Comparison of absorption and adsorption processes for CO_2 dehydration

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Abstract

Captured carbon dioxide (CO_2) must be dehydrated prior to transport or storage because of possibilities for corrosion and hydrate formation. CO_2 dehydration can be performed by absorption, typically into triethylene glycol (TEG) followed by desorption or by adsorption on a solid (typically a molecular sieve) followed by desorption. In this work, the process simulation program Aspen HYSYS is used to calculate material and heat balances for a TEG based absorption process and a molecular sieve adsorption process to achieve less than 30 ppm water in the dehydrated gas. The absorption and stripping columns were modelled using a specified Murphree stage efficiency on each absorption and stripping stage. In the base case, the absorption and adsorption pressure was 40 bar and the inlet temperature was 30 °C. An additional stripping column was added below the desorption column to obtain a low water content. In the molecular sieve based process, all the process units except the adsorption/stripping units were simulated in Aspen HYSYS. It is simulated reasonable process alternatives for CO_2 dehydration down to water levels of 30 and 5 ppm. The simulations combined with cost estimation indicate that a TEG based process is the most economic process both for dehydration down to 30 ppm and to 5 ppm water in dehydrated gas.

Keywords: Dehydration, Carbon capture, Adsorption, Absorption, Aspen HYSYS

1 Introduction

CO_2 dehydration is the process of reducing the water content of captured CO_2 down to an acceptable value prior to transport or storage. The reasons are to avoid problems like corrosion and hydrate formation. Possible specifications are discussed in the references (Cole et al., 2011; Uilhorn, 2013; Buit, 2011). Water specifications are normally in the range between 5 and 500 ppm (parts per million by volume).

The most mentioned processes for dehydration are based on absorption and adsorption. The most traditional method for large scale dehydration is by absorption into triethylene glycol (TEG). For very low water levels, adsorption processes (typically using molecular sieves) are claimed to be necessary (Kohl and Nielsen, 1997; Kemper et al., 2014). Processes for glycol dehydration of CO_2 down to water levels below 5 ppm (Øi and Fazlagic, 2014) using stripping gas and an extra stripping column have been simulated. Øi and Rai (2018) simulated the alternative including an extra stripping column and a Drizo process achieving a water level down to 1 ppm. Glycol based processes are evaluated and compared by Kinigoma and Ani (2016), Kong et al. (2019) and Affandy et al. (2020).

Most commercially planned processes for CO_2 dehydration are based on molecular sieve technologies, eg. the operating facility at Melkøya (Equinor, 2016), in Brevik (Norcem, 2019) and Fortum Oslo Varme (2020). However, CO_2 dehydration has also been performed large scale using glycol processes, eg. at the Quest project in Canada (Dharwadkar, 2011).

The main purpose of this paper is to perform simulation, dimension and cost estimation of a glycol based and molecular sieve dehydration process for a traditional specification of 30 ppm to compare the two alternatives. To our knowledge, such comparisons have not been documented in open literature before.

2 Process description

2.1 Process description of traditional process

A traditional process for CO_2 dehydration using TEG is shown in Figure 1. The inlet gas flows upwards in the contactor/absorber while lean glycol (glycol with little water) flows downwards. The rich glycol (with water) flows to a heat exchanger and a regenerator where the water is evaporated. The regenerated glycol is cooled in the heat exchanger and flows back to the contactor.

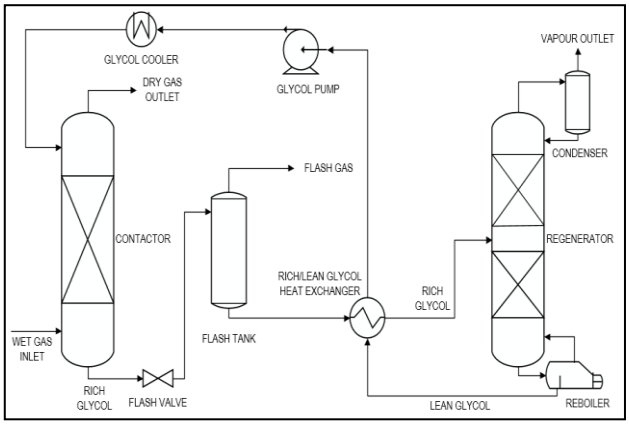

Figure 1. Process flow diagram of a standard TEG dehydration process (Øi and Rai, 2018)

A traditional adsorption based dehydration process has at least two columns filled with an adsorbent like molecular sieves. While one of the columns is in adsorption mode, the other is in desorption mode. After a scheduled time, the operation mode is switched between the columns by opening and closing control valves.

2.2 Process description of simulated processes

Figures 2 and 3 were used as a basis for process simulation. Figure 2 is based on information from Øi and Fazlagic (2014) and Øi and Rai (2018). Compared to Figure 1, the process in Figure 2 takes stripping gas from the flash gas which is contacted countercurrently with regenerated glycol in an extra stripping column. The advantage with using stripping gas and an extra stripping column is that the water content in regenerated glycol can be reduced considerably. This makes it possible to obtain considerably less water in dehydrated gas out from the absorber.

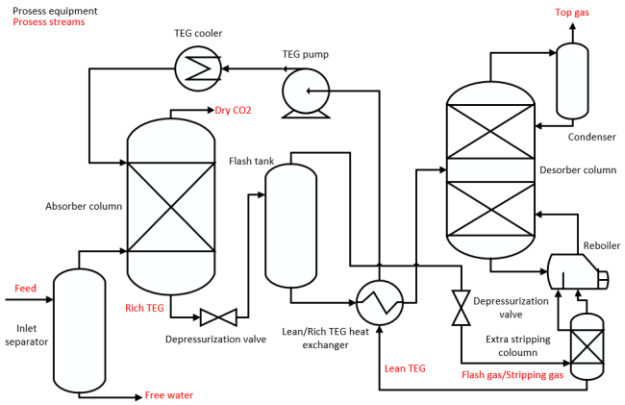

Figure 2 Flowsheet of TEG dehydration unit with extra stripping column and flash gas as stripping gas (Nitsche, 2020).

Figure 3 is a simplified version of the process information from Fortum (2020). The feed (wet CO_2) is first brought to an inlet separator to remove any free water. The CO_2 then flows into the column in adsorption mode where the water is adsorbed on molecular sieves. The dry CO_2 exits at the bottom. A portion of the dry CO_2 is heated and goes through the column operating in regenerating mode. The water is released from the molecular sieves and exits with the regeneration gas. This gas is now cooled, and the water is separated out. A compressor is used to recycle the gas back to mix it with the inlet gas.

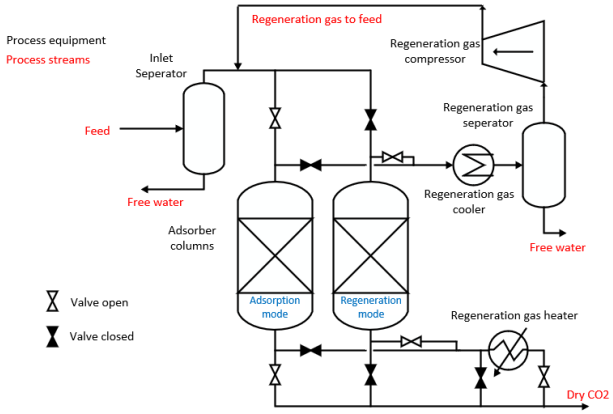

Figure 3. Process flow diagram of the molecular sieve based process (Nitsche, 2020).

3 Simulations

3.1 Specifications and simulation of TEG process and molecular sieve process

The simulation is performed using the glycol package in Aspen HYSYS based on the vapour/liquid equilibrium model Twu et al. (2005). The simulation is similar to the simulations in Øi and Fazlagic (2014) and in Øi and Rai (2018). In these simulations, the Peng-Robinson (PR) model and the Twu-Sim-Tassone (TST) model have been used. The specifications are given in Table 1. An Aspen HYSYS flow diagram is shown in Figure 4. The desorption column and the extra stripping column were simulated as one column in Aspen HYSYS with heating at an intermediate stage.

Table 1. Aspen model parameters and specifications for the TEG simulation

Parameter	Value
Feed flowrate [kg/h]	55000
CO_2 content in Feed [mol%]	0.9960
Water content in Feed [mol%]	0.40
Absorber column temperature [°C]	30
Absorber column pressure [kPa]	4000
Lean TEG temperature [°C]	35
Lean TEG pressure [kPa]	4000
Lean TEG circulation rate [kg/h]	1337
Number of stages in absorber column	8
Murphree efficiency in absorber column	0.5
Flash drum pressure [kPa]	110
Lean-Rich TEG heat exchanger ΔT_{min} [°C]	10
Number of stages in desorber column	7
Murphree efficiency in desorber column	1.0
Reboiler temperature [°C]	200
Desorber column pressure [kPa]	101.3
Reflux ratio in desorber column	0.5

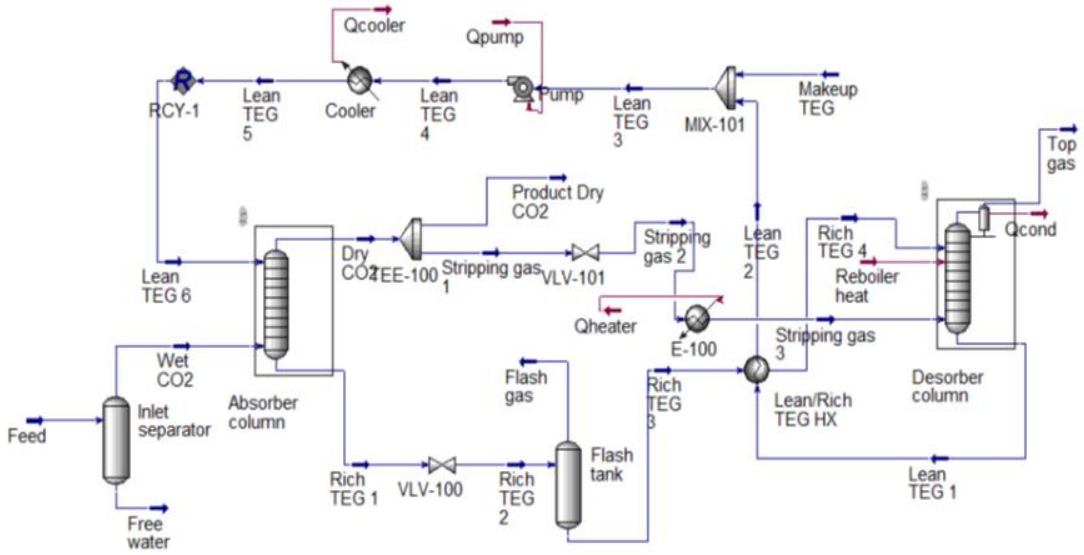

Figure 4. Aspen HYSYS flow diagram of the TEG dehydration process (Nitsche, 2020)

Table 2. Aspen model parameters and specifications for the mol sieve simulation

Parameter	Value
Feed flowrate [kg/h]	55000
CO_2 content in Feed [mol%]	99.6
Water content in Feed [mol%]	0.4
Regeneration gas flow rate [kmole/h]	125.3
CO_2 content in Regeneration gas (same as in Wet CO_2) [mol%]	99.79
Water content in Regeneration gas (same as Wet CO_2) [mol%]	0.21
Adsorber inlet and outlet temperature [°C]	30
Adsorber / regeneration inlet pressure [kPa]	4000
Pressure drop in regenerator [kPa]	5
Adsorber column outlet and inlet [kmole/h]	1373
Regeneration column inlet temperature [°C]	278

A simulation of the molecular sieve based process was performed based on the specifications in Table 2. The two adsorption/regeneration columns were not simulated in Aspen HYSYS, so the calculation was divided in three. An Aspen HYSYS flow diagram is shown in Figure 5. The first part starts with the feed and the regeneration gas and ends before the column in adsorption mode. The second and middle part starts after the column in adsorption mode and ends before the column in regeneration mode. The third starts after the column in regeneration mode and ends with the regeneration gas. The resulting flow in the regeneration gas in the third part equals the flow to the first part. The Aspen HYSYS flow diagram is shown in Figure 5.

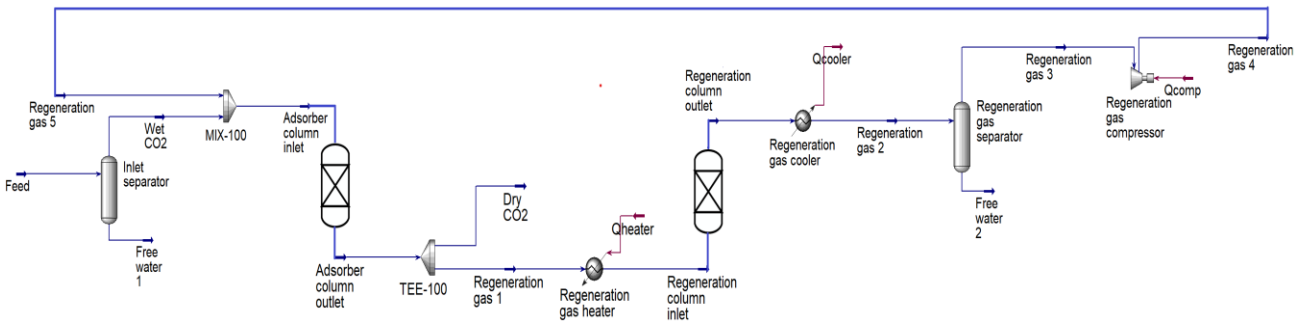

Figure 5. Aspen HYSYS flow diagram of the molecular sieve based process (Nitsche, 2020)

4 Dimensioning and cost estimation

4.1 Dimensioning specifications

The basis for the dimensioning is the material and heat balance from the Aspen HYSYS simulations.

For the TEG dehydration process, gas velocity was specified to 0.32 m/s to calculate the cross section and diameter. The estimated gas velocity through the structured packing is calculated from a traditional value of 2 m/s at atmospheric conditions divided by the square root of the pressure ratio (40). The packing height of the absorption and desorption column is 1 meter per stage with a specified stage efficiency. The total height of the absorption column, desorption column and extra stripping column were specified to be 17 m, 8 m and 7 m, respectively. The extra height is due to distributors, demister, gas inlet, outlet and sump. The heat transfer numbers (U-values in $W/(m^2K)$) were estimated to 300 for the lean rich heat exchanger, 900 for the reboiler, 500 for the condenser and 300 for the cooler.

The adsorption and stripping columns were dimensioned by assuming gas velocities (0.12 m/s) based on an Ergun equation from GPSA, relative water capacity (0.13 kg water/kg for 1/8") of the molecular sieves, retention time and operation time between switching between adsorption and stripping modes (12 hours). The adsorber height was calculated by finding the height of the saturation zone and the mass transfer zone. The total height and diameter for the two adsorbers were then specified to 6.1 m and 1.4 m, respectively.

The separator tanks were dimensioned by a traditional Souders Brown factor of 0.07 using data for physical properties from the Aspen HYSYS simulation. For the tanks, traditional design pressure based on operating pressure was assumed. Standard corrosion allowance was also assumed. The adiabatic efficiency for the compressor was specified to 0.75.

4.2 Cost estimation specifications

The Enhanced Detailed Factor (EDF) method from Ali et al. (2019) was used in the cost estimation. For each equipment unit, the Aspen In-plant version 10.0 was used to estimate the procured cost. Stainless steel was specified for all process units. Then an installation cost was calculated based on a detailed factor table (Ali et al., 2019). Then the unit cost was corrected for currency and year index.

Table 3. Assumptions made for CAPEX calculation

Parameter	Value
Currency exchange rate (20.11.18)	9.7135 NOK/EU
Currency exchange rate (20.11.20)	10.6613 NOK/EU
Cost index (Nov.2018)	109.8
Cost index (Nov.2020)	112.4

Table 4. Assumptions for OPEX calculations

Maintenance cost	4 % of CAPEX
Electricity price	0.50 NOK/kWh
Steam price	0.13 NOK/kWh
Operational time	8000 hours/yr

4.3 Scope of dimensioning and cost estimation

The cost analysis is limited to the equipment listed in the flowsheets in Figure 4 and 5. No pre-treatment like inlet gas purification is considered, and no treatment after processing like purification, compression, transport or storage is considered. The cost estimate is limited to installed cost of listed equipment. It does not include eg. land procurement, preparation, service buildings or owners cost.

5 Results and Discussion

5.1 CAPEX results

Based on the cost estimation described in section 4, the capital cost was calculated for the process based on glycol dehydration (the TEG unit) and the process based on molecular sieve adsorption. The results are presented in Figure 6.

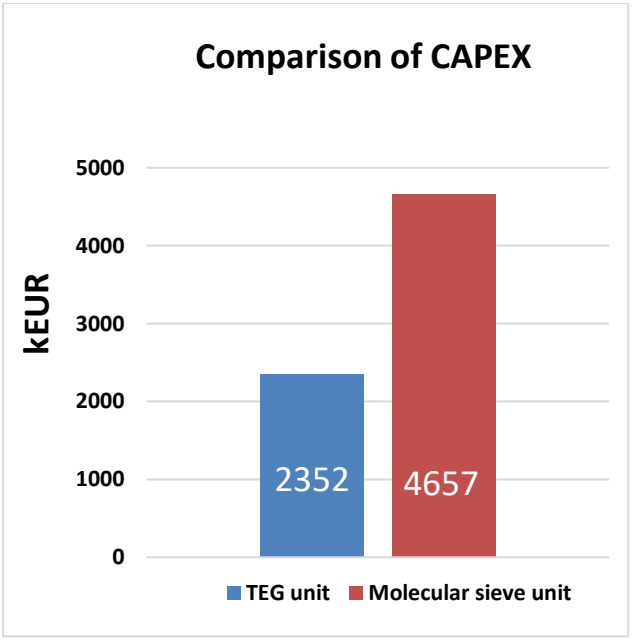

Figure 6. Comparison of CAPEX between the TEG and molecular sieve unit [kEUR] (Nitsche, 2020)

The comparison of the CAPEX shows that the capital cost is considerably higher for the molecular sieve based unit. There are two main reasons. The recirculation compressor unit is expensive, and the molecular sieve columns are large due to a lower gas velocity through the molecular sieve compared to the gas velocity in the absorption column.

The processes are compared for the base case conditions and selected specifications. The inlet and operating pressure of 30 bar is based on optimum absorption conditions between 30 and 50 bar from literature (Øi and Fazlagic, 2014). Other specifications as pressure drop and regeneration flow rate for the mol-sieve process are also recommended values from industry (GPSA, 1987). Other choices of the specifications are not expected to change much on the differences between the compared processes.

5.2 Opex results

The yearly operating cost was calculated for both dehydration processes. The dominant operation cost is energy which is due to heating, compression and pumping. Maintenance cost estimated as 4 % of CAPEX is also included. The results are presented in Figure 7.

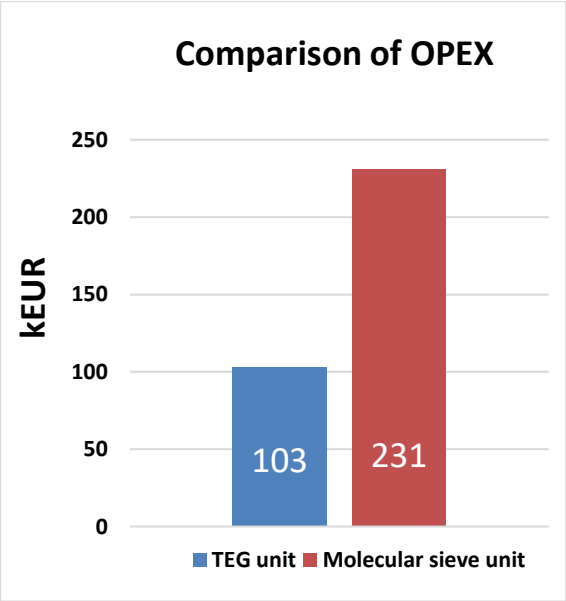

Figure 7. Comparison of yearly OPEX between the TEG and molecular sieve unit [kEUR] (Nitsche, 2020)

The comparison of OPEX also shows considerably higher operating cost for the molecular sieve based process. The two main reasons are that the heat demand is higher for the adsorption case because of more indirect heating, and that the compressor has a high energy demand. It is assumed that electricity is necessary to heat the regeneration gas. For the glycol unit, it is possible to use cheaper heat as steam.

If the same heat source (like steam or electricity) was used for both processes, the operating cost difference would be less. But because the heat demand is higher for the molecular sieve based process, the operating cost for the molecular sieve alternative would still be higher.

5.3 Results for 5 ppm water specification

Some references (Kohl and Nielsen1997; Kemper et al., 2014) claim that a molecular sieve based process is necessary to obtain low water levels. A glycol based process which achieved less than 5 ppm was simulated with a higher absorption column than in the standard case. This is compared with the molecular sieve process in Figure 8. The capital cost for the molecular sieve unit is assumed to be only slightly increased to obtain 5 ppm water in dehydrated gas.

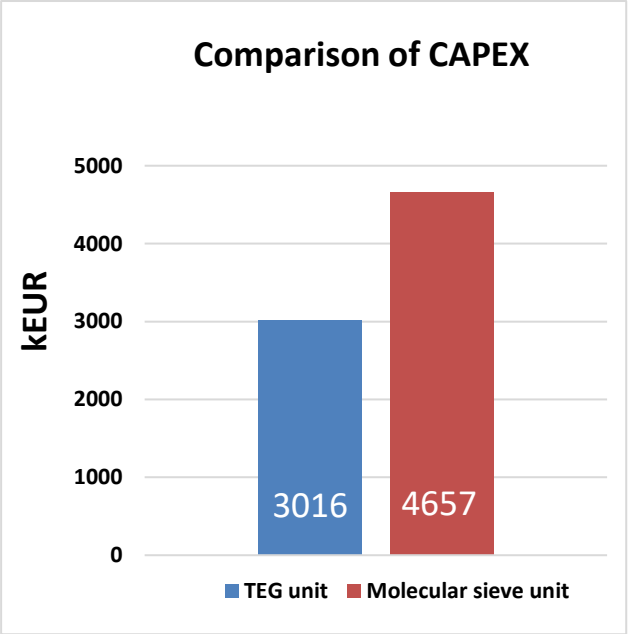

Figure 8. Comparison of CAPEX between the TEG and molecular sieve unit [kEUR] for dehydration down to 5 ppm (Nitsche, 2020)

The results show that the CAPEX is still considerably higher for the molecular sieve based process for obtaining less than 5 ppm in dehydrated gas.

There might be other criterias than cost when comparing a glycol based and molecular sieve based dehydration process like stability, robustness and risk. These factors are however assumed to be comparable for the two dehydration processes. There is no reason to claim that it is not possible to achieve 5 ppm water with both a glycol based and a molecular sieve based process.

6 Conclusion

In this work, the process simulation program Aspen HYSYS is used to calculate material and heat balances for a TEG based absorption process and a molecular sieve adsorption process to achieve less than 30 ppm water in the dehydrated gas. The absorption and stripping columns were modelled using a specified Murphree stage efficiency on each absorption and stripping stage. In the base case, the absorption and adsorption pressure were 40 bar, the inlet temperature was 30 °C, and the processes achieved less than 30 ppm water in the dehydrated gas. An additional stripping column was added below the desorption column. Both processes were cost estimated using the Aspen In-Plant cost estimation tool for the equipment cost, using a detailed factor method to estimate the capital cost and typical utility cost data for heat and electricity.

For the base case (with less than 30 ppm water in the dehydrated gas), the capital cost was calculated to 2.4 mill. EURO for the TEG unit and 4.7 mill. EURO for the molecular sieve process. The yearly operating cost was calculated to 0.1 mill. EURO for the TEG process and 0.23 mill. EURO for the molecular sieve process. The process was also calculated for dehydration down to 5 ppm. To achieve that in the TEG process, a higher absorption column is necessary. The cost of the TEG based process did not increase considerably, so the TEG absorption process was also most economical for those conditions.

It is simulated reasonable process alternatives for CO_2 dehydration down to water levels of 30 and 5 ppm. The simulations combined with cost estimation indicate that a TEG based process is the most economic process both for dehydration down to 30 ppm and to 5 ppm water in dehydrated gas.

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