption, wet CO$_2$ gas is removed of its water content so that dry CO$_2$ gas leaves the column at the top. The rich glycol, saturated with H$_2$O, is taken from the absorber bottom and heated up at the heat exchanger before being fed into the regeneration/desorber column. There, the glycol is regenerated by heat introduction in the reboiler into the desorber. The steam is condensed in a condenser at the top of the desorber column resulting in the release of water vapour. The regenerated lean glycol leaves the bottom of the desorption column and stripping gas is used to increase the percentage recovery of the lean glycol. After further cooling at the glycol cooler, the lean glycol can again be used for dehydrating CO$_2$ in the absorption column. At the flash drum, the rich glycol is flashed to remove dissolved gas. The flash gas, inert gas from external source or portion of gas dehydrated in the absorption column can be used as possible stripping gas, [5, 6, 9, 26]. Heat exchange between the rich glycol and the hot lean glycol can be improved by using two or more shell and tube heat exchanger in series. The increased heat recovery reduces fuel consumption in the reboiler and protects the glycol circulation pump from being overheated.
3.1.2 CO₂ dehydration-Adsorption Method

CO₂ dehydration-adsorption process is a batch process, with multiple desiccant beds used in cyclic operation to dry the gas on a continuous basis, see Figure 3.1.2-1 below.

In solid desiccant diagram above, three separate functions or cycles must alternatively be performed in each dehydrator tower. Cycle time (operation hours) is 8 to 24 hours, [14].

- Adsorbing or gas-drying cycle
- Heating or regeneration cycle
- Cooling cycle (prepares the regenerated bed for another gas-drying cycle)

Adsorption is encouraged by low temperature and high pressures while desorption (its reversal or regeneration) is encouraged by high temperature and low pressure, [15]. In the twin tower system above, wet gas first passes through an efficient microfiber inlet filter separator where free liquids, entrained mist and solid particles are removed. As the wet gas flows downward through the tower on the adsorption cycle, the water vapour is adsorbed in the top layers of the desiccant bed. When the bed is completely saturated with water vapour, the towers must be switched from the adsorbing cycle to the regeneration cycle.

In regeneration tower, regeneration gas is sent to a heater where it is heated up to temperature between 400°F (204°C) to 600°F (315.5°C), and then piped to the tower being regenerated. Part of the dry gas will be used for regeneration gas, [14]. In most plants, a flow controller regulates the volume of regeneration gas used. The desiccant bed will be properly regenerated when the outlet gas (peak-out) temperature has reached between 350°F (176.7°C) and 550°F (287.8°C). After the heating cycle, the desiccant bed is cooled by flowing unheated regeneration gas until the desiccant is sufficiently cooled. All of the regenerated gas is passed through an aerial gas cooler where it is cooled to condense the water removed from the regenerated desiccant bed. The water is then separated in the water knockout vessel before compressing the regeneration gas for another adsorption-dehydration cycles.
3.2 Concentration, Retention time, Water content and Glycol circulation rate analysis

3.2.1 Concentration, Retention time and Water content

**Concentration:**

In molecular diffusion of fluid streams in both absorption and adsorption, there is species concentration difference in the mixture. According to Incropera et al., [16], a mixture consists of two or more chemical constituents (species), and the amount of any species $i$ may be quantified in terms:

- its mass density, $\rho_i (kg/m^3)$ or
- its molar concentration, $C_i (kmol/m^3)$

The mass density and molar concentration are related through the species molecular weight, $M_i (kg/kmol)$ such that,

$$\rho_i = M_i C_i \quad (3-1)$$

Since $\rho_i$ represents the mass of species $i$ per unit volume of the mixture, the mixture mass density is,

$$\rho = \sum_i \rho_i \quad (3-2)$$

And the total no of moles per unit volume of the mixture is,

$$C = \sum_i C_i \quad (3-3)$$

Thus, molar concentration of species, $i$, will be,

$$C_i = \frac{\rho_i}{M_i} \quad (3-4)$$

For a mixture of ideal gases, the mass density and molar concentration of any constituent are related to the partial pressure of the constituent through the ideal gas law. That is,

$$\rho_i = \frac{P_i}{R_i T} \quad (3-5)$$

And

$$C_i = \frac{P_i}{\mathcal{R} T} \quad (3-6)$$

Where $R_i$ is the gas constant for species $i$ and $\mathcal{R}$ is the universal gas constant.

**Retention time (Hydraulic Retention time or Residence time):**

The hydraulic retention time (HRT), also known as hydraulic residence time or $\tau$ (tau), is a measure of the average length of time that a compound remains in a storage unit. It is defined as;

$$HRT = \frac{V}{Q} \quad (3-7)$$

Where,

$V$ = Volume of aeration tank ($m^3$).

$Q$ = Influent flowrate ($m^3/h$)

HRT is usually expressed in hours (or sometimes days).
For this report, \( V \) will be the effective volume of the Absorption or Adsorption tower.

**Water content:**

According to Mokhatab et al. [5], the key design parameter for the absorber are:

- Gas flow rate and specific gravity
- Gas temperature
- Operating pressure (Gas pressure)
- Outlet water content required

The water removal rate, \( W_r \), assuming the inlet gas is saturated can be determined as,

\[
W_r = \frac{Q_G(W_i - W_o)}{24} \tag{3-8}
\]

Where;

- \( W_r \) = Water removed [lb/hr]
- \( W_i \) = Water content of Inlet CO\(_2\) gas [lb/MMscf]
- \( W_o \) = Water content of Outlet CO\(_2\) gas [lb/MMscf]
- \( Q_G \) = Gas flow rate [MMscfd = Million standard cubic feet of gas per day]

### 3.2.2 Glycol circulation rate

Glycol circulation rate is determined on the basis of the amount of Water to be removed and it is usually between 2 and 6 gallons of TEG per pound of water removed, with 3 gallons TEG/Lb water being typical [5].

\[
Q_{TEG,min} = G \times W_r \tag{3-9}
\]

Where;

- \( Q_{TEG,min} \) = minimum TEG circulation rate, (gal TEG/hr)
- \( G \) = glycol-to-glycol water ratio, (gal TEG/Lb water removed).

Using the conversion factors, (See Appendix C), [20, 41, 42], the unit can be changed to a standard unit. Higher circulation rates provide little additional dehydration while increasing reboiler fuel and pumping requirements. Problems can arise if the TEG circulation rate is too low; therefore, a certain amount of over-circulation is desired. An excessive circulation rate may overload the reboiler and prevent good glycol regeneration. The heat required by the reboiler is directly proportional to the circulation rate. Thus, an excessive increase in circulation rate may decrease reboiler temperature, decreasing lean glycol concentration, and actually decrease the amount of water that is removed by the glycol from the gas. An overly restricted circulation rate can also cause problems with tray hydraulics, contactor performance, and fouling of glycol-to-glycol heat exchangers. Therefore, operators should include a margin of safety or comfort zone, when calculating reductions in circulation rates.

It is important that the glycol be near the gas temperature to:

- Prevent gas from exceeding equilibrium temperature
- Prevent foaming

But when the lean glycol concentration and number of trays are held constant, the required glycol circulation rate can be determined from the following equation, [15], :
\[
L_{cr} = \frac{(\Delta W/W_i)W_i Q_g}{24}
\]

(3-11)

Where:

- \(L_{cr}\) = Glycol circulation rate, \(\text{gal/hr}\)
- \(W_i\) = Water content of inlet gas, \(\text{Lb H}_2\text{O/MMscf}\)
- \(W_o\) = Desired outlet Water content, \(\text{Lb H}_2\text{O/MMscf}\)
- \(\Delta W = W_i - W_o\)
- \(Q_g\) = Gas flow rate, \(\text{MMscfd}\)

### 3.3 Specification for TEG dehydration process

According to Abbas et al., [32], the operating conditions and the range of possible compositions for the CO\(_2\) product stream for post-combustion capture technology, as obtained from several sources, [43-46], aligns with some specifications presented below. Aspen HYSYS base case simulation specifications for this thesis, as listed in Table 3.3-1 was from work of Mirela and Lars Erik, [26, 47]. Some specification changes were made based on results from literature reviews. From analysing of various studies on TEG dehydration of CO\(_2\) gas, 85% removal efficiency was selected.

**Table 3.3-1: Specifications for the TEG dehydration of CO\(_2\) wet gas, base case [26, 47]**

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet gas temperature</td>
<td>30 °C</td>
</tr>
<tr>
<td>Inlet gas pressure</td>
<td>40 bar = 4000 kPa</td>
</tr>
<tr>
<td>Inlet gas flow (See Appendix C)</td>
<td>501.1 kgmole/h = 10.06 MMscfd</td>
</tr>
<tr>
<td>CO(_2) in inlet gas</td>
<td>0.76 mole-%</td>
</tr>
<tr>
<td>Water in inlet gas</td>
<td>0.23 mole-%</td>
</tr>
<tr>
<td>Mixer inlet water flow</td>
<td>0.5 kgmole/h (1.102 lbmole/hr)</td>
</tr>
<tr>
<td>Water in outlet gas from Absorber(1st iteration)</td>
<td></td>
</tr>
<tr>
<td>Temperature, Lean TEG to Contactor</td>
<td>35 °C</td>
</tr>
<tr>
<td>Pressure, Lean TEG to Contactor</td>
<td>4000 kpa</td>
</tr>
<tr>
<td>Lean TEG rate (1st iteration)</td>
<td>3.583 kgmole/h</td>
</tr>
<tr>
<td>TEG content in lean glycol</td>
<td>99.04 mass-%</td>
</tr>
<tr>
<td>Water in lean TEG [27]</td>
<td>0.96 mass-%</td>
</tr>
<tr>
<td>Description</td>
<td>Value</td>
</tr>
<tr>
<td>----------------------------------------------------------------------------</td>
<td>------------------------</td>
</tr>
<tr>
<td>Number of stages in absorber</td>
<td>10</td>
</tr>
<tr>
<td>Murphree efficiency for each stage in absorber</td>
<td>0.5</td>
</tr>
<tr>
<td>Lean glycol pump pressure</td>
<td>4100 kPa</td>
</tr>
<tr>
<td>Pump efficiency (Range: 70-80%), [5]</td>
<td>80%</td>
</tr>
<tr>
<td>Pressure drop (ΔP) in Valve</td>
<td>620 kPa</td>
</tr>
<tr>
<td>Pressure after the depressurization valve</td>
<td>110 kPa</td>
</tr>
<tr>
<td>Temperature, TEG to regeneration</td>
<td>153 °C</td>
</tr>
<tr>
<td>Number of desorber stages</td>
<td>6 (4 + reboiler + condenser)</td>
</tr>
<tr>
<td>Murphree efficiency for each stage in desorber</td>
<td>1.0</td>
</tr>
<tr>
<td>Reflux ratio in stripper (for full reflux condenser)</td>
<td>0.5</td>
</tr>
<tr>
<td>Condenser temperature</td>
<td>102 °C</td>
</tr>
<tr>
<td>Reboiler temperature</td>
<td>200 °C</td>
</tr>
<tr>
<td>Desorber gas temperature</td>
<td>190 °C</td>
</tr>
<tr>
<td>Desorber gas pressure (Pressure in desorber)</td>
<td>101 kPa</td>
</tr>
<tr>
<td>Minimum ΔT in heat Exchanger (ΔT\text{min})</td>
<td>10 °C</td>
</tr>
<tr>
<td>Pressure drop (ΔP) range in TEG dehydrator; 5 to 10 psi (34.5 - 69 kPa)</td>
<td>62 kPa (9 psi)</td>
</tr>
<tr>
<td>Number of extra stripper stages (Equilibrium)</td>
<td>3</td>
</tr>
</tbody>
</table>
3.4 Specification for 3A Mol. Sieve dehydration process

For solid desiccant CO\(_2\) dehydration, 3A Molecular Sieve was chosen (See Appendix D).

- **3A Mol. Sieve** Chemical formula, \([15, 23, 24]\), is:
  \[ K_{12}[(A_1O_2)_{12}(S_iO_2)_{12}] \times nH_2O \quad (n = 27 \text{ when saturated}) \]  
  \[ \text{Molecular Weight of 3A Molecular Sieve} = (39+27+32+28+32)\times12+27\times18 \]
  \[ 3A_{(MW)} = 1896 + 486 = 2382 \text{ (g/mol)} \]
  \[ 3A_{\text{Effective Diameter}} (4\times8\text{ mesh size}) = 0.0109 \text{ ft} = 3.3 \text{ mm}. \]

Minimum tower diameter can be determined from Equation 3-12 below, \([15]\):

\[
d^2 = 3600 \left( \frac{Q_gTZ}{VP} \right) \tag{3-12}
\]

Where;
- \(d\) = Tower internal diameter, \((\text{inches})\)
- \(Q_g\) = Gas flow rate, \((\text{MMscfd})\)
- \(T\) = Gas temperature, \((\circ\text{R})\)
- \(Z\) = Compressibility factor
- \(V\) = Superficial gas velocity, \((\text{ft/min})\)
- \(P\) = Tower operating pressure, \((\text{Psia})\)

The regeneration gas velocity is very important especially when effluent moisture content less than 1 ppm are needed. Other design specifications are listed in Table 3.4-1 below.

**Table 3.4-1: Specifications for 3A Molecular Sieve dehydration, base case,\([14, 15, 20]\), (see Appendix D).**

<table>
<thead>
<tr>
<th>Specification Type</th>
<th>Design value used</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet wet Gas/Adsorption temperature</td>
<td>30°C</td>
</tr>
<tr>
<td>Adsorption inlet wet CO(_2) pressure</td>
<td>800 Psi = 5516 kPa</td>
</tr>
<tr>
<td>Allowable adsorption superficial velocity</td>
<td>30ft/min(At 800Psi)=0.152m/s</td>
</tr>
<tr>
<td>Adsorption period</td>
<td>8 – 12 hours</td>
</tr>
<tr>
<td>Gas Feed rate (See Appendix C and D)</td>
<td>200 MMscfd = 9962 kgmole/h (assumed)</td>
</tr>
<tr>
<td><strong>Contents</strong></td>
<td><strong>Zeolites Molecular Sieves _ Heat of Adsorption for water , [48].</strong></td>
</tr>
<tr>
<td>----------------------------------------------------------------------------</td>
<td>---------------------------------------------------------------------</td>
</tr>
<tr>
<td><strong>Regeneration pressure</strong></td>
<td>1800 BTU/lbm H2O = 7536.24 kJ/kg.K (see Appendix C)</td>
</tr>
<tr>
<td><strong>Regeneration temperature</strong></td>
<td>200 Psi = 1379 kPa</td>
</tr>
<tr>
<td><strong>Minimum Regen Superficial velocity (Range = 5- 10ft/min ,[6] )</strong></td>
<td>260°C</td>
</tr>
<tr>
<td><strong>200 Psi)= 0.0457m/s</strong></td>
<td>9ft/min</td>
</tr>
<tr>
<td><strong>Regeneration Gas rate (assumed)</strong></td>
<td>19 MMscfd = 946.4 kgmole/h</td>
</tr>
<tr>
<td><strong>Regen Gas heater inlet temperature</strong></td>
<td>288°C</td>
</tr>
<tr>
<td><strong>Regeneration time</strong></td>
<td>8 hours (5 hrs heating time and 3 hrs cooling time)</td>
</tr>
<tr>
<td><strong>Cycle time (Operation hours)</strong></td>
<td>16hrs (8hrs Adsorption &amp; 8hrs Regen.)</td>
</tr>
<tr>
<td><strong>Design pressure drop (ΔP), Range=5-8 Psi (34.5-55kPa)</strong></td>
<td>7 Psi (48kPa)</td>
</tr>
<tr>
<td><strong>External void fraction, ε, for ΔP calculation [6]</strong></td>
<td>0.37</td>
</tr>
<tr>
<td><strong>Static Equilibrium capacity</strong></td>
<td>20% (Water adsorbed-dry basis)</td>
</tr>
<tr>
<td><strong>Surface-to-volume ratio, ( \frac{A}{V} )</strong></td>
<td>750cm²/cm³ = 75000 m²/m³</td>
</tr>
<tr>
<td><strong>Total bed height, L</strong></td>
<td>8 ft (1.8m)</td>
</tr>
<tr>
<td><strong>Bed height/Diameter (L/D) ratio, Design range=2.5 – 4.0</strong></td>
<td>2.7</td>
</tr>
<tr>
<td><strong>Bed diameter (Calculated)</strong></td>
<td>2.96 ft (0.9m)</td>
</tr>
</tbody>
</table>
4 Process simulation

The process simulation of the base cases in chapter 3.1 are presented here. Generally, the property packages available in Aspen HYSYS allow one to predict properties of mixtures ranging from well-defined light hydrocarbon systems to complex oil mixtures and highly non-ideal (non-electrolyte) chemical systems. In this simulation, Aspen HYSYS recommended property package was used, [49, 50].

4.1 Base Case-Absorption simulation

A traditional TEG dehydration process as presented in Figure 3.1-1 has been simulated in the simulation program, Aspen HYSYS version 8.6, using the Peng Robinson equation of state and Glycol package in the 2nd recycle block. The result is presented below;

![Aspen HYSYS process flow diagram (PFD) for TEG dehydration process.](image)

**Figure 4.1-1: Aspen HYSYS process flow diagram (PFD) for TEG dehydration process.**

**Simulation calculation sequence:**

The calculation sequence is the same as the base case. Mixer and separator was used initially in the simulation to get the required specification of the Wet CO₂ gas. This gas feed stream was calculated first. Then the absorption column and the rest of the process was calculated step by step. The Flash gas was used as stripping gas as stated in the process description, Chapter 3.1.1. Recycle blocks were used in two process flow lines in the design; first to ensure that the extra column vapour outlet stream equals the stripping gas stream to the regeneration column and finally to ensure that the lean glycol stream from the cooler equals the lean glycol stream into the absorption column. Stream cutter was implemented in the course of adding recycle block-2. From the stream cutter transition, P-H flash was changed to T-P flash to ensure the process flow convergence. Clicking ignored in the recycle function while modeling will achieve same function as stream cutter. Worksheet tables for the energy stream and material stream was generated and the results are presented in chapter 7.

Using the base case specifications in Table 3.3-1, the water content in dehydrated gas which was initially 22 ppm from 1st iteration was simulated to approximately 48.9 ppm with Peng Robinson model.
4.2 Base Case-Adsorption simulation

The adsorbent used in the Aspen HYSYS Simulation is 3A Molecular Sieve. 3A Mol. Sieve chemical formula, [15, 23, 24], is:

\[ K_{12}[ (A_1O_2)_{12} (S_iO_2)_{12}] \times nH_2O \quad (n = 27 \text{ when saturated},[15]) \]

Molecular Weight of 3A = \((39+27+32+28+32)\times12 + 4.5\times18 = 1896 + 486 = 2382 (g/mol)\).

This chemical formula was inserted as a new component in Aspen HYSYS with all its properties modified. Other Specifications used for the simulation are stated in Table 3.4-1. The design considerations was based on literature data as all efforts made to get vendors design specifications and data were unsuccessful.

![Figure 4.2-1: Aspen HYSYS PFD for 3A Mol. Sieve dehydration process](image)

**Simulation calculation sequence:**

The calculation sequence is the same as the base case. In this simulation, vessel is used in place of adsorption tower in Aspen HYSYS simulation. It was impossible to input the parameters of 3A Molecular sieve specifications as stated in chapter 3.4 in the simulation calculation. Since 3A Mol. Sieve characteristics is for solid while Aspen HYSYS software is for gases and liquids analysis, there is need to use another software that has an adsorption tower bed input parameters.
5 Process equipment dimensioning

This section covers simplified dimensioning methods for standard process equipment like heat exchanger, columns/towers, pump, etc. Results from Aspen HYSYS simulation was used for the calculation of equipment dimension. The purpose of the dimensioning is to be a basis for cost estimation, thus the investment cost of the equipment can be determined.

5.1 Dimension of Absorption Equipment

For a Traditional TEG absorption process with extra stripping column, the following equipment were dimensioned;

- Absorption/Contactor column
- Regeneration/Desorption column and Extra stripping column
- Flash Drum (Separator Used in design)
- Shell and Tube Heat Exchanger
- Reboiler

Separators:

In glycol dehydration base case, two separators were used in its simulation. These separators are dimensioned with vessel equation parameters. The separators are all made of stainless steel (SS316) with a density of 8238 kg/m³, from Incropera et al, Table A.1, [16]. For vertical separators, vessel diameter, length and shell volume are necessary for its dimensioning. According to the engineering data book, GPSA, [14] and John Campbell, [51], these parameters can be evaluated by the equations below;

\[ D_v = \sqrt{\frac{4Q_g}{\pi F_g V_g}} \]  

(5-1)

Where:

- \( D_v = D \) = Vessel diameter (m)
- \( Q_g \) = Gas flow rate at the actual flowing condition or volumetric flow rate \( (m^3/s) \)
- \( V_g \) = Velocity of the gas \( (m/s) \)
- \( F_g \) = Gravity force (for vertical separators, \( F_g = 1 \))

Since \( F_g = 1 \);

\[ D_v = \sqrt{\frac{4Q_g}{\pi V_g}} \]  

(5-2)

For vertical column diameter determination, a suitable gas velocity of 2 m/s was selected, (typical range= 1-3 m/s). The total cross-sectional area is,

\[ A_T = \pi DL \]  

(5-3)

The length of the vertical column will be,

\[ L = D \frac{L}{D} \]  

(5-4)

The \( L/D \) ratio at 4000 kPa (580 psi) was assumed to be 4.5 based on \( L/D \) reference guidelines stated in Appendix D. The shell volume equation is;

\[ V_{sh} = \pi * t_w * L * D \]  

(5-5)
Using ASME pressure vessel required shell thickness chart for cylindrical shell and Eugene, [52], an approximate wall thickness, \( t_w \), of 0.06 m (2.5 inches) was selected. Solving iteratively and using some simulation values and Equations 5-2 to 5-5, Table 5.1-1 for separator dimension specification was developed below.

Table 5.1-1: Separator dimension specification

<table>
<thead>
<tr>
<th>Separators</th>
<th>V-100</th>
<th>V-101 (Flash Drum)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas volumetric flow rate [m³/s]</td>
<td>3.294 m³/s = 11860 m³/h</td>
<td>0.0368 m³/s = 132.5 m³/h</td>
</tr>
<tr>
<td>Velocity of the gas [m/s]</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Vessel diameter [m]</td>
<td>1.45</td>
<td>0.15</td>
</tr>
<tr>
<td>( L/D ) ratio</td>
<td>4.5</td>
<td>4.5</td>
</tr>
<tr>
<td>Vessel length [m]</td>
<td>6.525</td>
<td>0.675</td>
</tr>
<tr>
<td>Total cross-sectional area [m²]</td>
<td>29.72</td>
<td>3.18</td>
</tr>
<tr>
<td>Wall thickness [m]</td>
<td>0.06</td>
<td>0.06</td>
</tr>
<tr>
<td>Shell volume [m³]</td>
<td>1.78</td>
<td>0.02</td>
</tr>
<tr>
<td>Density (SS316) [kg/m³] [16]</td>
<td>8238</td>
<td>8238</td>
</tr>
</tbody>
</table>

**Shell and tube heat exchanger:**

The Glycol-Glycol exchanger is for countercurrent-flow heat exchange, see figure below.

![Figure 5.1-1: Countercurrent flow heat exchange](image)

The following equations below are used for the heat exchanger dimension:

\[
q = U A \Delta T \tag{5-6}
\]

\[
\Delta T = F_T \times \Delta T_{LM} \tag{5-7}
\]

\[
\Delta T_{LM} = \frac{\Delta T_2 - \Delta T_1}{\ln\left(\frac{\Delta T_2}{\Delta T_1}\right)} \tag{5-8}
\]

\[
\Delta T_1 = T_{ho} - T_{ci} ; \quad \Delta T_2 = T_{hi} - T_{co} \tag{5-9}
\]

\[
F_T = f(R, P) \tag{5-10}
\]
\[ R = \frac{T_{hi} - T_{ho}}{T_{co} - T_{ci}} \quad ; \quad P = \frac{T_{hi} - T_{co}}{T_{hi} - T_{ci}} \quad (5-11) \]

Where;

\( q \) = heat transfer per unit time \((J/s = W)\)

\( U \) = overall heat transfer coefficient \((W/m^2.K)\)

\( A \) = heat transfer area \((m^2)\)

\( \Delta T_{LM} \) = logarithmic mean temperature difference \( (LMTD) \)

\( T_{hi}, T_{ho} \) = temperature of hot water in and hot water out respectively \((K)\)

\( T_{co}, T_{ci} \) = temperature of cold water out and cold water in respectively \((K)\)

\( F_T \) = LMTD correction factor, \((0 < F_T < 1)\)

\( R \) = heat capacity flowrates

\( P \) = thermal effectiveness of the exchanger

From TEG Aspen simulation, the following values were obtained, Table 5.1-2.

**Table 5.1-2: Tube and Shell HX temperatures data calculated by Aspen HYSYS**

\[ T_{hi}=192.6^\circ C \quad ; \quad T_{ho}=116.4^\circ C \quad ; \quad T_{ci}=105^\circ C \quad ; \quad T_{co}=29.81^\circ C \] . \( F_T \) was traced using \( R=1.01 \) and \( P=0.46 \) in LMTD correction factor figure, [14], for 1 shell pass/2 tube passes. Solving Equations 5-6 to 5-11, dimension of shell and tube heat exchanger table was developed.

**Table 5.1-3: Shell and tube heat exchanger dimensioning**

<table>
<thead>
<tr>
<th>Heat Exchanger</th>
<th>E-100</th>
</tr>
</thead>
<tbody>
<tr>
<td>( q = ) Duty [W]</td>
<td>113000 [kJ/h] = 31388.89 [W] (See Appendix C)</td>
</tr>
<tr>
<td>( \Delta T_{LM} ) [K]</td>
<td>87.09</td>
</tr>
<tr>
<td>( F_T )</td>
<td>0.863</td>
</tr>
<tr>
<td>( \Delta T ) [K]</td>
<td>75.16</td>
</tr>
<tr>
<td>( U ) [W/m(^2).K] (Assumed)</td>
<td>15</td>
</tr>
<tr>
<td>A [m(^2)]</td>
<td>27.84</td>
</tr>
</tbody>
</table>
**Absorber:**
Absorber towers, storage tanks, stripping and distillation towers fall under pressure vessels. The absorber dimension method applied are from earlier master’s thesis, [53, 54], and it is shown below:

\[
A_{\text{absorber}} = \frac{\dot{V}_{\text{absorber}}}{3600 \times V_g}
\]  

(5-12)

\(\dot{V}_{\text{absorber}}\) (\(m^3/h\)) is the gas flow calculated through Aspen HYSYS simulation. A suitable gas velocity of 2 \(m/s\) was selected. For absorber diameter calculation,

\[
D_{\text{absorber}} = \sqrt{\frac{4 \times A_{\text{absorber}}}{\pi}}
\]  

(5-13)

The absorber shell volume was calculated using Equation 5-5. The total packing volume was calculated with Equation 5-14 below,

\[
Packing\ \text{volume} = \frac{\pi \times \text{packing height} \times (D_{\text{absorber}}^2)}{4}
\]  

(5-14)

From GPSA, [14], a total height of the contactor column is based on the number of trays or packing required plus an additional 6-10 ft (1.8–3 m) to allow space for vapour disengagement above the top tray, inlet gas distribution below the bottom tray, and rich glycol surge volume at the bottom of the column. Typical tray spacing in TEG contactors is 24 inches (0.61m), [5, 14]. Packing Height (\(z\)) = HTU\#NTU = height of transfer unit\#number of transfer unit. NTU is similar to number of theoretical trays. It was assumed that each stage is of 1m height, which makes the total packing height as:

\[
h_{\text{packing, absorber}} = N_{\text{absorber}} \times 1m
\]  

(5-15)

**Table 5.1-4: Dimension of the Absorption column**

<table>
<thead>
<tr>
<th>Absorption Column (HYSYS output data)</th>
<th>T-100</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas volumetric flow rate [m(^3)/s]</td>
<td>9073 m(^3)/h = 2.52 m(^3)/s</td>
</tr>
<tr>
<td>Gas velocity in absorber [m/s]</td>
<td>2</td>
</tr>
<tr>
<td>Number of stages</td>
<td>10</td>
</tr>
<tr>
<td><strong>Calculated Results for Absorber</strong></td>
<td></td>
</tr>
<tr>
<td>Wall thickness [m]</td>
<td>0.06</td>
</tr>
<tr>
<td>Absorber Diameter [m]</td>
<td>1.26</td>
</tr>
<tr>
<td>Packing height [m] [53] (estimated)</td>
<td>22 , that is ( (3<em>2)+(0.61</em>10)+10)</td>
</tr>
<tr>
<td>Total packing volume [m(^3)]</td>
<td>27.4</td>
</tr>
<tr>
<td>Absorber shell volume [m(^3)]</td>
<td>5.23</td>
</tr>
</tbody>
</table>
**Regeneration/Desorption column:**

Desorber dimension calculation is referred to Rafid, [53], and it is shown below;

Vessel diameter calculation:

X-axis position:

\[
x - \text{axis} = \frac{\dot{m}_{\text{liq}}}{\dot{m}_{\text{vap}}} \frac{\rho_{\text{vap}}}{\rho_{\text{liq}}} \sqrt{\rho_{\text{liq}}} \tag{5-16}
\]

Sounders and Brown factor:

\[
C_{bs} = -0.0283 \cdot \ln(x - \text{axis}) + 0.0452 \tag{5-17}
\]

Flooding velocity:

\[
v_f = C_{bs} \left( \frac{\dot{m}_{\text{liq}}}{\dot{m}_{\text{vap}}} \right)^{0.2} \sqrt{\frac{\rho_{\text{liq}} - \rho_{\text{vap}}}{\rho_{\text{vap}}}} \tag{5-18}
\]

90% flooding is assumed, thus Gas velocity:

\[
v_{\text{gas}} = v_f \cdot 0.9 \tag{5-19}
\]

Vessel diameter:

\[
D_{\text{desorber}} = \sqrt{\frac{4 \cdot \dot{m}_{\text{vap}}}{0.85 \cdot \pi \cdot \rho_{\text{vap}} \cdot v_{\text{gas}} + 3600 \cdot v_{\text{gas}}} \tag{5-20}
\]

Desorber Area:

\[
\pi D^2 \frac{4}{4} \tag{5-21}
\]

The wall thickness of vessel is assumed to be 0.06m. Parameters from Aspen HYSYS simulation and desorber calculation results are listed in Table 5.1-5.

**Table 5.1-5: Dimension of the Desorption column**

<table>
<thead>
<tr>
<th>Density (SS316) [kg/m³]</th>
<th>8238</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Aspen HYSYS output data</strong></td>
<td><strong>T-101</strong></td>
</tr>
<tr>
<td>Vapour volume flow [m³/h]</td>
<td>60.61</td>
</tr>
<tr>
<td>Liquid volume flow [m³/h]</td>
<td>0.5633</td>
</tr>
<tr>
<td>Mass density for liquid [kg/m³]</td>
<td>966.3</td>
</tr>
<tr>
<td>Mass density for vapour [kg/m³]</td>
<td>1.106</td>
</tr>
<tr>
<td>Liquid mass flow [kg/h]</td>
<td>544.3</td>
</tr>
<tr>
<td>Vapour mass flow [kg/h]</td>
<td>67.04</td>
</tr>
<tr>
<td><strong>Vessel calculation results</strong></td>
<td><strong>T-101</strong></td>
</tr>
<tr>
<td>X-axis</td>
<td>0.274679</td>
</tr>
<tr>
<td>Cbs</td>
<td>0.035289</td>
</tr>
<tr>
<td>Flooding velocity [m/s]</td>
<td>1.585</td>
</tr>
<tr>
<td></td>
<td>Gas velocity [m/s]</td>
</tr>
<tr>
<td>-------------------------</td>
<td>-------------------</td>
</tr>
<tr>
<td></td>
<td>1.426</td>
</tr>
</tbody>
</table>

**Aspen HYSYS output data for Reboiler, Condenser, Glycol cooler and Glycol pump:**

Table 5.1-6: Reboiler, Condenser, Glycol pump and Glycol cooler HYSYS output data

<table>
<thead>
<tr>
<th></th>
<th>Reboiler</th>
<th>Condenser</th>
<th>Glycol cooler</th>
<th>Glycol pump</th>
</tr>
</thead>
<tbody>
<tr>
<td>Duty [kJ/h]</td>
<td>215100</td>
<td>61980</td>
<td>382500</td>
<td>5252</td>
</tr>
<tr>
<td>Power [kW]</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>1.459</td>
</tr>
<tr>
<td>Mass flow [kg/h]</td>
<td>544.3</td>
<td>67.04</td>
<td>1068</td>
<td>1068</td>
</tr>
<tr>
<td>ΔP [bar]</td>
<td>-</td>
<td>-</td>
<td>0.2</td>
<td>40.61</td>
</tr>
<tr>
<td>Efficiency</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>80%</td>
</tr>
<tr>
<td>Pressure [kPa]</td>
<td>101</td>
<td>101</td>
<td>4080</td>
<td>4100</td>
</tr>
<tr>
<td>Temperature [°C]</td>
<td>200</td>
<td>102</td>
<td>35</td>
<td>130.3</td>
</tr>
<tr>
<td>Volume [m³]</td>
<td>2</td>
<td>2</td>
<td>0.10</td>
<td>-</td>
</tr>
<tr>
<td>Act. Volume flow [m³/h]</td>
<td>-</td>
<td>-</td>
<td>0.9551</td>
<td>1.024</td>
</tr>
</tbody>
</table>
Reboiler:

Using Equation 5-6, the reboiler heat transfer area dimension was calculated. Thus,

\[ A_{\text{Reboiler}} = \frac{q}{3600 \cdot U \cdot \Delta T} \]  

(5-22)

Where:

\[ q = 215100 \text{ kJ/h} \] (see Table 5.1-6 above)

\[ \Delta T = \Delta T_{LM} \cdot F_T \]

To change hour in kJ/h to seconds in kW as 1 J/s is equal to 1 W, \( q \) is divided by 3600.

The following assumptions were also made:

\[ U [\text{KW/m}^2.\text{K}] = 2.5, \quad [55] \]

\[ F_T = 1.0 \]

\[ \Delta T_{min} = 10 \text{ °C} \cdot 1 = 10 \]

Therefore, area of the reboiler will be;

\[ A_{\text{Reboiler}} = \frac{215100}{(3600 \cdot 2.5 \cdot 10)} = 2.39 \text{ m}^2 \]
5.2 Dimension of Adsorption Equipment

Figure 3.1.2-1 shows a solid dehydration twin tower for adsorption process. For its dimension, the following equipment would be evaluated:

- Adsorption tower
- Regeneration and cooling tower
- Regeneration gas Heater
- Regeneration gas Cooler
- Compressor
- Water Knockout vessel

**Adsorption tower:**

Adsorption tower is a pressure vessel, thus most of its dimensioning will be calculated with vessel equations as stated in section 5.1 and equations from GPSA, [14].

Using Equation 3-12, adsorption tower minimum diameter was dimensioned, thus

\[ d^2 = 3600 \left( \frac{Q_g T Z}{VP} \right) \]

\[ d = \text{Tower internal diameter, (inches)} \]

\[ Q_g = 200 \text{ MMscfd (see chapter 3.4)} \]

\[ V = 30 \text{ ft/min} \]

\[ P = 800 \text{ Psia} = 5516 \text{ kPa} \]

\[ T = 30 \text{ °C}, \quad T(^°\text{R}) = 545.67 \text{ (see Appendix C)} \]

\[ Z_{\text{Adsorption}} = 0.75 \text{ (Interpolating for compressibility factor of CO}_2\text{ at 30°C, 55 bar, [56])} \]

\[ d^2 = 3600 \left( \frac{200 \times 545.67 \times 0.75}{30 \times 800} \right) \]

\[ d = \sqrt{12277.575} \]

\[ d_{\text{Adsorption tower}} = 110.804_{\text{inches}} = 2.81_{\text{meters}} \]

According to GPSA, [14], the weight of adsorption tower vessel steel can be calculated as,

\[ \text{Weight of Steel (lb)} = 155(t_w + 0.125)(L_s + L_{MTZ} + 0.75D_{bed} + 3)D_{bed} \quad (5-23) \]

Where;

\[ L_{MTZ (ft)} = \text{length of mass transfer zone} \]

\[ L_{S (ft)} = \text{length of the saturation zone} \]

\[ t_w (\text{inches}) = \text{wall thickness} \]

\[ D_{bed (ft)} = \text{diameter of the adsorbent bed} \]

\[ 0.125_{\text{inches}} = \text{is the corrosion allowance} \]

The term, \(0.75D_{bed}\), accounts for the weight of the tower heads while 3 inches value provides the space for the inlet distributor, support and hold-down balls (see Appendix G).

\[ t_w (\text{inches}) = \frac{12D_{bed}P_{design}}{(2*18800)-1.2P_{design}} \quad (5-24) \]
Where;

\[ P_{\text{design (Psi)}} = \text{design pressure} \]

18800 \text{Psi} = \text{Allowable tensile stress for SA516 Grade 70 steel - pressure vessel.} \\

\[ L_s = \frac{S_s}{\pi D^2 \times (\text{bulk density})} \] \hspace{1cm} (5-25)

Where;

\[ S_{s(\text{lb})} = \text{mass of desiccant on the saturation zone.} \]

But, length of adsorbent bed, L, is;

\[ L = L_s + L_{MTZ} \] \hspace{1cm} (5-26)

\[ L_s = L - L_{MTZ} \] \hspace{1cm} (5-27)

Calculating iteratively using Equations 5-23 to 5-27:

The value of L and \( D_{\text{bed}} \) was gotten from Table 3.4-1. L=8ft (1.8m) while \( D_{\text{bed}} = 2.96 \)ft (0.9m). Using Equation 1-15, \( L_{MTZ} \) for adsorption tower will be,

\[ L_{MTZ, \text{Adsorption}} (ft) = 2.5 + 0.025(30) = 3.25 \text{ ft} = 0.99 \text{ m} \]

\[ L_{s(\text{m})} = 1.8 - 0.99 = 0.81 \text{ (2.66 ft).} \]

\[ t_w(\text{inches}) = \frac{12 + 2.96 + 800}{(2 + 18800) - (1.2 + 800)} = 0.7755 \text{ inches} = 0.02 \text{ m} \]

Weight of Steel \( l_{(\text{lb})} = 155(0.7755 + 0.125)(2.66 + 3.25 + (0.75 \times 2.96) + 3) \times 2.96 = 4598.35 \text{ Lb} = 2085.78 \text{ kg (see Appendix C for its unit conversion.)} \)

Length of the vertical tower, \( L_{VT} \), was calculated with equation 5-4. L/D ratio at 800 Psi was estimated to be 5.0 (see Appendix D).

\[ L_{VT, \text{(Adsorption)}} = D \times \frac{L}{D} = 2.81 \times 5 = 14.05 \text{ m} \]

With Equation 5-5, Adsorber shell volume was calculated to be;

\[ V_{sh} = \pi \times t_w \times L_{VT} \times D = \pi \times 0.02 \times 14.05 \times 2.81 = 2.48 \text{ m}^3 \]

From Equation 5-3;

\[ A_T = \pi D L_{VT} = \pi \times 2.81 \times 14.05 = 124.03 \text{ m}^2 \]

The dimension calculation result was tabulated in Table 5.2-1 below.

**Table 5.2-1: Adsorption tower dimensions**

<table>
<thead>
<tr>
<th>Adsorber superficial gas velocity</th>
<th>30ft/min = 0.152m/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of adsorption tower [m]</td>
<td>2.81</td>
</tr>
<tr>
<td>Length of mass transfer zone [m]</td>
<td>0.99</td>
</tr>
<tr>
<td>Length of the saturation zone [m]</td>
<td>0.81</td>
</tr>
<tr>
<td>Vessel Wall thickness [m]</td>
<td>0.02</td>
</tr>
</tbody>
</table>
### Contents

<table>
<thead>
<tr>
<th>Weight of steel vessel [kg]</th>
<th>2085.78</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vessel L/D ratio</td>
<td>5.0</td>
</tr>
<tr>
<td>Length of the vertical tower [m]</td>
<td>14.05</td>
</tr>
<tr>
<td>Adsorber shell volume [m^3]</td>
<td>2.48</td>
</tr>
<tr>
<td>Adsorber cross-sectional area [m^2]</td>
<td>124.03</td>
</tr>
<tr>
<td>ASME 2001 allowable tensile stress for SA516 Grade 70 steel (Carbon steel)</td>
<td>18800 Psi = 1296.2 bar</td>
</tr>
</tbody>
</table>

---

### Regeneration and cooling tower:

For regeneration tower minimum diameter,

\[ d^2 = 3600 \left( \frac{Q_g T Z}{V P} \right) \]

\( Q_g = 19 \) MMscfd (see chapter 3.4)

\( V = 9 \) ft/min

\( P = 200 \) Psi = 1379 kPa

\( T = 260 \) °C, \( T(°R) = 959.67 \) (see Appendix C)

\( Z_{Regeneration} = 0.99 \) (Compressibility factor of CO \(_2\) at 260°C, 14 bar, [56])

\[ d^2 = 3600 \left( \frac{19 \times 959.67 \times 0.99}{9 \times 200} \right) \]

\[ d = \sqrt{36102.785} \]

\[ d_{Regeneration\ tower} = 190.007 \text{ inches} = 4.83 \text{ meters} \]

### Regen/Cooling tower iteration using Equations 5-23 to 5-27:

From Table 3.4.1, the value of \( L=8\)ft (1.8m) while \( D_{bed}=2.96\)ft (0.9m). Using Equation 1-15, \( L_{MTZ} \) for regeneration and cooling tower will be,

\[ L_{MTZ\ Regen/cooling}(ft) = 2.5 + 0.025(9) = 2.725 \text{ ft} = 0.83 \text{ m} \]

\[ L_s(\text{m}) = 1.8 - 0.83 = 0.97\text{ m (3.18 ft)} \]

\[ t_w(\text{Regen})(\text{inches}) = \frac{12D_{bed}+P_{design}}{2(18800)-1.2P_{design}} = \frac{12+2.96+200}{(2+18800)-(1.2+200)} = 0.1901 \text{ inches} = 0.0048 \text{ m} \]

**Weight of Steel (lb) = 155(0.1901 + 0.125)(3.18 + 2.725 + (0.75 * 2.96) + 3) * 2.96 = 1608.32 Lb = 729.52 kg (see Appendix C).**

With equation 5-4, length of the vertical regeneration tower, \( L_{VT} \), was calculated. L/D ratio at 200 Psi was estimated to be 2.4 (see Appendix D).
\[ L_{VT(Adsorption)} = 4.83 \times 2.4 = 11.59 \text{ m} \]

With Equation 5-5, Adsorber shell volume was calculated to be;

\[ V_{sh} = \pi \times t_w \times L_{VT} \times D = \pi \times 0.0048 \times 11.59 \times 4.83 = 0.84 \text{ m}^3 \]

From Equation 5-3;

\[ A_T = \pi D L_{VT} = \pi \times 4.83 \times 11.59 = 175.87 \text{ m}^2 \]

Regeneration and cooling tower calculation result dimensions was tabulated in Table 5.2-2 below

**Table 5.2-2: Regeneration and cooling tower dimensions**

<table>
<thead>
<tr>
<th>Regeneration/cooling tower superficial gas velocity</th>
<th>9ft/min = 0.0457m/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of regeneration tower [m]</td>
<td>4.83</td>
</tr>
<tr>
<td>Length of mass transfer zone [m]</td>
<td>0.83</td>
</tr>
<tr>
<td>Length of the saturation zone [m]</td>
<td>0.97</td>
</tr>
<tr>
<td>Vessel Wall thickness [m]</td>
<td>0.0048</td>
</tr>
<tr>
<td>Weight of steel vessel [kg]</td>
<td>729.52</td>
</tr>
<tr>
<td>Vessel L/D ratio</td>
<td>2.4</td>
</tr>
<tr>
<td>Length of the vertical regeneration tower [m]</td>
<td>11.59</td>
</tr>
<tr>
<td>Regeneration/cooling tower shell volume [m³]</td>
<td>0.84</td>
</tr>
<tr>
<td>Regeneration/cooling tower cross-sectional area [m²]</td>
<td>175.87</td>
</tr>
<tr>
<td>Allowable tensile stress for SA516 Grade 70 steel</td>
<td>18800 Psi = 1296.2 bar</td>
</tr>
<tr>
<td>(Carbon steel)</td>
<td></td>
</tr>
</tbody>
</table>
6 Cost estimation methods

To be able to evaluate the choice of design options, economic viability of a project in terms of project profitability and to make a decision on whether to invest on a project, there is need to carry out its cost estimation. The cost estimation methods used in this studies are from Lecture materials by Nils Henrik Eldrup,[57] publications by Rafid, [53] and Robin Smith, [21].

6.1 Classification of cost

CO2 dehydration processes cost can be divided into two main categories, viz.

- Capital Expenditure (CAPEX):
  It is the total amount of investment/money needed to supply the necessary plant and manufacturing facilities and the working capital for operation of the facilities. It can be broken down into five major parts, [21];
  i. Battery limits investment: includes process equipment and structures or buildings to house it but excludes site storage, pollution control, etc. In addition to the purchased cost of the equipment, investment is required to install the equipment. Installation cost include;
    ✓ Piping, valves and control systems
    ✓ Foundations, insulation and painting
    ✓ Engineering fees and contingency
  ii. Utility investment: it covers capital investment in utility plant and include equipment for electricity generation and distribution, steam generation, process/cooling water, effluent treatment, firewater, compressed air.
  iii. Off-site investment: it includes auxiliary buildings such as offices, medical, personnel, warehouses, maintenance shops; roads and paths; fire protection systems; communication systems; waste disposal systems, etc.
  iv. Working capital: Money invested before there is a product to sell and it includes raw materials for plant start-up, money to meet payroll when starting up, etc.
  v. Total capital cost: It can be obtained by applying installation factors to the purchase cost of individual items of equipment.

- Operational Expenditure (OPEX):
  The following are covered in the operational cost of a project design;
  i. Raw materials cost.
  ii. Catalyst and raw materials consumed in manufacturing/production other than raw materials.
  iii. Utility operating cost: It is the most significant variable operating cost after the cost of raw materials and it includes,
    ✓ Fuel and electricity
    ✓ Steam and cooling water
    ✓ Compressed air, inert gas and refrigeration
  iv. Labor cost: It depends on whether the process is batch or continuous, the level of automation, the number of processing steps and the level of production.
  v. Maintenance cost: It depends on whether processing material are solid or gas and liquid. Handling solids and liquid corrosive process fluids increases maintenance costs.
6.2 Cost Estimation of Base Case (Absorption and Adsorption) processes

The cost of a specific item of equipment will be a function of;

- size
- materials of construction
- design pressure
- design temperature

This section covers the cost estimation of the base case using cost estimation method by Nils Eldrup, [57]. A minor CAPEX and OPEX has been performed for both case.

6.2.1 Installation factor

Installation cost calculation is dependent on two factors:

- Total installation factor: it depends on equipment cost and type of material.
- Material factor: it influences the cost of equipment and piping for the equipment of different material other than carbon steel.

All the cost factors can be found in Appendix E, [57]. The formula to calculate the total installed cost factor of equipment is given by Equation 6-1, [57].

\[
f_i = [f_{TC} - f_P - f_E]_{CS} + [f_M \cdot (f_P + f_E)]_{SS}
\]  
(6-1)

Where;

- \(f_i\) = Total installation factor
- \(f_{TC}\) = Total cost factor; \(f_M\) = Material factor
- \(f_P\) = Piping cost factor; \(f_E\) = Equipment cost factor
- \(CS\) = Carbon steel; \(SS\) = Stainless steel

Installed equipment cost can be calculated with Equation 6-2,

\[
Total\ \text{Installed equipment cost} = Equipment\ \text{cost}(C_E) \cdot f_i
\]  
(6-2)

The material factor for materials other than carbon steel (CS) are listed in table 6.2.1-1 below.

Table 6.2.1-1: Material factors, [57].

<table>
<thead>
<tr>
<th>Material</th>
<th>Material factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stainless Steel (SS316) Welded</td>
<td>1.75</td>
</tr>
<tr>
<td>Stainless Steel (SS316) Machined</td>
<td>1.30</td>
</tr>
<tr>
<td>GRP</td>
<td>1.00</td>
</tr>
<tr>
<td>Exotic</td>
<td>2.50</td>
</tr>
</tbody>
</table>

Exotic material is titanium or high quality stainless steel, [54], while GRP is Glassfibre reinforced plastic material.
6.2.2 Installation cost calculation for the base cases

The equipment cost, $C_E$, for each of the equipment in the base case process was first calculated before the installation cost calculation. According to Smith, [21],

$$C_E = C_B \left( \frac{Q}{Q_B} \right)^M \quad (6-3)$$

Where;

$C_E =$ equipment cost with capacity/size $Q$

$C_B =$ known base cost for equipment with capacity/size $Q_B$

$M =$ constant depending on equipment type.

Nils Eldrup, [57], applied Equation 6-3 in its cost estimation method. Constant $M$ can be obtained from the reference material by Smith, [21], in its Table 2.1. To bring up-to-date an equipment cost, say from year 2010 to 2017, Equation 6-4 below can be applied, [21];

$$\frac{C_{E2017}}{C_{E2010}} = \frac{COST INDEX_{2017}}{COST INDEX_{2010}} \quad (6-4)$$

$$C_{E2017} = C_{E2010} \times \frac{COST INDEX_{2017}}{COST INDEX_{2010}} ;$$

But in Eldrup, [57].

$$C_{E2017} = C_{E2010} \times \frac{INFLATION INDEX_{2017}}{INFLATION INDEX_{2010}} \quad (6-5)$$

Cost index from 1969 to 2000 are stated in the reference material, [58], specifically its Table 2.12. Inflation index from 2002 to 2013 and historical exchange rates was applied in this thesis cost estimation analysis. It could be found in Appendix F.

TEG dehydration equipment - Installation cost calculation

Cost calculation in this section was done with Nils Eldrup cost estimation method. Year of current analysis was assumed to be 2013 as $C_B$ and inflation index from 2014 to 2017 was not available in the literature for the study (see Appendix F). Table 6.2.2-1 shows some of the known base cost with its capacity.

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Size</th>
<th>Equipment cost</th>
<th>Currency</th>
<th>Year</th>
<th>Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vessel</td>
<td>200 m³</td>
<td>1550</td>
<td>kNOK</td>
<td>2010</td>
<td>SS316</td>
</tr>
<tr>
<td>Heat exchanger</td>
<td>550 m³</td>
<td>98.9</td>
<td>kUSD</td>
<td>2008</td>
<td>CS</td>
</tr>
<tr>
<td>Pump</td>
<td>30 litre/sec =108 m³/h</td>
<td>128</td>
<td>kNOK</td>
<td>2013</td>
<td>CS</td>
</tr>
<tr>
<td>Compressor</td>
<td>1000 kW</td>
<td>12500</td>
<td>kNOK</td>
<td>2013</td>
<td>CS</td>
</tr>
<tr>
<td>Storage tank</td>
<td>45 m³</td>
<td>124</td>
<td>kNOK</td>
<td>2003</td>
<td>GRP</td>
</tr>
<tr>
<td>Condenser, [53]</td>
<td>94.8m²</td>
<td>400</td>
<td>kNOK</td>
<td>2011</td>
<td>Exotic</td>
</tr>
<tr>
<td>Lean Glycol Cooler, [53]</td>
<td>2195m²</td>
<td>3390</td>
<td>kNOK</td>
<td>2011</td>
<td>Exotic</td>
</tr>
</tbody>
</table>
Applying Equations 6-1 to 6-5, Total installation cost for absorption-dehydration base case was estimated as presented below.

**Vessel (Separator) cost estimation:**

From Equation 6-3: \[ C_E = C_B \left( \frac{Q}{Q_B} \right)^M = 1550 \times \left( \frac{1.78}{200} \right)^{0.65} = 72.0 \]

Inflation cost, \[ C_{E2013} = C_{E2010} \times \frac{INFLATION\ INDEX_{2013}}{INFLATION\ INDEX_{2010}} = 72.0 \times \frac{116.6}{111.7} = 75.2 \text{kNOK} \]

From Appendix E, the material factor for stainless steel (SS316) welded is 1.75.

Therefore, Total equipment cost = 75.2 / 1.75 = 43

Installation factor: In Appendix E, 43 is in the range 20-100. Equipment and piping cost are also included in vessel calculation.

For SS316: \[ f_M \times (f_P + f_E) = 1.75 \times (1.51 + 1) = 4.39 \]

For CS: \[ f_{TC} - f_P - f_E = 12.13 - 1.51 - 1 = 9.62 \]

\[ f_i = 9.62 + 4.39 = 14.01 \]

Total installed cost = 43 \times 14.01 = 602.43

**Rich/Lean Heat Exchanger cost estimation:**

Heat Exchanger cost, \[ 2008 = (98.9\text{kUSD} \times 5.64) \times \left( \frac{27.84}{550} \right)^{0.68} = 73.4 \]

5.64 is the exchange rate of NOK/USD for 2008 (see Appendix F).

Inflation cost, \[ 2013 = 73.4 \times \frac{116.6}{106.7} = 80.2 \text{kNOK} \]

Total equipment cost in CS = 80.2

Inflation factor: 80.2 is in the range 20-100. Heat exchanger does not have material factor, piping and equipment cost. Thus \[ f_i = f_{TC} = 12.13 \]

Total installed cost = 80.2 \times 12.13 = 972.83 kNOK

**Glycol Pump cost estimation:**

Glycol Pump cost, \[ 2013 = 128 \times \left( \frac{1.024}{108} \right)^{0.35} = 25.1 \]

Change from CS to SS316; Pump equipment cost = 25.1 \times 1.30 (Machined) = 32.6

Total Equipment cost, \[ CS = 25.1 \]

Installation factor: 25.1 falls in the range 20-100. Thus considering the piping and equipment cost for pump,

\[ f_i = (12.13 - 1.51 - 1) \times 1.30(1.51 + 1) = 9.62 + 3.26 = 12.88 \]

Total installed cost = 25.1 \times 12.88 = 323 kNOK

The calculation results of the cost estimation analysis as presented above are tabulated in Table 6.2.2-2. Vessel calculation steps was also applied in the cost estimation of flash drum, absorber and desorber. Its results was presented in table below.
### Table 6.2.2-2: TEG dehydration _ Cost Estimation calculation results

<table>
<thead>
<tr>
<th>No</th>
<th>P (kPa)</th>
<th>Temp. (°C)</th>
<th>Size</th>
<th>Material</th>
<th>Equipment Cost (kNOK)</th>
<th>Equipment cost in CS (kNOK)</th>
<th>$f_i$</th>
<th>Total installed cost (kNOK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4000</td>
<td>30</td>
<td>1.78 m$^3$</td>
<td>SS316</td>
<td>75.2</td>
<td>43</td>
<td>14.01</td>
<td>602.43</td>
</tr>
<tr>
<td>1</td>
<td>3318</td>
<td>29.81</td>
<td>0.02 m$^3$</td>
<td>SS316</td>
<td>4.06</td>
<td>2.32</td>
<td>26.48</td>
<td>61.43</td>
</tr>
<tr>
<td>1</td>
<td>4000</td>
<td>31.14</td>
<td>5.23 m$^3$</td>
<td>SS316</td>
<td>151.47</td>
<td>86.55</td>
<td>14.01</td>
<td>1212.57</td>
</tr>
<tr>
<td>1</td>
<td>101</td>
<td>123.9</td>
<td>0.326 m$^3$</td>
<td>SS316</td>
<td>24.94</td>
<td>14.25</td>
<td>26.48</td>
<td>377.34</td>
</tr>
<tr>
<td>1</td>
<td>110</td>
<td>105</td>
<td>27.84 m$^2$</td>
<td>CS</td>
<td>80.2</td>
<td>80.2</td>
<td>12.13</td>
<td>972.83</td>
</tr>
<tr>
<td>1</td>
<td>4100</td>
<td>130.3</td>
<td>1.024 m$^3$/h</td>
<td>SS316</td>
<td>32.6</td>
<td>25.1</td>
<td>12.88</td>
<td>323</td>
</tr>
</tbody>
</table>

$f_i$ = Total installation factor

### 3A Mol. sieve dehydration equipment - Installation cost calculation

Using Vessel calculation steps and dimension values as presented in chapter 5.2, installation cost estimation was done for Adsorption and Regeneration/cooling tower.

**Adsorption tower cost estimation:**

Adsorption tower vessel $\text{Size} = 2.48 \text{ m}^3$; $P = 5516 \text{ kPa}$; $T = 30^\circ \text{C}$

Material = SA516 Gr.70 Carbon steel

Adsorption tower cost, $2013 = 1550 \times \left(\frac{2.48}{200}\right)^{0.65} = 89.34$

Inflation cost, $2013 = \frac{C_{E_{2010}} \times \text{INFLATION INDEX}_{2013}}{\text{INFLATION INDEX}_{2010}} = 89.34 \times \left(\frac{116.6}{111.7}\right) = 93.26 \text{ kNOK}$

The material factor for stainless steel (SS316) welded is 1.75. (see Appendix D)

Thus, Total equipment cost $= 93.26 / 1.75 = 53.29$
Installation factor: In Appendix E, 53.29 is in the range 20-100. Equipment and piping cost are also included in vessel calculation.

For SS316: \( f_M \times (f_P + f_E) = 1.75 \times (1.51 + 1) = 4.39 \)

For CS: \( f_{TC} - f_P - f_E = 12.13 - 1.51 - 1 = 9.62 \)

\( f_i = 9.62 + 4.39 = 14.01 \)

Total installed cost = \( 53.29 \times 14.01 = 746.59 \) kNOK

**Regeneration and cooling tower cost estimation:**

Regeneration tower

vessel Size = 0.84 m³  \( P = 1379 \) kPa; \( T = 260^\circ C \)

Material = SA516 Gr.70 Carbon steel

Regen/cooling tower cost, \( 2013 \) = \( 1550 \times \left( \frac{0.84}{200} \right)^{0.65} = 44.20 \)

Inflation cost, \( 2013 \) = \( 44.20 \times \left( \frac{116.6}{111.7} \right) = 46.14 \) kNOK

\( f_M \) for stainless steel (SS316) welded is 1.75.

Thus, Total equipment cost = \( 46.14 \times 1.75 = 26.37 \) kNOK

Installation factor: 26.37 is in the range 20-100.

For SS316: \( f_M \times (f_P + f_E) = 1.75 \times (1.51 + 1) = 4.39 \)

For CS: \( f_{TC} - f_P - f_E = 12.13 - 1.51 - 1 = 9.62 \)

\( f_i = 9.62 + 4.39 = 14.01 \)

Total installed cost = \( 26.37 \times 14.01 = 369.4 \) kNOK

**Compressor cost estimation:**

Here, compressor power of 250 kW = 335 hp was assumed. Constant, \( M = 0.46 \) . [21].

Regen/cooling tower cost, \( 2013 \) = \( 12500 \times \left( \frac{250}{1000} \right)^{0.46} = 6606 \)

There is no inflation as year of analysis and known base cost in Table 6.2.2-1 is 2013.

Total equipment cost = 6606 kNOK

Equipment cost, \( CS \) = 6606 kNOK

Installation factor: 6606 is in the range 5000 - 15000

Compressor has no piping, equipment and material factor cost.

Thus \( f_i = f_{TC} = 3.89 \)

Total installed cost = \( 6606 \times 3.89 = 25697 \) kNOK

The adsorption cost calculation results are presented in Table 6.2.2-3.
Table 6.2.2-3: 3A Molecular Sieve dehydration _ Cost Estimation calculation results

<table>
<thead>
<tr>
<th></th>
<th>Aspen output data</th>
<th>Calculated cost</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>No</td>
<td>P</td>
</tr>
<tr>
<td>Adsorption Tower</td>
<td>1</td>
<td>4000</td>
</tr>
<tr>
<td>(Pressure vessel)</td>
<td>1</td>
<td>3318</td>
</tr>
<tr>
<td>Vessel</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>(Regeneration &amp; cooling tower)</td>
<td>1</td>
<td>-</td>
</tr>
</tbody>
</table>

In Table 6.2.2-3, regen gas heater, cooler and water knockout vessel installation cost were not presented because of irregularities in 3A molecular sieve Aspen HYSYS simulation.

6.2.3 Energy estimation method

Energy consumption in the reboiler (TEG Absorption) and in 3A Mol. Sieve Adsorption (compressor and regen gas heater) for a one year period can be calculated with Equation 6-6 below. [53, 54]

$$Cost_{energy,1y} = \frac{Energy\ price \cdot T_{op,1y} \cdot Q}{3600}$$ (6-6)

Where:

$T_{op,1y} = 8000$ hr/yr. (Annual plant operation time)

Energy price = 0.13 NOK / (kWh), [53]

Q = Duty or heat flow in the reboiler, compressor and regeneration gas heater (kJ/h or kW)

For Reboiler:

$$Cost_{energy,1y} = \frac{0.13 \cdot 8000 \cdot 215100}{3600} = 62140\ NOK/yr$$

Compressor uses electrical energy to generate power. But compressor and regen gas heater energy cost was not calculated because of 3A mol. Sieve simulation problem.
6.2.4 Net present value calculation and Economic potential of a project

According to Nils Eldrup, [57], net present value (NPV) can be calculated with Equation 6-7:

\[ NPV = \sum_{n}^{\infty} \text{Cash flow} \times \frac{1}{(1+p)^n} \]  

Where;

\[ \frac{1}{(1+p)^n} = \text{discount factor} \]

p = rate of return

n = period number

For energy calculations, Rafid, [53] used \( Cost_{\text{energy},1y} \) to represent \( \text{Cash flow} \).

Assuming for a new project installation, we have an investment of 20000 NOK and an assumed income, variable and fixed cost. With \( p = 10\% \) rate of return, the NPV can be calculated as tabulated in Table 6.2.4-1 below;

**Table 6.2.4-1: Example of NPV analysis of a new project installation.**

<table>
<thead>
<tr>
<th>n</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>2014</strong></td>
<td><strong>2015</strong></td>
<td><strong>2016</strong></td>
<td><strong>2017</strong></td>
<td><strong>2018</strong></td>
<td><strong>2019</strong></td>
<td><strong>2020</strong></td>
</tr>
<tr>
<td>Income</td>
<td>0</td>
<td>5000</td>
<td>7500</td>
<td>7500</td>
<td>7500</td>
<td>7500</td>
<td>7500</td>
</tr>
<tr>
<td>Variable cost</td>
<td>0</td>
<td>-1000</td>
<td>-1100</td>
<td>-1100</td>
<td>-1200</td>
<td>-1200</td>
<td>-1200</td>
</tr>
<tr>
<td>Fixed cost</td>
<td>-200</td>
<td>-200</td>
<td>-200</td>
<td>-200</td>
<td>-200</td>
<td>-200</td>
<td>-200</td>
</tr>
<tr>
<td>Investment</td>
<td>-20000</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Cash flow</td>
<td>-20200</td>
<td>3800</td>
<td>6200</td>
<td>6200</td>
<td>6100</td>
<td>6100</td>
<td>6100</td>
</tr>
<tr>
<td>( \frac{1}{(1+p)^n} )</td>
<td>1</td>
<td>0.91</td>
<td>0.83</td>
<td>0.75</td>
<td>0.68</td>
<td>0.62</td>
<td>0.56</td>
</tr>
<tr>
<td>NPV</td>
<td>-20200</td>
<td>3458</td>
<td>5146</td>
<td>4650</td>
<td>4148</td>
<td>3782</td>
<td>3416</td>
</tr>
<tr>
<td>Acc. NPV</td>
<td>-20200</td>
<td>-16742</td>
<td>-11596</td>
<td>-6946</td>
<td>-2798</td>
<td>984</td>
<td>4400</td>
</tr>
</tbody>
</table>

Cash flow = Income – investment – operating cost (variable cost and fixed cost). If NPV is negative, it is not a good investment. With Accumulated (Acc.) NPV, the number of years it will take an investment in a project to start making profit can be estimated. In the example above, it is 5 years.

**Economic potential of a project:**

The economic potential of a project can be calculated as, [21];

\[ EP = \text{Value of products} – \text{fixed costs} – \text{variable costs} – \text{taxes} \]
7 Results/Base case simulation result

The analytical result and base case simulation result are presented in this section. The analytical results for dimension are presented in Tables 5.1-1, 5.1-3, 5.1-4, 5.1-5, 5.2-1, 5.2-2 while the cost estimation results are presented in Tables 6.2-2, 6.2-3 above.

TEG dehydration simulation results:

Table 7-1 and 7-2 shows the material streams and energy streams for the process.

Table 7-1: Aspen HYSYS_TEG dehydration material streams simulation results

<table>
<thead>
<tr>
<th>Material Streams</th>
<th>CO2 in inlet</th>
<th>CO2 in Condenser</th>
<th>Heat Gas</th>
<th>Gas to Separator</th>
<th>Wet CO2 gas</th>
<th>Water out</th>
<th>Dry CO2 Gas</th>
<th>Reflux</th>
<th>Wet CO2 to Hats</th>
<th>Dry CO2 to Hats</th>
<th>Hats Gas</th>
<th>Wet CO2 to Hats</th>
<th>Dry CO2 to Hats</th>
<th>Condensation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
<td>30.09</td>
</tr>
<tr>
<td>Pressure</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
<td>420</td>
</tr>
</tbody>
</table>

Table 7-2: Aspen HYSYS_TEG dehydration energy streams simulation results

Concentration:

The iteration result obtained here will be compared with the simulation results.

Solving Iteratively:

From Equation 3-1, the concentration of CO2 will be equal to: \( C_{CO2} = \frac{\rho_{CO2} M_{CO2}}{M_{CO2}} \)

\[ M_{CO2} = 44.01 \text{ kg/kmol} \]

\[ CO2 \text{ in inlet gas} = 0.76 \text{ mole-\%} \]

And from Table 3.3-1, \( T_{CO2} = 30^\circ \text{C} = 303.15 \text{ K} \), which is the inlet gas temperature.

To be able to get the mass density, \( \rho_{CO2} \), an interpolation was done from Table A.4 of Incropera et al [16].

After Interpolation, \( \rho_{CO2} = 1.7553 \text{ kg/m}^3 \)

\[ C_{CO2} = \frac{1.7553}{44.01} = 0.03988 \text{ kmol/m}^3 = 39.88 \text{ mol/m}^3 \]

Thus the Total Molar Concentration, \( C = 39.88 \times 0.76 = 30.3 \text{ mol/m}^3 \)
Hydraulic residence time:
Equation 3-7 was applied in calculating the hydraulic retention time, HRT, of most equipment and vessels. Using dimension values, the calculation results are presented in Table 7.3.

Table 7-3: HRT of Absorption and Adsorption equipment

<table>
<thead>
<tr>
<th>Equipment/Vessels</th>
<th>V (m³)</th>
<th>Q (m³/s)</th>
<th>HRT (seconds)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Separator (V-100)</td>
<td>1.78</td>
<td>3.294</td>
<td>0.5</td>
</tr>
<tr>
<td>Flash Drum (V-101)</td>
<td>0.02</td>
<td>0.0368</td>
<td>0.5</td>
</tr>
<tr>
<td>Absorber (T-100)</td>
<td>5.23</td>
<td>2.52</td>
<td>2.1</td>
</tr>
<tr>
<td>Desorber (T-101)</td>
<td>0.326</td>
<td>0.039</td>
<td>8.4</td>
</tr>
<tr>
<td>Adsorption tower</td>
<td>2.48</td>
<td>_</td>
<td>_</td>
</tr>
<tr>
<td>Regen/cooling tower</td>
<td>0.84</td>
<td>_</td>
<td>_</td>
</tr>
</tbody>
</table>
8 Comparison of Absorption and Adsorption

The major operating cost of TEG absorption is the reboiler energy. While the major operating costs of 3A Mol. Sieve adsorption are, [20];

- The energy required for regeneration in regeneration gas heater
- And the compression power required to overcome bed pressure drop.

To minimize the heat load, the adsorption beds are insulated. Insulation may be external or internal. Internal insulation saves energy during bed regeneration because it eliminates heating of the vessel walls and reduces the regeneration time. However, insulation imperfections and cracks may cause wet gas to bypass the adsorbent, [14]. Internal insulation also requires a larger diameter pressure vessel, which adds to capital costs.

Comparison of base case processes:

TEG absorption and 3A Mol. sieve adsorption comparison will be carried out based on its,

i. Energy consumption
ii. Qualitative comparison: This compares differences between
   - Operations
   - Merits and demerits
   - Process requirements
   - Safety and environmental considerations.

Energy consumption:

Energy cost of reboiler is 62140 NOK/yr. Energy consumption of both regen gas heater and compressor electrical energy should be relatively higher when compared with TEG energy consumption as molecular sieve has higher heat requirement, [6].

Qualitative comparison:

i. From specifications of TEG and 3A Mol. Sieve, specifically chapter 3.3 and 3.4, 3A Mol. Sieve has higher temperature for regeneration, thus it has higher operating cost, [5]. Kohl, [6], also stated that operating costs for dry-desiccant systems are typically 20 to 30% higher than simple glycol dehydration units.

ii. From the cost estimation analysis in chapter 6.2.2, the total installation cost for both absorber and desorber column is 1589.91 kNOK while for adsorption and regen/cooling tower, it is 1115.99 kNOK. Unlike TEG dehydrator, desiccant dehydrator (3A Mol. Sieve Twin tower system- Figure 3.1.2-1) do not use pumps, contactors, and fired reboiler/regenerator. The only capital cost is for the adsorption and regeneration/cooling towers. Thus TEG process has high equipment cost while 3A Mol. Sieve process has lower equipment cost.

iii. With TEG dehydration, less than 50 ppm water content in dehydrated CO$_2$ dry gas can be calculated, [4, 26, 27], while 3A Mol. Sieve is capable of dehydration to less than 0.1 ppm water content, [4-6, 14, 15, 20].

iv. Operational problems:
   Kidnay, [20], stated that when considering susceptibility to inlet feed contamination, one should keep in mind that replacing a solvent is much easier and cheaper than changing an adsorbent bed.
   The operational problems in TEG dehydration are insufficient dehydration, foaming caused by contaminants in the glycol, glycol losses due to vaporization,
glycol over circulation/under circulation, [5, 15]. The major operational problems in Molecular sieve are bed contamination, liquid carryover, hydrothermal damaging of adsorbent bed and leakages of molecular sieves through the support grids ceramic balls and buffer gel, (see Appendix G). To overcome these operational problems, there is need to implement good design specifications.

v. Safety and Environmental considerations:
The most unique safety consideration in molecular sieve is when adsorbent beds are being changed. The bed must be thoroughly purged, preferably with nitrogen, to remove adsorbed hydrocarbons before the adsorbent is dumped. A potential exist for hydrocarbons on the adsorbent to ignite when exposed to air because the adsorbent heats as it adsorbs moisture from the air, [20]. A trained safety expert should be present to help ensure safe dumping and filling operations. Its dumping produces dust, thus operators must wear protective clothing and dust masks. Major environmental concern in glycol dehydration is BTEX emissions. Ethylene glycol is toxic to humans and must be handled properly.
9 Discussion of results

The purpose of this study was to compare CO\(_2\) dehydration processes after CO\(_2\) capture. These processes were evaluated, TEG absorption dehydration and 3A Molecular sieve adsorption dehydration. From the comparison carried out in chapter 8, the following views were presented;

- Based on energy consumption, it will be more economical to use TEG dehydration for the base case process.
- For large scale process unit, TEG dehydration will be more reasonable to use as it has lower operating cost and lower energy consumption while for small scale, 3A molecular sieve is preferable because of lower equipment cost.
- When considering water content specification in the dehydrated dry gas, 3A Molecular sieve is capable of dehydration to less than 0.1 ppm water content. In this report, 22 ppm was obtained in 1\(^{st}\) iteration with TEG dehydration. From the research of Mirela, [26], Peng-Robinson model was applied in TEG dehydration to obtain a water dew point as low as 9.6 ppm. This implies that TEG and Mol. Sieve can obtain a product specification of less than 9.6 ppm water content. Lars Erik Qi in his conference paper, [27], also claims that it is possible to achieve lower water content specification less than 5 ppm with TEG dehydration.

9.1 General Uncertainties in the calculations

There were uncertainties in 3A molecular sieve simulation as its solid bed specifications and equipment simulation was not applicable with Aspen HYSYS software. In cost estimation, I was unable to get a current inflation index or cost index from most reference materials. In Molecular sieve adsorption, most efforts were made to get vendors design data and process flow design requirements. This was not successful, thus there might be need to still make efforts to engage the vendors stated in Table 2.2-1.

9.2 Further work

- There is need to source for updated inflation index from published Oil and Gas Journal, and acceptable Chemical Engineering Magazine. This will be used to bring the cost estimation year up to date.
- The uncertainties in 3A Molecular Sieve simulation can be corrected by using CHEMCAD software version 7. There might be other software that can be used for 3A adsorption, thus there is need for further work with the most adaptable software. With the most adaptable software, 3A Molecular sieve adsorption can be properly simulated with intent to use its output data in its dimensioning and cost estimation.
10 Conclusion

A number of suitable technologies for CO$_2$ dehydration already exist, but due to most industrial recommendations, TEG absorption and 3A Molecular Sieve adsorption was compared in this research. It was possible to carry out simulation, dimension and cost estimation of both processes with intent to evaluate its comparison and proffer reasonable process solution based on project installation expectations.
References


Appendices

Appendix A  Task Description
Appendix B  Technical Background on Corrosion and Hydrates
Appendix C  Unit Conversion Factors
Appendix D  Design properties selection guide for TEG and Molecular Sieve dehydration
Appendix E  Installation Factors
Appendix F  Cost Data: Inflation Index _ Historical Exchange rates
Appendix G  Typical cross-section of an Adsorber bed
Appendix A - Task Description

Title: Comparison of CO\textsubscript{2} dehydration processes after CO\textsubscript{2} capture

USN supervisor: Professor Lars Erik Øi

Task description:

The aim is to develop tools for comparing processes for CO\textsubscript{2} dehydration after CO\textsubscript{2} capture.

1. Literature search on dehydration methods based on adsorption and glycol absorption for captured CO\textsubscript{2}. The search may include processes from commercial suppliers of dehydration plants.

2. Process descriptions of dehydration processes for natural gas and compressed CO\textsubscript{2}. The CO\textsubscript{2} dehydration can be performed after or between CO\textsubscript{2} compression stages.

3. Dimensioning and cost estimation of dehydration processes using e.g. Excel or possibly Aspen HYSYS.

4. Comparison of adsorption and absorption processes. Evaluation of which processes are reasonable for different conditions.

Task background:

Several Master Projects have been performed at USN/HiT about calculation and simulation of different CO\textsubscript{2} capture processes. USN/HiT has collaborated with different companies (TelTek, Statoil, Aker Kværner, Norcem, Yara, Skagerak and Gassnova) which work with plans for CO\textsubscript{2} capture. There have also been performed several Master projects on dehydration of natural gas, and also Master projects on dehydration of captured CO\textsubscript{2} in 2014, 2015 and 2016. Papers based on this work have been presented at conferences autumn 2014 and autumn 2016.

Student category: PT or EET

Practical arrangements:

The work can be carried out any place.

Signatures:

Student (date and signature): 28/02/2017

Supervisor (date and signature): 29/2/19
Appendix B - Technical Background on Corrosion and Hydrates

**Corrosion:**

CO₂ forms carbonic acid in the presence of water [20].

\[
\text{CO}_2 + \text{H}_2\text{O} = \text{H}_2\text{CO}_3 \quad \text{(Carbonic acid)}
\]

Carbonic acid is a weak acid which is only partly dissociated, with PH in the range of 3.3 to 3.7. Under high pressure conditions the degree of dissociation increases and the PH falls as the acid becomes stronger. Acidic impurities such as H₂S, NOx and SOx also causes corrosion. In the presence of water, H₂S and SO₂ will form sulphuric acid which is corrosive to carbon steel. CO₂ corrosion rate can be accelerated with the presence of H₂S. It is therefore important to prevent water dewing, thus preventing/minimizing corrosion from CO₂ as well as the impurities present [59].

NACE Standard, [60], may be used to assist in material selection. Though carbon steel is significantly cheaper and may be used in the presence of dry CO₂, the options exists to use carbon steel or stainless steel. Material selection is governed by the corrosion rate. The dryness level required is dependent upon the individual process conditions. A corrosion prevention, monitoring and control programme should be established. Internal and external corrosion may be prevented by the use of protective coatings, injection of corrosion inhibitors, choice of corrosion-resistant metals and cathodic protection [4, 22, 61]. Corrosion inhibitors are cationic surfactant chemicals, which, when added in a small concentration, effectively reduce the internal corrosion rate of a metal.

**Hydrates:**

Hydrates are ice-like solid crystalline compounds which occurs when water molecules form a cage-like structure around smaller guest molecules [15, 22]. The most common guest molecules are methane, ethane, isobutene, nitrogen, CO₂ and H₂S. It can form in the presence of both free and dissolved water [41]. It can form in both vapour and liquid CO₂.

Hydrate formation is dependent on:

- Temperature
- Pressure
- Composition

Hydrate formation are also affected by the type and amount of impurities present. CO₂ reaction with impurities such as ammonium impurities forms ammonium carbonate / bicarbonate solids which may block pipelines. Inhibitors are added to the gas to depress the hydrate or freezing temperature and the use of dry CO₂ prevents these solid crystalline formation.

The following inhibitors can be used; MeOH (Methyl hydroxide or methanol – CH₃OH), EG and DEG (DEG preferred above -10°C, gives less loss than EG and MeOH).

Hydrates can also cause serious problems such as;

- Destroying the pipeline systems.
- Changing the natural gas quality.
- Plugging the pipeline when it accumulates.

From the technical perspective, the permanent solution to the prevention of hydrate formation and corrosion is to ensure water removal prior to pipeline transportation using a dehydration plant [22].
Appendix C – Unit Conversion Factors

Some of the most commonly used conversion factors are as listed below, [20];

**Flow:**
- 1 MMscfd = 49.81 (kgmole/h) = 179316 (kgmole/s) = 109.8 (lbmole/hr)
- 1 (lb/hr) = 0.453592 (kg/hr)
- 1 (gal/hr) = 0.003785412 (m³/hr)
- 1 (gal [UK]/hr) = 0.004546092 (m³/hr)
- 1 gal/min = 0.1336805 ft³/min = 1.42857 bbl/h = 6.309020 × 10⁻⁵ m³/s

**Density:**
- 1 (kg/m³) = 1000 (ppm)
- 1 lbm/ft³ = 0.1336806 lbm/gal= 0.01601846 g/cm³ = 16.01846 kg/m³

**Mass:**
- 1 pound (lb) = 7,000 grains = 16.0 ounces (oz) = 453.592 grams (g) = 0.4535924 (kg)

**Volume:**
- 1 cubic foot (ft³) = 7.48052 gallons (gal) = 1,728 cubic inches = 0.1781076 barrels (42 U.S. gal) of oil (bbl) = 28.31685 litres (L) = 0.02831685 cubic meters (m³)

**Area/Unit Volume:**
- 1 cm²/cm³ = 100 m²/m³

**Length:**
- 1 Ångstrom = 1e⁻⁷ mm= 1e⁻¹⁰ m = 1e⁻⁸ cm , [20].
- 1 foot (ft) = 12.0 inches (in) = 30.480 centimetres (cm) = 0.30480 meters (m)

**Pressure:**
- 1 atmosphere (atm) = 1.01325 bar = 14.696 lbf/in² = 760 mm Hg (at 32°F) = 1.013250 × 10⁵ pascal (Pa)

**Temperature:**
- °C = (°F -32)/1.8
- K = °C + 273.15
- °F = 1.8(°C) + 32
- °R = °F + 459.67
- °R = 1.8(K)

**Force:**
- 1 pound (lbf) = 4.448 × 10² dyne (dyn) = 4.448222 Newtons (N)

**Energy:**
- 1 British Thermal Unit (Btu) (IT) = 252.1644 cal (tc) = 3.930148 × 10⁻⁴ hp= 1.055056 × 10³ joules (J) = 2.930711 × 10⁻⁴ kWh
- (1 Btu [IT] = 1.00067 Btu [tc])
- (Note: Customarily the Btu refers to the International Steam Table [IT] Btu, and the calorie refers to the thermochemical calorie [tc])

**Power:**
- 1 kJ/h = 0.2777777778 W
- 1 hp (US) = 2544.433 Btu (IT)/h = 550 ft lb/s = 745.6999 watts (W)
- 1 kW = 1.341022 hp

**Specific Energy per Degree:**
- 1 Btu/lbm. °F (IT) = 1.0 cal/g. °C (IT) = 4.186800 kJ/kg.K

**Velocity/Speed:**
- 1 ft/min = 0.00508 (m/s)
- Also, multiply 1 m/s by 197 to obtain ft/min.
Appendix D - Design properties selection guide for TEG and Molecular Sieve dehydration

The following Physical properties table was sourced from the following reference materials, [14, 20].

<table>
<thead>
<tr>
<th></th>
<th>Ethylene Glycol</th>
<th>Diethylene Glycol</th>
<th>Triethylene Glycol</th>
<th>Tetracyrane Glycol</th>
<th>Methanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C₂H₄O₂</td>
<td>C₂H₆O₂</td>
<td>C₂H₆O₄</td>
<td>C₂H₁₀O₄</td>
<td>CH₃OH</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>62.1</td>
<td>106.1</td>
<td>150.2</td>
<td>194.2</td>
<td>32.04</td>
</tr>
<tr>
<td>Boiling Point* at 760 mm Hg, °F</td>
<td>387.1</td>
<td>472.6</td>
<td>545.9</td>
<td>597.2</td>
<td>148.1</td>
</tr>
<tr>
<td>Boiling Point* at 760 mm Hg, °C</td>
<td>197.3</td>
<td>244.8</td>
<td>285.5</td>
<td>314</td>
<td>64.5</td>
</tr>
<tr>
<td>Vapor Pressure at 77°F (25°C) mm Hg</td>
<td>0.12</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>120</td>
</tr>
<tr>
<td>Density (g/cc) at 77°F (25°C)</td>
<td>1.110</td>
<td>1.113</td>
<td>1.119</td>
<td>1.120</td>
<td>0.790</td>
</tr>
<tr>
<td></td>
<td>(g/cc) at 140°F (60°C)</td>
<td>1.085</td>
<td>1.088</td>
<td>1.092</td>
<td>1.092</td>
</tr>
<tr>
<td>Pounds Per Gallon</td>
<td>9.26</td>
<td>9.29</td>
<td>9.34</td>
<td>9.34</td>
<td>6.59</td>
</tr>
<tr>
<td>at 77°F (25°C)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Freezing Point, °F</td>
<td>8</td>
<td>17</td>
<td>19</td>
<td>22</td>
<td>-144.0</td>
</tr>
<tr>
<td>Pour Point, °F</td>
<td>—</td>
<td>-65</td>
<td>-73</td>
<td>-42</td>
<td></td>
</tr>
<tr>
<td>Viscosity in centipoise at 77°F (25°C)</td>
<td>16.5</td>
<td>28.2</td>
<td>37.3</td>
<td>44.6</td>
<td>0.52</td>
</tr>
<tr>
<td></td>
<td>at 140°F (60°C)</td>
<td>4.68</td>
<td>6.99</td>
<td>8.77</td>
<td>10.2</td>
</tr>
<tr>
<td>Surface Tension at 77°F (25°C), dynes/cm</td>
<td>47</td>
<td>44</td>
<td>45</td>
<td>45</td>
<td>22.5</td>
</tr>
<tr>
<td>Refractive Index</td>
<td>1.450</td>
<td>1.446</td>
<td>1.454</td>
<td>1.457</td>
<td>0.328</td>
</tr>
<tr>
<td>at 77°F (25°C)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Specific Heat</td>
<td>0.58</td>
<td>0.55</td>
<td>0.53</td>
<td>0.52</td>
<td>0.60</td>
</tr>
<tr>
<td>at 77°F (25°C) Btu/lb·°F</td>
<td>240</td>
<td>255</td>
<td>350</td>
<td>400</td>
<td>53.6</td>
</tr>
<tr>
<td>Flash Point, °F (PMCC)</td>
<td>245</td>
<td>280</td>
<td>330</td>
<td>375</td>
<td></td>
</tr>
<tr>
<td>Fire Point, °F (C.O.C.)</td>
<td>245</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* Glycols decompose at temperatures below their atmospheric boiling point. Approximate decomposition temperatures are:

Ethylene Glycol  329°F  Triethylene Glycol  404°F
## Typical Operating Conditions of TEG Dehydrators

<table>
<thead>
<tr>
<th>Contactor</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet pressures</td>
<td>&lt;2000 psig (139 bar)</td>
</tr>
<tr>
<td>Inlet temperatures</td>
<td>60°F to 100°F (16°C to 38°C)</td>
</tr>
<tr>
<td>(Lower temperatures enhance absorption capacity but can lead to hydrate formation at high pressure.)</td>
<td></td>
</tr>
<tr>
<td>Pressure drop</td>
<td>5 to 10 psi (34 to 69 kPa)</td>
</tr>
<tr>
<td>Glycol circulation rate</td>
<td>2 to 5 gal/lb H₂O removed, with 3 common.</td>
</tr>
<tr>
<td>(17 to 42 L/kg)</td>
<td></td>
</tr>
<tr>
<td>Tray efficiencies</td>
<td>25 to 30%</td>
</tr>
<tr>
<td>Dew points</td>
<td>&gt;–25°F (–32°C) (Enhanced regeneration required for lower dew point temperatures.)</td>
</tr>
<tr>
<td>Glycol losses</td>
<td></td>
</tr>
<tr>
<td>Vaporization</td>
<td>–0.012 gal/MMscf (1.6 L/MM Sm³)</td>
</tr>
<tr>
<td>Total</td>
<td>0.025 gal/MMscf (3.3 L/MM Sm³)</td>
</tr>
<tr>
<td>Regenerator (reboiler and still)</td>
<td></td>
</tr>
<tr>
<td>Column internals</td>
<td>Packed equivalent to 3 or 4 trays</td>
</tr>
<tr>
<td>Reboiler temperatures</td>
<td>375°F to 400°F (191°C to 204°C)</td>
</tr>
<tr>
<td>Flash tank Pressure</td>
<td>50 to 75 psig (446 to 618 kPa)</td>
</tr>
<tr>
<td>Temperature</td>
<td>150°F (66°C)</td>
</tr>
<tr>
<td>Retention times</td>
<td></td>
</tr>
<tr>
<td>C₄+ Lean Gas</td>
<td>~10 minutes.</td>
</tr>
<tr>
<td>C₄+ Rich Gas</td>
<td>~20 minutes (Use three-phase separator.) TEG absorbs about 1 scf gas/gal TEG at 1,000 psig and 100°F (0.0076 Sm³/L at 70 barg and 38°C)</td>
</tr>
</tbody>
</table>

* For treatment of gas streams that contain high concentrations of C₄+, adequate time needs to be allowed for removal of the less-volatile components from the glycol to minimize hydrocarbon losses in the still overhead.

*Source: Engineering Data Book, (2004b).*

Reference Source for TEG operating conditions, [14, 15].

## Typical Operating Conditions for Molecular Sieve Dehydration Units

| Feed rate | 10 to 1500 MMscfd (0.3 to 42 MMSm³/d) |
| Superficial velocity | Approximately 30 to 35 ft/min (9 to 11 m/min) |
| Pressure drop | Approximately 5 psi (35 kPa), not to exceed 10 psi (69 kPa) |
| Cycle time | Four to 24 hours; 8 or a multiple thereof is common |
| Temperatures and pressures |  |
| Adsorption | Temperatures: 50 to 115°F (10 to 45°C) |
| | Pressures: to 1500 psig (100 barg), |
| Regeneration | Temperatures: 400 to 600°F (200 to 315°C) |
| | Pressures: Adsorption pressure or lower. |

Reference Sources for Typical Molecular Sieve operating conditions above, [6, 14, 20, 62].
Appendices

Reference source for Adsorption and Regeneration Superficial Velocity above, [14].

Reference source for Length/Diameter ratio (L/D) in Separator and Vessel sizing, [63].
## Basic Characteristics of Molecular Sieves

<table>
<thead>
<tr>
<th>Basic Type</th>
<th>Nominal Pore Diameter (Angstroms)</th>
<th>Available Form</th>
<th>Equilibrium H₂O Capacity (% w/w)</th>
<th>Molecules Adsorbed**</th>
<th>Molecules Excluded</th>
<th>Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>3A</td>
<td>Powder 1/16-in. Pellets 1/8-in. Pellets</td>
<td>23 21 20</td>
<td>Molecules with an effective diameter &lt;3 angstroms, including H₂O and H₂.</td>
<td>Molecules with an effective diameter &gt;3 angstroms, e.g. ethanol.</td>
<td>Ethanol and water.</td>
<td>Water purification.</td>
</tr>
<tr>
<td>5A</td>
<td>Powder 1/16-in. Pellets 1/8-in. Pellets</td>
<td>21.5 21.5</td>
<td>Molecules with an effective diameter &lt;5 angstroms, including C₂H₅OH**, n-C₃H₇OH**, C₃H₆ to C₅H₁₀, and all hydrocarbons.</td>
<td>Molecules with an effective diameter &gt;5 angstroms, e.g. iso compounds and all &lt; hydrocarbons.</td>
<td>Isobutane and larger.</td>
<td>Isobutane purification.</td>
</tr>
<tr>
<td>13X</td>
<td>Powder 1/16-in. Pellets 1/8-in. Pellets</td>
<td>28.5 28.5</td>
<td>Molecules with an effective diameter &lt;10 angstroms.</td>
<td>Molecules with an effective diameter &gt;0 angstroms, e.g. (C₂H₅)₃N</td>
<td>Used commercially for general gas drying, air after fuel purification (simultaneous removal of H₂O and CO₂) and liquid hydrocarbon and natural gas sweetening (H₂S and mercaptan removal).</td>
<td></td>
</tr>
</tbody>
</table>

Reference source for Basic characteristics of Molecular sieve, [22].
Appendix E – Installation Factors

<table>
<thead>
<tr>
<th>Material</th>
<th>Code</th>
<th>Qty</th>
<th>Unit</th>
<th>Price</th>
<th>Total</th>
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<tbody>
<tr>
<td>Steel</td>
<td>SAE</td>
<td>0.01</td>
<td>TON</td>
<td>0.01</td>
<td>0.01</td>
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<tr>
<td>Concrete</td>
<td>CNT</td>
<td>0.02</td>
<td>CBM</td>
<td>0.02</td>
<td>0.02</td>
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<tr>
<td>Wood</td>
<td>WOOD</td>
<td>0.03</td>
<td>M3</td>
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<td>0.03</td>
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</table>

Total Cost: $0.06

Appendices
Appendix F - Cost Data: Inflation Index _ Historical Exchange rates

Reference for Inflation Index Table, [57].

Historical Exchange Rates Table: Reference source - Eldrup, [57] and www.xe.com/currencytables (from 2012 to 2017)

<table>
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<th>Year</th>
<th>NOK/USD</th>
<th>NOK/GBP</th>
<th>NOK/EURO</th>
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<tbody>
<tr>
<td>2017</td>
<td>8.57</td>
<td>11.08</td>
<td>9.34</td>
</tr>
<tr>
<td>2016</td>
<td>8.44</td>
<td>10.63</td>
<td>8.98</td>
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<tr>
<td>2015</td>
<td>8.64</td>
<td>13.02</td>
<td>9.18</td>
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<tr>
<td>2014</td>
<td>6.92</td>
<td>10.90</td>
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<tr>
<td>2013</td>
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<td>8.33</td>
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<tr>
<td>2012</td>
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<td>9.08</td>
<td>7.37</td>
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<tr>
<td>2011</td>
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<td>2010</td>
<td>6.05</td>
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<td>8.01</td>
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<td>2007</td>
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<tr>
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<tr>
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<tr>
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<tr>
<td>2003</td>
<td>7.08</td>
<td>11.57</td>
<td>8.00</td>
</tr>
<tr>
<td>2002</td>
<td>7.97</td>
<td>11.95</td>
<td>7.51</td>
</tr>
</tbody>
</table>
Appendix G – Typical cross-section of an Adsorber bed

Look Inside.
A Typical Cross-Section of an Adsorber Bed

Flow Direction

Protection Layer
- to prevent the adsorbent being blown about by turbulence of incoming gas and improve inlet flow distribution
- to protect the adsorbent bed if there is risk of liquid carry-over which otherwise may damage the molecular sieve

Molecular Sieve Bed
The molecular sieve bed can exist of only one type of molecular sieve or different types. Molecular sieves of different structures/chemical nature can optimize the removal of multiple components. A combination of large and small beads is used to minimize pressure drop while retaining optimum adsorption kinetics.

to distribute regeneration gas and prevent molecular sieve blinding support screen

Buffer Gel

Large Ceramic Balls

Small Ceramic Balls

Large Molecular Sieve Beads

Small Molecular Sieve Beads

Small Ceramic Balls

Large Ceramic Balls

GRACE Davison

SYLOBEAD®