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Amine LPG Sweetening Process
عملية تحلية الغاز البترولي المسال باستخدام الأمين

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الآيـــــة

بسم الله الرحمن الرحيم

قَالَ رَبِّ اشْرَحْ لِي صَدْرِي (25) وَيَسِّرْ لِي أَمْرِي (26) وَاحْلُلْ عُقْدَةً مِنْ لِسَانِي (27) يَفْقَهُوا قَوْلِي (28)

صدق الله العظيم

سورة طه

Dedication

To our parents, the two persons that gave the tools and values necessary to be where we are standing today. To all brothers, sisters, friends, teachers, colleague, relatives, & anyone who assisted, advised, &supported us and our, project. To all SPE members around the world, we would be honor to dedicate this project.

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Abstract

LPG is one of the top products in refineries contains impurities like H2S, are very harmful due to its corrosive and toxic characteristics, use to Tertiary amines (MDEA) to removes these impurities, called LPG sweetening process, the simulation and optimization of LPG sweetening process using HYSYS process version 11

H_2S concentration in sweet LPG is within permissible limit of 0-10 ppm

التجـريــد:

يعتبر الغاز البترولي المسال أحد المنتجات الاولى في المصافي. يحتوي الغاز البترولي المسال على شوائب مثل غاز كبريتيد الهيدروجين وهو ضار بسبب سميته وخصائصه المسببة للتآكل.

باستخدام الإصدر 11 من برنامج الهايسس يستخدم ثلاثي ميثيل ألامين لإزالة هذه الشوائب في عملية تسمى بتحلية الغاز .

تركيز غاز كبريتيد الهايدروجين بعد عملية التحلية صفر .

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Introduction

Chapter 1

Introduction

1.1 Introduction

Refineries mainly process crude oil to produce valuable petroleum products like fuel gas, LPG, gasoline, naphtha, ATF, kerosene, diesel, gas oil, residue and sulfur. Refineries also have hydrogen plant to meet hydro-treating requirements and nitrogen for utility requirements, Petroleum products like ethylene, propylene, cumene, cyclohexane, benzene, xylene, methanol and ammonia are obtained from petrochemical complex. LPG is still considered one of the important products due to its domestic usage and commercial value. (K. Jayakumar1, 2017)

1.2 Liquified petroleum gas LPG

Also called LP gas, many of several liquid mixtures of the volatile hydrocarbons propene, propane, butene, and butane. It was used as early as 1860 for a portable fuel source, and its production and consumption for both domestic and industrial use have expanded ever since. A typical commercial mixture may also contain ethane and ethylene, as well as a volatile mercaptan, an odorant added as a safety precaution.

LPG reaches the domestic consumer in cylinders under relatively low pressures. The largest part of the LPG produced is used in central heating systems, and the next largest as raw material for chemical plants. LPG commonly is used as fuel for gas barbecue grills and gas cooktops and ovens, for gas fireplaces, and in portable heaters. In Europe, LPG water heaters are common. It is also used as an engine fuel and for backup generators. Natural gas and crude oil process is main sources of LPG (britannica, n.d.)

1.2.1 Properties of LPG

LPG is primarily propane and butane, the properties of LPG (properties of propane and butane).

LPG has density heavier than Air (Propane Density) – and specific gravity (Propane specific gravity)

LPG chemical formula – molecular formula: C_3H_8 or C_4H_{10} and Combustion formula

$$C3H8 + 5\ O2 \rightarrow 3\ CO2 + 4\ H2O + \text{Heat (complete combustion)}$$

Table (1.1.1) LPG properties

LPG (propane) gas melting/freezing temperature	-188 °C or -306.4 °F
LPG (propane) gas boiling point temperature	42 °C or -44 °F
LPG gas flame temperature	1967 ºC or 3573 ºF
LPG-Propane auto ignition temperature	470 °C or 878 °F
LPG-Propane ignition temperature (in air)	470°C – 550°C (878°F – 1020°F)
LPG vapour pressure	637 kPa @ 27°C (128 PSIG @ 80°F)
LPG energy content	25 MJ/L or 91,547 BTU/Gal (60°F)
Gaseous expansion of LPG	1 L (liquid) = 0.27 M3 (gas)
LPG limits of flammability	2.15% to 9.6% LPG/air
Molecular weight of LPG components	Propane is 44.097 kg/kmole – Butane (n-butane) is 58.12 kg/kmole
Specific Gravity of liquid LPG propane	0.499 (25°C)
Molecular weight	44.097 kg/kmole

1.3 Problem Statement:

In Refineries gas sweetening process is inevitable when LPG contains acid gases like H_2S. Removal of these acid gases is essential since their presence poses severe corrosion problem to the process equipment. Tertiary amines (MDEA) is used as solvent for sweetening purpose.

1.4 Objective:

- The objective of this project is to remove hydrogen sulfide H_2S from a gas stream, to meet requirement of LPG handling, and to avoid forms of acidic solutions that will cause corrosion process equipment.
- Study the effect of various feed temperature on the percentage removal of acid gas is studied and the percentage of sweet LPG recovered

Chapter 2

Literature Review

Chapter 2

Literature review

2.1 Introduction

The demand for liquid hydrocarbon sweetening facilities has increased with the rise in the production of liquefied petroleum gas (LPG). The most common contaminants present in LPG are hydrogen sulfide (H2S), mercaptans (RSH), carbon dioxide (CO2), carbonyl sulfide (COS), carbon disulfide (CS2) and elemental sulfur. (Hanan Jalal Qeshta a, 2015)

2.1.1 Hydrogen sulfide (H_2S)

H_2S is an extremely hazardous and toxic compound. It is a colorless, flammable gas, which can be dangerous in relative low concentrations. H_2S can be characterized by the smell of rotten eggs and can be found in e.g. sewage, fertilizers, wastewater treatment plants and gas wells.

The gas is often produced under conditions where rotten organic matter containing sulfur is decomposed in a low oxygen atmosphere. The smell of H_2S can be detected by the human nose in concentrations below 1 part per million (ppm). The smell will increase as the concentration increases. In concentration up to 30 ppm the rotten smell will be present. Above this concentration the smell will change into a more sickening sweet smell. This is dangerous because H_2S can be present without anyone observing any particularly smell. When H2S reaches this level, it starts to be a threat to the life of humans. (Hansen, 2014)

Table (2.2.1) symptoms from exposure to H_2S

LOW	0 – 10 ppm	Irritation of the eyes, nose and throat
MOD	10 – 50 ppm	Headache Dizziness Nausea and vomiting Coughing and breathing difficulty
HIGH	50 – 200 ppm	Severe respiratory tract irritation Eye irritation/acute conjunctivitis Shock Convulsions Coma Death in severe cases

H2 S is highly undesirable in liquefied petroleum gas (LPG) for several reasons: » Storage. When storing produced LPGs for later distribution, H_2S causes corrosion in the expensive sphere tanks. » Polymer yield. Sulfur compounds reduce the polymer yield in polyolefin like polypropylene. » Catalysts. H_2S is known to poison catalysts in reactions that use LPGs as feedstock. » Emissions. When burning propane or any other LPG, H_2S will oxidize to SO_2, a particularly harmful emission

2.3 Sweetening process

Processes within oil refineries or chemical processing plants that remove hydrogen sulfide are referred to as "sweetening" processes because the odor of the processed products is improved by the absence of hydrogen sulfide.

Gas sweetening is sometimes referred to as amine treating can be used in refineries, petrochemical plants, natural gas processing plants its more referred to as gas sweetening(paqell)

Gases containing H_2S or both H_2S and CO_2 are commonly referred to as sour gases or acid gases in the hydrocarbon processing industries.

Methods for gas sweetening can be divided into two categories: adsorption and absorption processes. (paqell.com, n.d.)

2.3.1 Reasons for Sweetening

1. Safety and environmental protection
2. Product Specification
3. Corrosion prevention
4. Improved Heating Values
5. Economics(sometimes)

2.3.2 Methods of gas sweetening

Methods of gas sweetening can be divided into two categories: adsorption and absorption process

Adsorption is a physical/chemical method where the gas is concentrated on the surface of a solid or liquid to remove impurities of H2S. The absorption process is performed by either dissolution, which is a physical process or by reactions with other compounds, which are chemical processes. (Hansen, 2014)

2.4 Amines

Amines are compounds formed from ammonia (NH3) by replacing one or more of the hydrogen atoms with another hydrocarbon group. Replacement of a single hydrogen produces a primary amine, replacement of two hydrogen atoms produces. (Meyers, n.d.)

a secondary amine, and replacement of all three of the hydrogen atoms produces a tertiary amine. Primary amines are the most reactive, followed by the secondary and tertiary amines. The amines are used in water solutions in concentrations ranging from approximately 10 to 65 wt% amines. These amines are also used in many oil refineries to remove sour gases from liquid hydrocarbons such as liquified petroleum gas (Meyers, n.d.)

2.4.1 Types of amines

Until the 1970s, MEA was the first amine considered for any sweetening unit. In the 1970s, MEA switches to DEA mainly, and in the past 20 years, there is an interest in MDEA and mixed amines.5

Methyl diethanolamine as a solvent has been favored in the past few years because of its many advantages, such as low corrosion, environmental friendliness, high loading capacity, resistance to thermal and oxidative degradation, and low heat of regeneration, over other amines. However, the main disadvantage of this solvent is its slow reaction rate with CO_2, however, it has selectivity to H_2S removal. (Sajjad Sharif Dashti, n.d.)

2.4.1.1 Mon ethanolamine (MEA)

MEA is the strongest alkaline between the amines, for that reason MEA will be the one reacting most rapidly with the acid gas. MEA is able to remove both hydrogen sulfide and carbon dioxide from gas streams. MEA has a low molecular weight compared to the other amines, and has a greater carrying capacity for acid gases on a unit per weight or volume basis. (NOORHAN ABBAS FADHEL, n.d.)

2.4.1.2 Diethanolamine (DEA)

DEA is in many ways similar to MEA, where DEA is a secondary amine and MEA a primary. All side groups are ethanol. DEA’s reaction with carbonyl sulfide and carbon disulfide is very slow, and it is not always possible to detect reaction between those species. DEA is non-selective and removes H2S and CO2. It is more volatile than MEA, which will result in a more efficient recovering process, where the loss by evaporation will be small. (NOORHAN ABBAS FADHEL, n.d.)

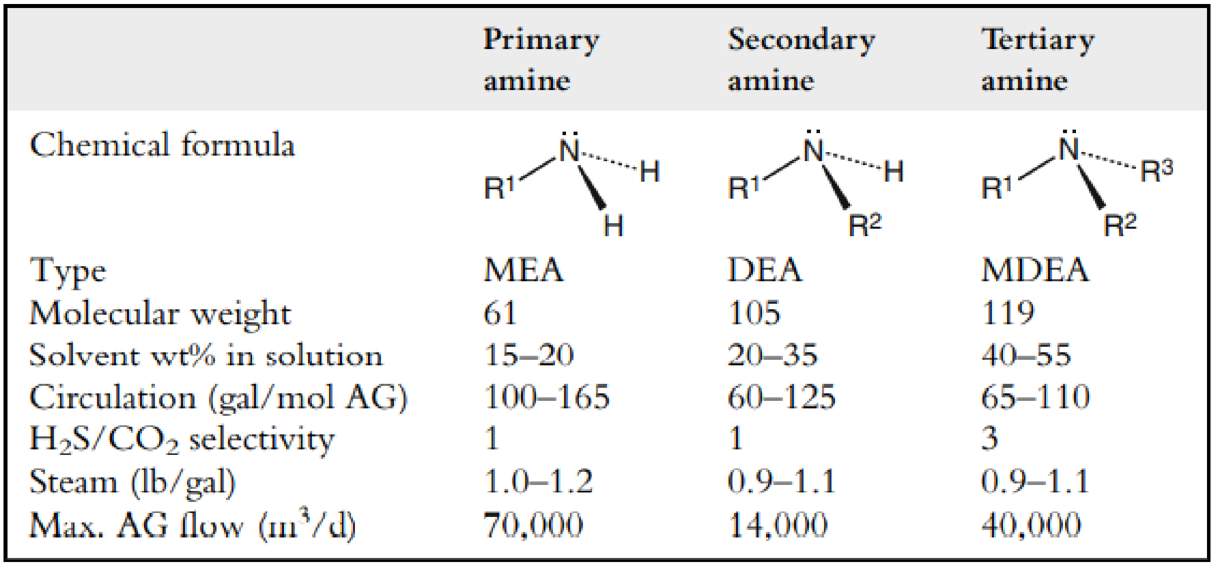
2.4.1.3 Methyldiethanolamine (MDEA)

Triethanolamine (TEA) was the first amine applied for gas sweetening. In modern gas treatment, it has been replaced by MDEA, since they are similar in their efficiency, but MDEA is less toxic.

MDEA is a tertiary amine like TEA, and they react the same way in gas sweetening processes. MDEA is less reactive with H2S and CO2, and sometimes the content of these will not be reduced enough to meet the demands for sweet gas. The flow and the temperature have to be raised to compensate for less efficiency compared to the other amines.

Due to the tertiary structure, MDEA is a more compact molecule, and therefore it is reacting slower because it is harder for the volatile component to get close to the center of the molecule. Nevertheless, the use of MDEA will still be realistic in some processes as a sweetening agent, due to its low toxicity. (NOORHAN ABBAS FADHEL, n.d.)

Table (3.2.2) comparison of amine solvent



	Primary amine	Secondary amine	Tertiary amine
Chemical formula			
Type	MEA	DEA	MDEA
Molecular weight	61	105	119
Solvent wt% in solution	15–20	20–35	40–55
Circulation (gal/mol AG)	100–165	60–125	65–110
H_2S/CO_2 selectivity	1	1	3
Steam (lb/gal)	1.0–1.2	0.9–1.1	0.9–1.1
Max. AG flow (m^3/d)	70,000	14,000	40,000

2.5 Previous studies

Hanan Jalal Qeshta a, b , Salaheddin Abuyahya a , Priyabrata Pal a , Fawzi Banat ,2015

LPG sweetening process using tertiary alkanolamine (methyldiethanolamine; MDEA) by Aspen HYSYS version 8.0.. The effects of operating parameters such as temperature and pressure on the proposed process were also studied. A steady state model was developed for determining the sensitivity of parameters affecting the process. The most suited feed LPG temperature was determined to be 45 C. The optimum MDEA concentration and flow rate was found to be 35.0 wt% and 24.43 m3 /h, respectively. The parameters which indirectly affect the extraction process such as reboiler operating pressure, rich MDEA temperature. (Hanan Jalal Qeshta a, 2015)

Ali Samadi Afshar, Sayed Reaza Hashemi, 2011 Sulfrex demercaptanization process is used to remove volatile and corrosive mercaptans from liquefied petroleum gases by caustic solution. This process consists of two steps. Removing low molecular weight mercaptans and regeneration exhaust caustic. Some parameters such as LPG feed temperature, caustic concentration and feed’s mercaptan in extraction step and sodium mercaptide content in caustic, catalyst concentration, caustic temperature, air injection rate in regeneration step are effective factors. (Ali Samadi Afshar, 2011)

Ruiting Liu, Daohong Xia, Yuzhi Xiang, and Yongliang Tian,2005, In order to provide the detailed technical guidance for the industrial operation in LPG sweetening, the caustic concentration not only has influence on the dispersion of catalyst sulfonated cobalt phthalocyanine (CoSPc), but also has effects on the transformation of mercaptans to mercaptides and further to disulfides (Ruiting Liu, n.d.)

JERRY A. BULLIN 1992 The use of amine mixtures employing methyldiethanolamine (MDEA), monoethanolamine (MEA), and diethanolamine (DEA) have been investigated for a variety of cases using a process simulation program called TSWEET . At high pressures, amine mixtures have little or no advantage in the cases studied. As the pressure is lowered, it becomes more difficult for MDEA to meet residual gas requirements and mixtures can usually improve plant performance. (BULLIN, 2005)

Chapter 3

Methodology

Chapter 3

Methodology

3.1 Process Description

Sour gas inters the contactor tower and rises through the descending amine solution .Purified gas flows from the top of tower. And the amine Solution, carrying absorbed acid gas, leaves from the bottom of tower to Separator to separate any insoluble gases Rich amine is heated by hot regenerated lean amine in the heat exchanger .Rich amine is further heated in the regeneration still column, by heat supplied from the reboiler. Steam and acid gases separated from rich amine are condensed and cooled, respectively in the reflux condenser. Condenser steam is separated in reflux accumulator and returned to the still. Acid gasses may be vented, incinerated, or directed to sulfur recovery system. Hot regenerated lean amine is cooled in solvent aerial cooler and circulated to the contractor tower, completing the cycle. A variety of heat sources can be used for the still reboiler- direct fired, waste heat, hot oil and steam system. The method will be used in this project is chemical absorption

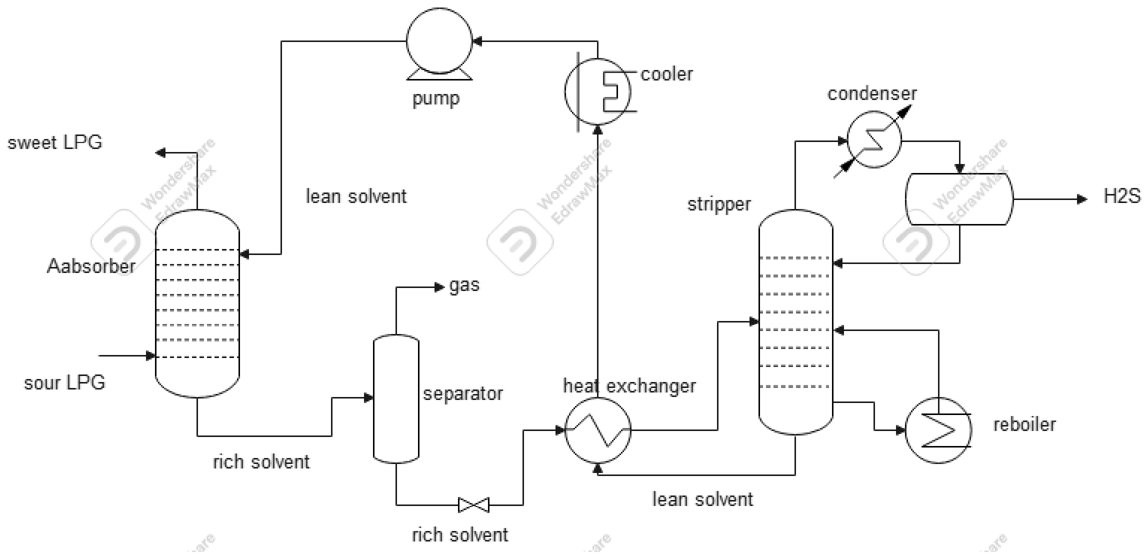


Figure (1.3.1) sweeting process flow sheet

3.2 Chemical absorption

In absorption (also called gas absorption, gas scrubbing, and gas washing), a gas mixture is contacted with a liquid (the absorbent or solvent) to selectively dissolve one or more components by mass transfer from the gas to the liquid. The components transferred to the liquid are referred to as solute or absorbate.

Absorption is used to separate gas mixture; remove impurities, contaminants, pollutants, or catalyst poisons from gas; or recovery valuable chemicals.

These processes are characterized by a high capability of absorbing large amounts of acid gases. They use a solution of a relatively weak base, such as mono-ethanolamine. The acid gas forms a weak bond with the base which can be regenerated easily. Mono- and di-ethanolamine are frequently used for this purpose. (Hansen, 2014)

3.2.1 Process chemistry

Where, H2S is reacted instantaneously with MDEA to form methyldiethanolamine-sulphide salt

$$R_2NCH_3 + H_2S \longleftrightarrow R_2NHCH_3HS$$

3.3 Material Balance

3.3.1 Introduction:

Material balances are important first step when designing a new process or analyzing an existing one. They are almost always prerequisite to all other calculations in the solution of process engineering problems.

The General Balance Equation A balance (or inventory) on a material in a system (a single process unit, a collection of units, or an entire process) may be written in the following general way:

$$\text{Input} + \text{generation} - \text{output} - \text{consumption} = \text{accumulation}$$

This general balance equation may be written for any material that enters or leaves any process system; it can be applied to the total mass of this material or to any molecular or atomic species involved in the process. The general balance equation may be simplified according to the process at hand. For example, by definition, the accumulation term for steady-state continuous process is zero. Thus the above equation becomes.

$$\text{Input} + \text{generation} = \text{output} + \text{consumption}$$

For physical process, since there is no chemical reaction, the generation and consumption terms will become zero, and the balance equation for steady-state physical process will be simply reduced to:

$$\text{Input} = \text{Output}$$

The main objective of mass balance is to collect physical for feedstock and products and to make hand calculation of plant mass balance. The best way to tackle a material balance problem will depend on the information given, the information required from the balance, and the constraints that arise from the nature of the problem.

Table (4.3.1) Sour LPG composition

Component	Mass%	M.wt	Kg/hr	Kmol/hr
Methane	1.05%	16.042	315	19.636
Ethan	7.58%	30.07	2274	75.624
Propane	15.08%	44.09	4524	102.608
Propene	17.59%	24.08	5277	125.404
i-butan	8.55%	85.12	2565	30.134
n-butane	23.47%	85.12	7122	83.67
i-butene	9.61%	56.1	2883	51.390
1-butene	5.05%	56.1	1515	27.005
Trans-butene 2	6.56%	56.1	1968	35.080
Cis-2-butene	4.45%	56.1	1335	23.797
n-pentane	0.28%	72.15	84	1.164
1-pentane	0.20%	70.13	60	0.856
$\mathbf{H_2S}$	0.13%	34.08	39	1.144
H2	0.07%	2.016	21	10.417
$\mathbf{H_2O}$	0.06%	18.016	18	0.999
Total			30000	588.929

3.3.2 Material Balance of absorber

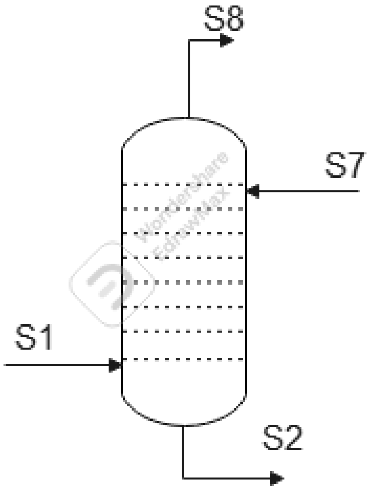


Figure (2.3.2) absorber

Stream 1 sour LPG $= 30000\ \text{kg/hr}$

Stream 7 Lean amine $= 17750\ \text{kg/hr}$

Gas recovery $= 97\%$

Stream 8 Sweet gas $=30000 \times 0.97 = 29100\ \text{kg/hr}$

H_2S In Sour gas $= 39\text{kg/hr}$

H_2S In Sweet gas 0.5 ppm $29100 \times 0.5/10^6 = 0.01455\ \text{kg/hr}$

H_2S In Rich Amine $39 - 0.01455 = 38.99\ \text{kg/hr}$

M.wt of MDEA $= 119.16\ \text{kg/kmol}$

M.wt of H_2O 18 kg/kmol

Solvent 35% MDEA & 65% Water

Mole% $= \dfrac{\frac{\text{wt1}}{\text{MT1}}}{\frac{\text{wt1}}{\text{Mt1}}+\frac{\text{wt2}}{\text{MT2}}}$

Concentration of MDEA in water = 45 wt%

Mole % of MDEA= $\frac{\frac{0.45}{119.16}}{\frac{0.45}{119.16}+\frac{0.55}{18}} * 100 = 11\%$

Mole of H_2O =$\frac{\frac{0.55}{18}}{\frac{0.55}{18}+\frac{0.45}{119.}} * 100 = 89\%$

M.wt of Lean Amine $= \mathrm{M.wt\ of\ MDEA} \times \mathrm{mol\%} + \mathrm{M.wt\ of\ H_2O} \times \mathrm{mol\%}$

$(119.16 \times 0.11) + (18 \times 0.89) = 29.13\ \mathrm{kg/kmole}$

Mole of lean amine = rate of lean solution in stream $7/\mathrm{M.wt}$ of lean amine

$$17750/29.13 = 609.39\ \mathrm{kmole/hr}$$

Over all Material Balance

Stream 1 + Stream 7 =Stream 2 + Stream 8

Rich Amine $= 18650\ \mathrm{kg/hr}$

Table (5.3.2) over all Material Balance of absorber

Component	In kg/hr		in total	Out kg/hr		Out total
	S1 Sour gas	S5 Lean amine		S2 rich amine	S8 treated gas	
LPG	29961	0	29961	861	29099.99	29961
H2S	39	0	39	38.99	0.1455	39.01
MDEA	0	17750	17750	17750	0	17750
Total	30000	17750	47750	18650	29100	47750

3.3.3 Material Balance of Separator

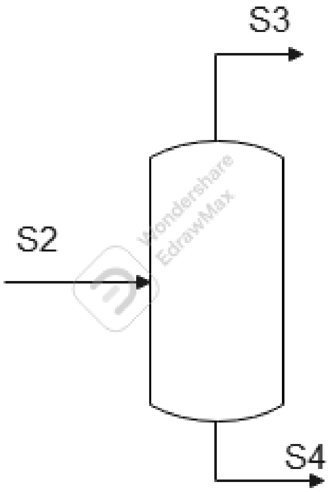


Figure (3.3.3) Separator

$\text{In} = \text{out}$

Assume that overhead gases 4.5%

Stream 3 over head gases $= \text{ total rich amine out } * \ 0.045$

$18650 * 0.045 = 839.25$

Stream 4 rich amine = total rich amine – overhead gases

$$18650 - 839.25 = 17810.75$$

Table (6.3.3) over all material balance of Separator

Stream	In	Out
S2 rich amine	18650	
Stream 3		839.25
Stream 4		17810.75
Total	18650	18650

3.3.4 Material Balance of Striper

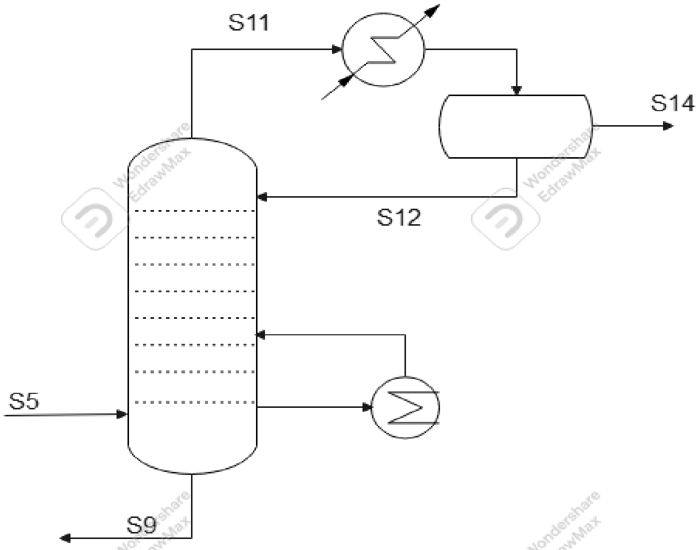


Figure (4.3.4) Stripper

Assume reflux rate 5%

Stream5 = 17810.75

Stream 9 = 17750

$\text{Stream } 12 \ = \ 0.05 \text{ Stream } 11$

$(17810.75 + 0.05S11) = (S11 + 17750)$

$\text{Stream } 11 \ = \ 63.946\text{kg/hr}$

$\text{Stream } 12 = 3.158 \text{ kg/hr}$

Table (7.3.4) over all material balance of Stripper

Stream	In	Out
Stream 5 (rich amine)	17810.75	
Stream 9(lean amine)		17750
Stream 11 (acid gas)		63.908
Stream 12 (reflux)	3.158	
Total	17813.908	17813.908

3.3.5 Reflux Drum Material Balance:

Table (8.3.5) over all material balance of reflux Drum

Stream	In	Out
Stream11	63.908	
Stream12 (Reflux)		3.158
Stream14		60.75
Total	63.908	63.908

3.4 Energy Balance:

Cp of material at any Temperature $(℃) = a + bT + cT^2 + dT^3$ (himmelblau, n.d.)

Energy balance around process units

Temperature reference for energy balance calculation =25℃

Table (9.3.6) Cp of LPG component at temperature 298 k^°

Component	Mass%	M.wt	CP (J/mol.k)	CP (kj/kg.k)	Cp*xi
Methane	1.05%	16.042	35.68	2.22E+00	2.34E-02
Ethan	7.58%	30.07	52.39	1.74E+00	1.32E-01
Propane	15.08%	44.09	73.47	1.67E+00	2.51E-01
Propene	17.59%	42.08	64.32	1.53E+00	2.69E-01
i-butan	8.55%	85.12	96.65	1.14E+00	9.71E-02
n-butane	23.74%	85.12	98.35	1.16E+00	2.74E-01
i-butene	9.61%	56.1	88.09	1.57E+00	1.51E-01
1-butene	5.05%	56.1	118	2.10E+00	1.06E-01
Trans-butene 2	6..56%	56.1	87.67	1.56E+00	1.03E-01
Cis-2-butene	4.45%	56.1	80.15	1.43E+00	3.36E-02
n-pentane	0.28%	72.15	119.8	1.66E+00	4.65E-03
1-pentane	0.20%	70.13	108.2	1.54E+00	3.09E-03
H_2S	0.13%	34.08	34.19	1.00E+00	1.30E-03
H_2	0.07%	2.016	28.78	1.43E+01	9.99E-03
H_2O	0.06%	18.016	33.58	1.86E+00	1.12E-03
Total					1.49E+00

3.4.1 Energy Balance of absorber:

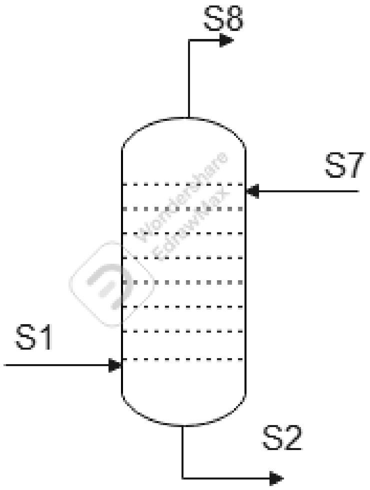


Figure (5.3.2) absorber

$Q_{1=mcp\Delta t}$

Sour gas

$M = 30000 kg/h$

$T = 44℃$

Cp of sour LPG= 1.49E+00

$30000 \times 1.49E + 00(44 - 25) = 8.49E + 05$ kj/kr

Sweet gas

M=29100 $T = 40$ ℃

Q_8 sweet gas $= 29100 \times 1.49E + 00(40 - 25) = 6.51E + 005$ kj/hr

Cp of lean amine

$M = 17750$ $T = 43℃$

Cp of MDEA =3.6 kj/kg. ℃

Cp of $\mathbf{H_2O}$ = 4.19kj/kg. ℃

$\text{Cp of lean solution} = \text{cp of MDEA} \times \text{mol\%} + \text{cp of} H_2O \times \text{mol\%}$

$$= (3.6 \times 0.11) + (4.19 \times 0.89) = 4.1251\ \text{kj/kg.k}$$

$Q_7\ \text{lean amine} = 17750 \times 4.1248\ (43 - 25) = 1.23E + 06\ \text{kj/h}$

Table (10.3.7) over all energy of absorber

Stream	In	Out
$\mathbf{Q_1}$ sour LPG	8.49E+05	
$\mathbf{Q_2}$ rich amine		1.52E+06
$\mathbf{Q_7}$ lean amine	1.32E+06	
$\mathbf{Q_8}$ Sweet gas		6.51E+05
Total	2.17E+06	2.17E+06

3.4.2 Energy Balance of Heat Exchanger (amine - amine):

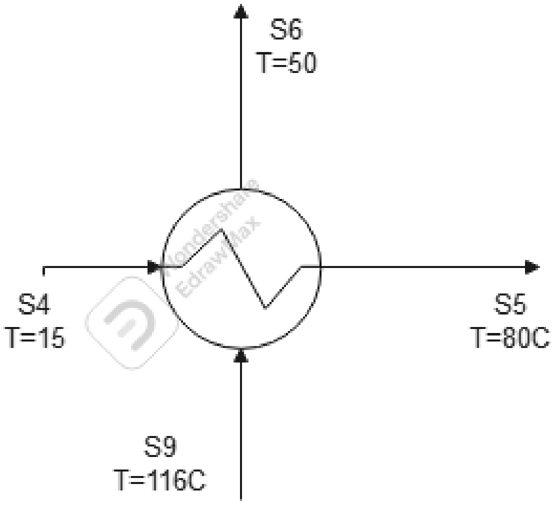


Figure (6.3.5) Heat Exchanger

$\text{Cp of rich solution} = \text{cp of } H_2S * \text{mol\%} + \text{cp of lean} * \text{mol\%}$

M.wt of lean solution $= 29.13\text{kg/mol}$

Mole of lean amine $= 609.39\ \text{kmol/hr}$

mole fraction of $H_2S =$ mole of H_2S/mole of $H_2S +$ mole of lean

$$= 1.144/(1.144 + 696.16) = 0.0019$$

Mole of fraction of lean $=1 - 1.0019 = 0.998$

cp of $H_2S = 0.236 + 974t * 10^{-5}$

Cp of H_2S at $25C^{\circ} = 0.240\text{kj/kg. k}$

Cp of rich solution $= 4.118\text{kj/kg. k}$

S_9 Lean amine $= 17750\text{kg/hr}$

S_5 Rich solution $= 17810.8\ \text{kg/hr}$

$Q_4 = Q_2 = 1.52E + 06\text{kj/hr}$

Heat of lean solution in stream line 9$=$ mcpΔt

$17750 * 4.1251(116 - 50) = 4830000\ \text{kj/hr}$

Heat of rich solution in stream 5$=$ mcpΔt

$17810 * 4.118(80 - 15) = 4767202.7\ \text{kj/hr}$

Table (11.3.8) over all energy Balance of amine-amine Heat Exchanger

Stream	In	Out
$\mathbf{Q_4}$ Rich amine	1.52E+06	
$\mathbf{Q_5}$ Rich amine		4.77E+06
$\mathbf{Q_6}$ lean amine		1.58E+0.6
$\mathbf{Q_9}$ lean amine	4.83E+0.6	
Total	6.35E+06	6.35E+06

3.4.3 Energy Balance of Heat Exchanger (Amine - water):

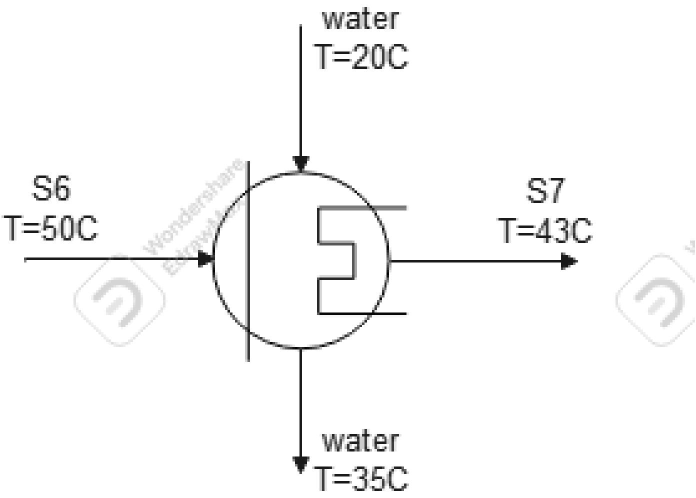


Figure (7.3.6) Cooler

Inlet temperature of water $= 20℃$

Outlet temperature of water $= 35℃$

Heat gain by water = heat loss from lean

Heat loss from lean

$Q_7 = \text{mcp}\Delta\text{t}$

$Q_7 = 17750 * 4.1251(35 - 20)$ =1.10E+06 kj/hr

Table (12.3.9) over all energy Balance of amine-water Heat Exchanger

Stream	In	Out
$\mathbf{Q_7}$ lean amine	1.10E+06	
Water		1.10E+06
Total	1.10E+06	1.10E+06

3.4.4 Energy Balance of stripper

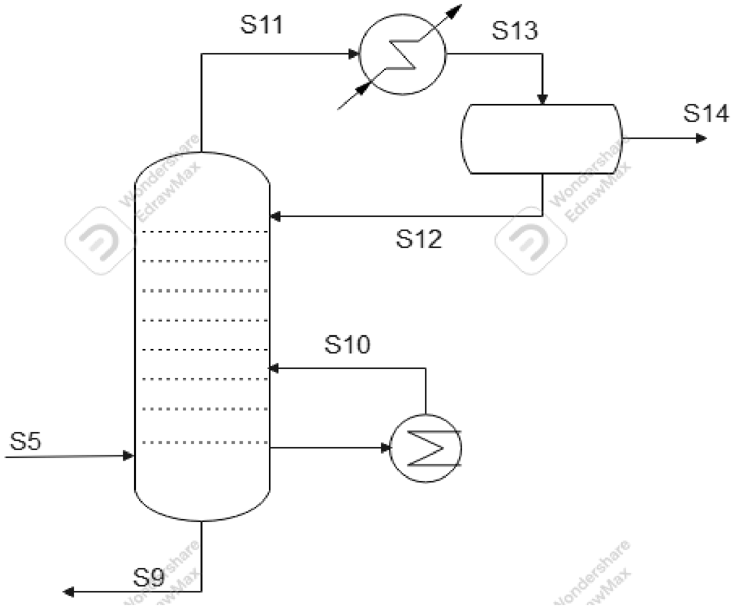


Figure (8.3.7) Stripper

Heat of Rich solution of stream5 $= 4.77E + 06kj/hr$

Heat of reflux in Stream 10 = $Q_{10} = mcp\Delta t$

$M = 3.158kg/hr$

$T = 30℃$

cp of $H_2O = 4.18$ kj/hg. ℃

$Q_{12} = 3.158 * 4.18(30 - 25) = 66$ kj/hr

Heat of acid gas = cp of $H_2S *$ mol% + cp of$H_2O *$ mol%

Cp of $H_2S = 0.24$ kj/kg. ℃

Kmol of H_2O =kg of reflex/M.wt of $H_2O = 3.158/18 = 0.1754kmol/hr$

Kmol of stream 11= kmol of H_2S +kmol of H_2O

$$1.144 + 0.175 = 1.3194\ \text{kmol/hr}$$

Mole fraction of $H_2S = 1.144/1.3194\ = 0.8670$

Mole fraction of $H_2O = 1 - 0.8670 = 0.133$

Cp of acid gas $= (0.24 * 0.8670) + (4.18 * 0.133) = 0.76402\text{kj/kg.℃}$

$Q_{11} = \text{mcp}\Delta\text{t}$

$\text{M} = 63.98\text{kg/hr}$

$\text{T} = 50℃$

$Q_{11} = 63.908 * 0.76402\ (50 - 25) = 1220.67\ \text{kj/hr}$

Over all energy balance of Stripper

$Q_5 + Q_{12} + Q_{10} = Q_9 + Q_{11}$

$Q_{10} = 66500\ \text{kj/hr}$

Table (13.3.10) over all energy of Stripper

Stream	In	Out
$\mathbf{Q_5}$ rich amine	4.77E+06	
$\mathbf{Q_9}$ lean amine		4.83E+06
$\mathbf{Q_{10}}$ reboiler	6.65E+04	
$\mathbf{Q_{11}}$acid gas		1.22E+03
$\mathbf{Q_{12}}$ reflex	6.60E+01	
Total	4.83E+06	4.83E+06

3.4.5 Energy balance of Condenser:

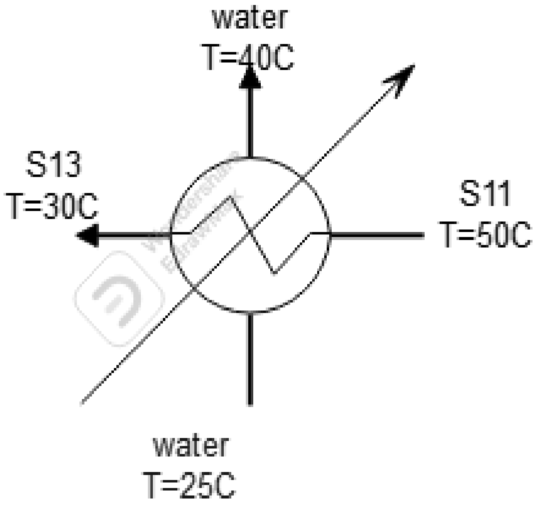


Figure (9.3.8) Condenser

Assume:

Inlet temperature of H_2O =25℃

Outlet temperature of $H_2O = 40^\circ C$

Heat of stream 11 (acid gas $1220\ kj/hr$

Heat of stream 13 = $Q_{11} = mcp\Delta t + \lambda * m$

T average $(50 + 30)/2 = 40^\circ C$

From steam table λat $40^\circ C = 167.5\ kj/kg$

Cp of water vapor $= 1.87 kj/kg.{}^\circ C$

S_{11}(Acid gas) $= 63.908 kg/hr$

S_{12} (Reflex) $= 3.158 kg/hr$

Q_{13} =$63.908 * 1.87(30 - 25) + 167.5 * 3.158 = 1130\ kj/hr$

Heat gain by water =$Q_{11} - Q_{13} = 1220 - 1130 = 94\ kj/hr$

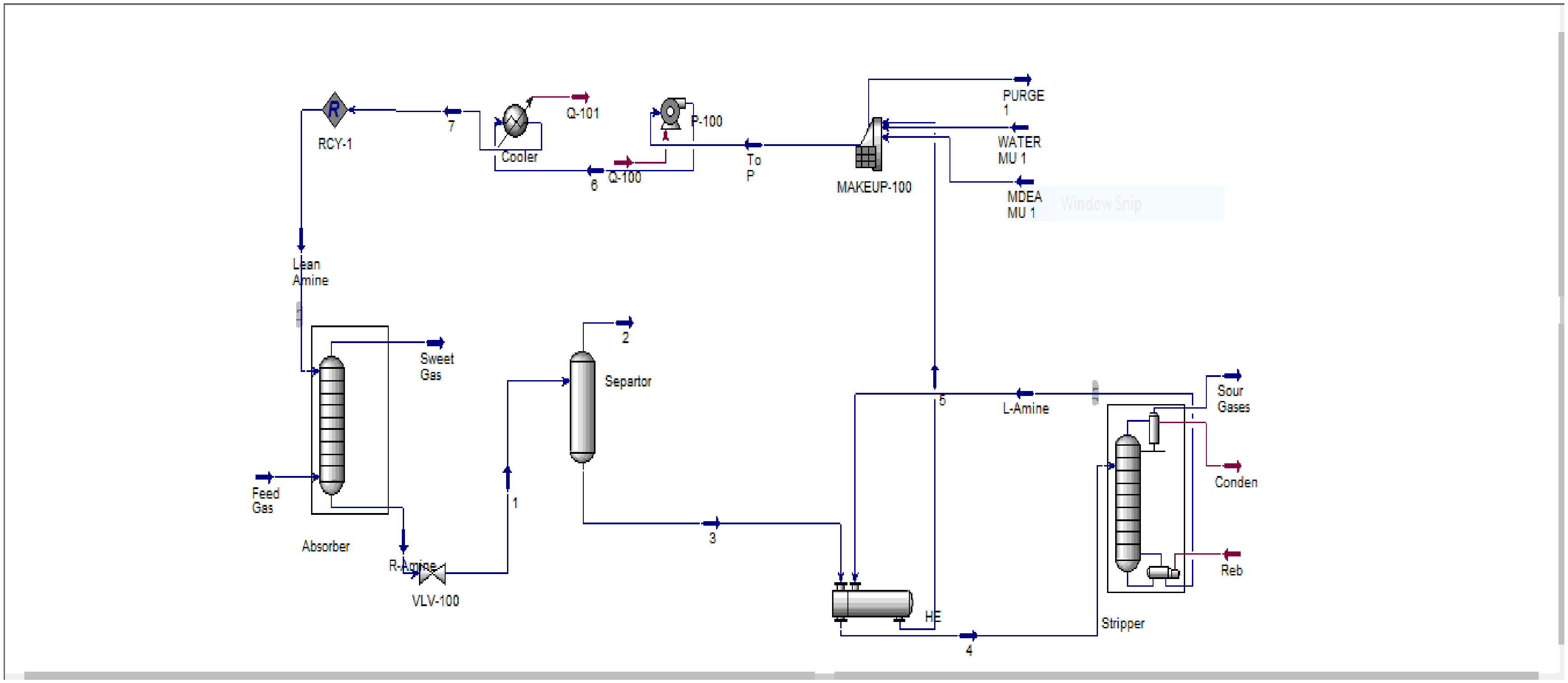
Table (14.3.11) over all energy of Condenser

Stream	In	Out
$\mathbf{Q_{11}}$ acid gas	1.22E+03	
$\mathbf{Q_{13}}$ acid gas		1.13E+03
Water		9.40E+01
Total	1.22E+03	1.22E+03

3.5 Hysys process simulator:

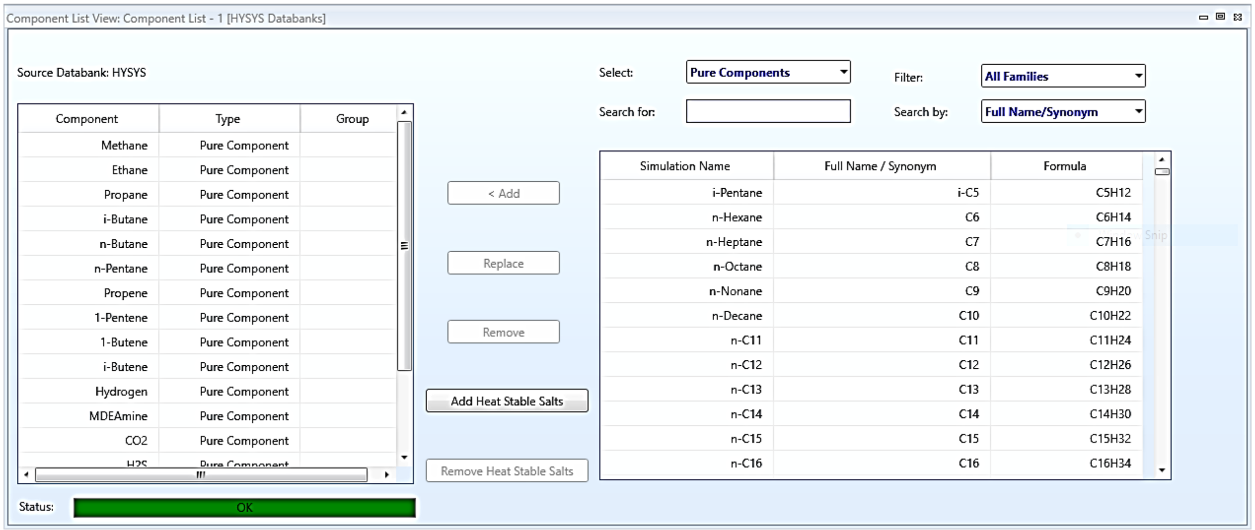
3.5.1 Introduction

Hysys is a process simulation environment designed to serve many processing industries especially oil and gas refining, rigorous steady state and dynamic models for plant design, performance monitoring, troubleshooting, operational improvement business planning and asset management can be created using HYSYS. The built-in property packages in HYSYS provide accurate thermodynamic, physical and transport property predictions for hydrocarbon, non-hydrocarbon, petrochemical and chemical fluids. .


RCY-1
7
Cooler
Q-101
P-100
6
Q-100
To
P
MAKEUP-100
PURGE
1
WATER
MU 1
MDEA
MU 1
Lean
Amine
Sweet
Gas
2
Separtor
Feed
Gas
Absorber
1
R-Amine
VLV-100
3
5
L-Amine
Sour
Gases
Conden
Reb
HE
4
Stripper

3.5.2 Simulation steps

First of all we have select the component



Source Databank: HYSYS

Select: Pure Components

Filter: All Families

Search for:

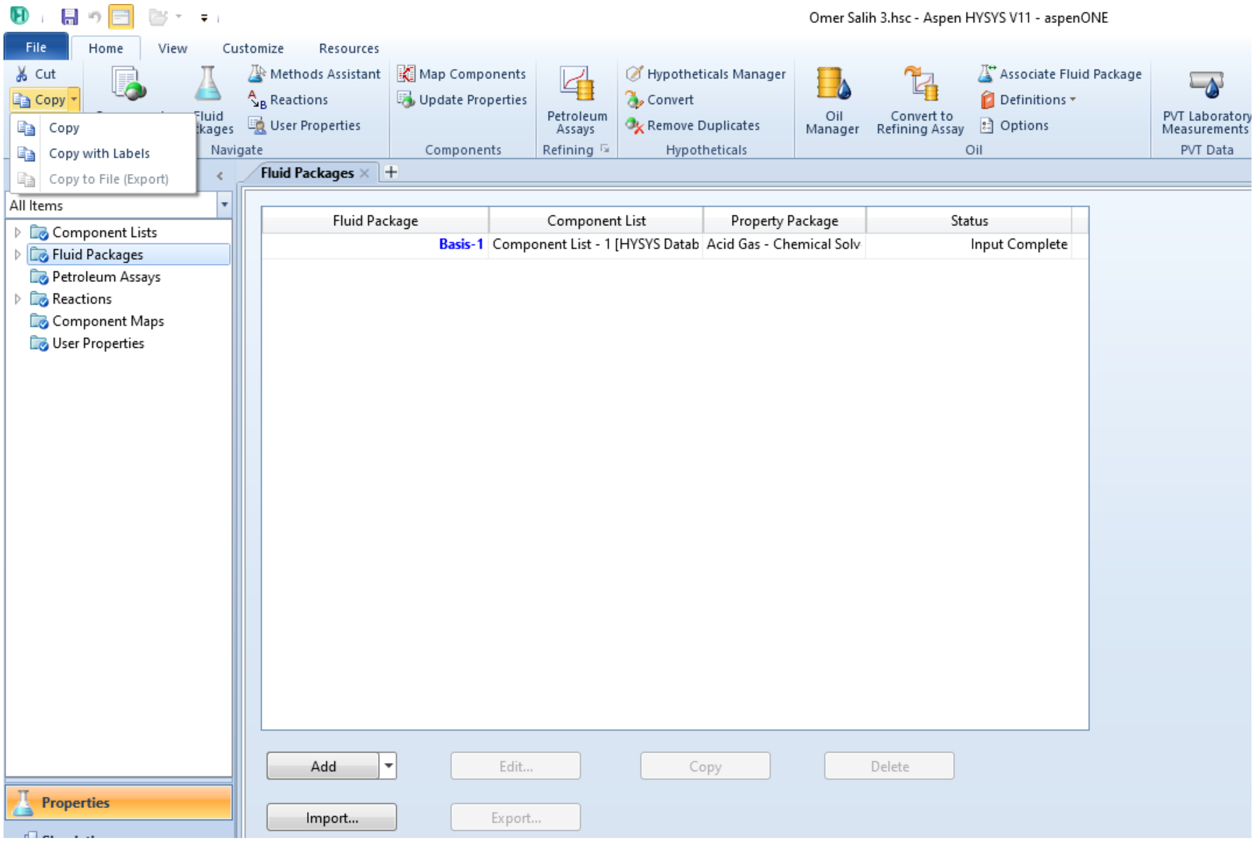
Search by: Full Name/Synonym

Component	Type	Group
Methane	Pure Component	
Ethane	Pure Component	
Propane	Pure Component	
i-Butane	Pure Component	
n-Butane	Pure Component	
n-Pentane	Pure Component	
Propene	Pure Component	
1-Pentene	Pure Component	
1-Butene	Pure Component	
i-Butene	Pure Component	
Hydrogen	Pure Component	
MDEAmine	Pure Component	
CO2	Pure Component	
H2S	Pure Component	

Simulation Name	Full Name / Synonym	Formula
i-Pentane	i-C5	C5H12
n-Hexane	C6	C6H14
n-Heptane	C7	C7H16
n-Octane	C8	C8H18
n-Nonane	C9	C9H20
n-Decane	C10	C10H22
n-C11	C11	C11H24
n-C12	C12	C12H26
n-C13	C13	C13H28
n-C14	C14	C14H30
n-C15	C15	C15H32
n-C16	C16	C16H34

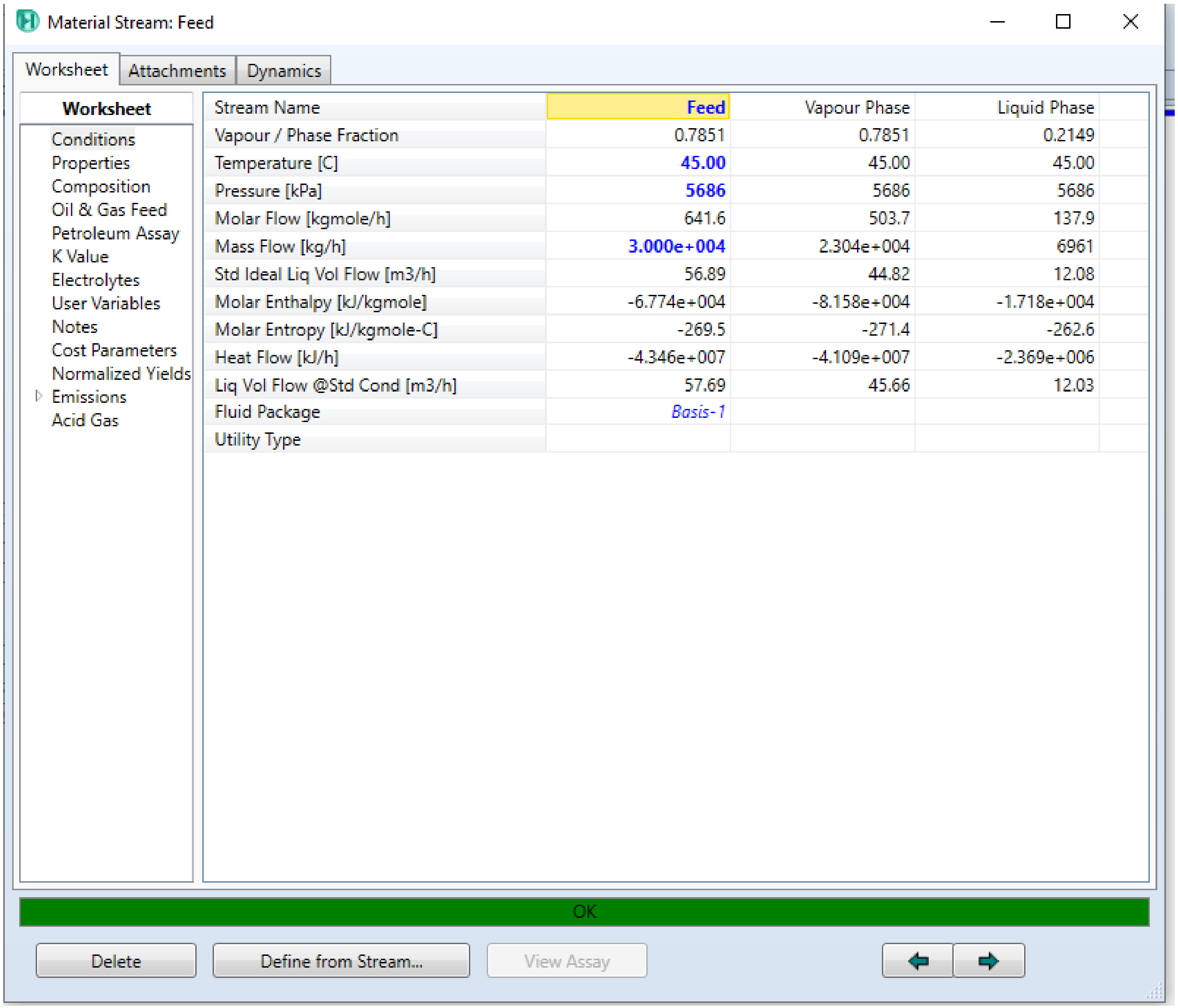
Status: OK

Then selecting the fluid package

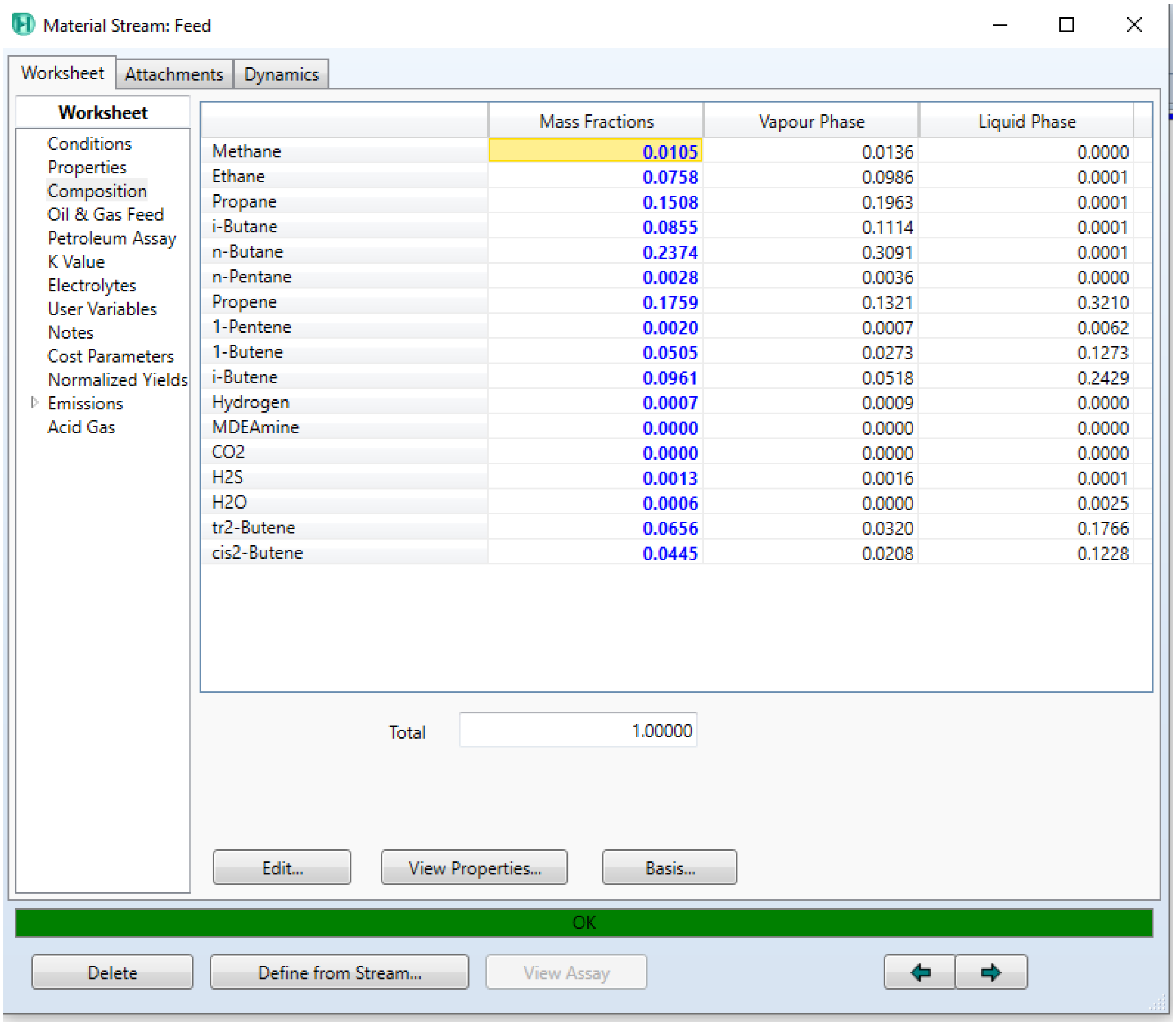


Fluid Package	Component List	Property Package	Status
Basis-1	Component List - 1 [HYSYS Datab	Acid Gas - Chemical Solv	Input Complete

Adding LPG stream composition and condition



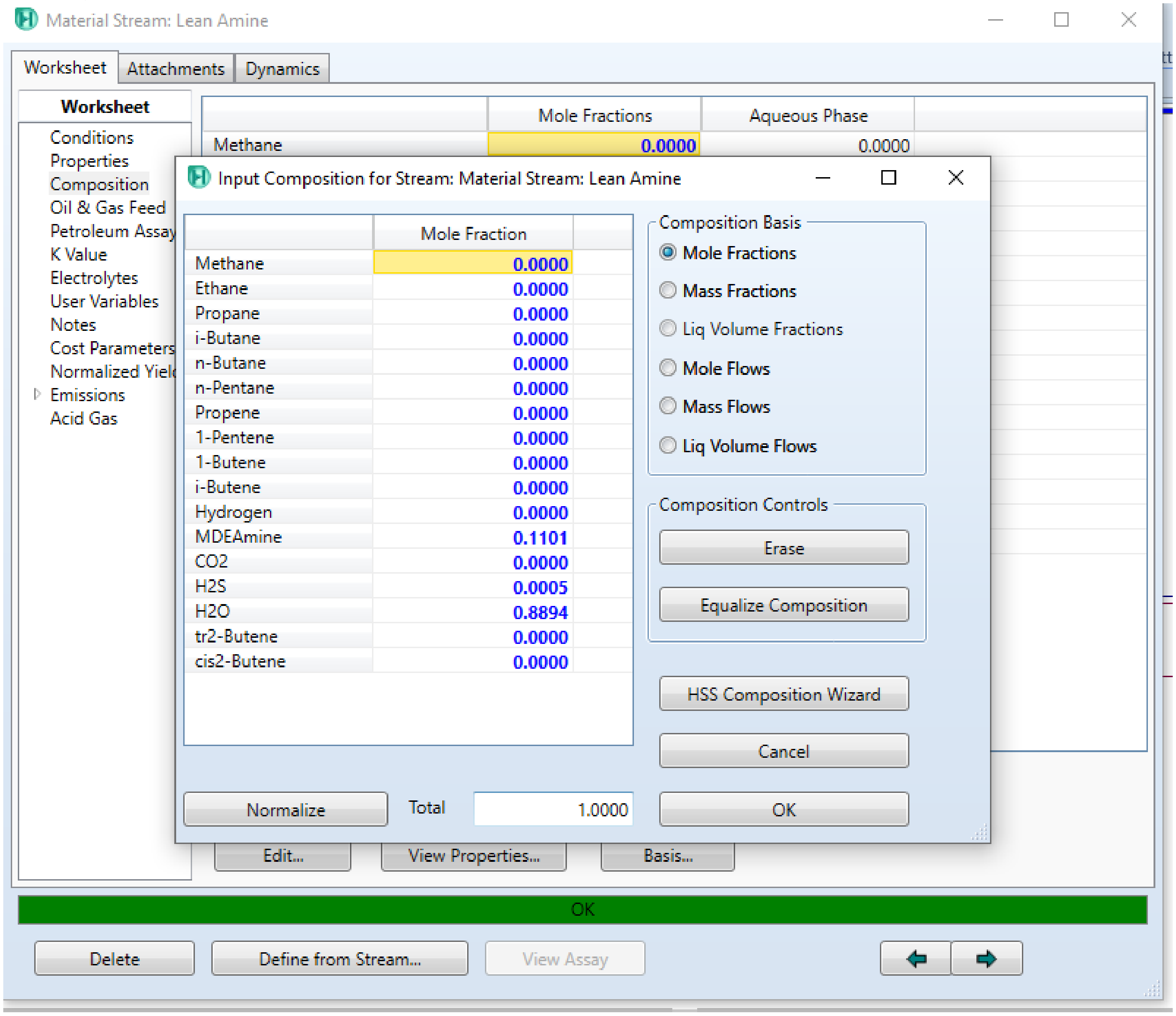
Stream Name	Feed	Vapour Phase	Liquid Phase
Vapour / Phase Fraction	0.7851	0.7851	0.2149
Temperature [C]	45.00	45.00	45.00
Pressure [kPa]	5686	5686	5686
Molar Flow [kgmole/h]	641.6	503.7	137.9
Mass Flow [kg/h]	3.000e+004	2.304e+004	6961
Std Ideal Liq Vol Flow [m3/h]	56.89	44.82	12.08
Molar Enthalpy [kJ/kgmole]	-6.774e+004	-8.158e+004	-1.718e+004
Molar Entropy [kJ/kgmole-C]	-269.5	-271.4	-262.6
Heat Flow [kJ/h]	-4.346e+007	-4.109e+007	-2.369e+006
Liq Vol Flow @Std Cond [m3/h]	57.69	45.66	12.03
Fluid Package	Basis-1		
Utility Type			



	Mass Fractions	Vapour Phase	Liquid Phase
Methane	0.0105	0.0136	0.0000
Ethane	0.0758	0.0986	0.0001
Propane	0.1508	0.1963	0.0001
i-Butane	0.0855	0.1114	0.0001
n-Butane	0.2374	0.3091	0.0001
n-Pentane	0.0028	0.0036	0.0000
Propene	0.1759	0.1321	0.3210
1-Pentene	0.0020	0.0007	0.0062
1-Butene	0.0505	0.0273	0.1273
i-Butene	0.0961	0.0518	0.2429
Hydrogen	0.0007	0.0009	0.0000
MDEAmine	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000
H2S	0.0013	0.0016	0.0001
H2O	0.0006	0.0000	0.0025
tr2-Butene	0.0656	0.0320	0.1766
cis2-Butene	0.0445	0.0208	0.1228

Total 1.00000

Adding amine composition and condition

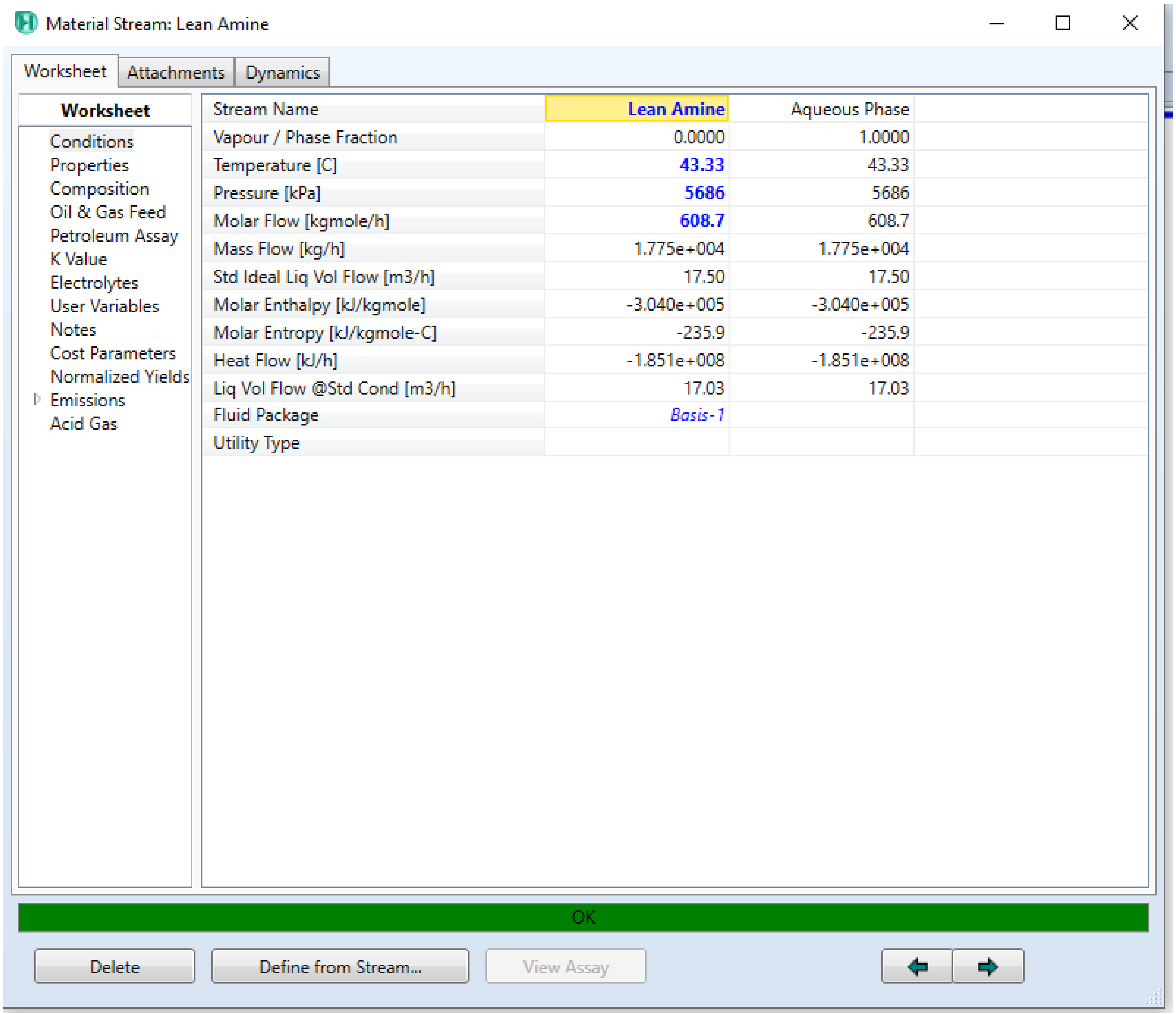


	Mole Fractions	Aqueous Phase
Methane	0.0000	0.0000

	Mole Fraction
Methane	0.0000
Ethane	0.0000
Propane	0.0000
i-Butane	0.0000
n-Butane	0.0000
n-Pentane	0.0000
Propene	0.0000
1-Pentene	0.0000
1-Butene	0.0000
i-Butene	0.0000
Hydrogen	0.0000
MDEAmine	0.1101
CO2	0.0000
H2S	0.0005
H2O	0.8894
tr2-Butene	0.0000
cis2-Butene	0.0000

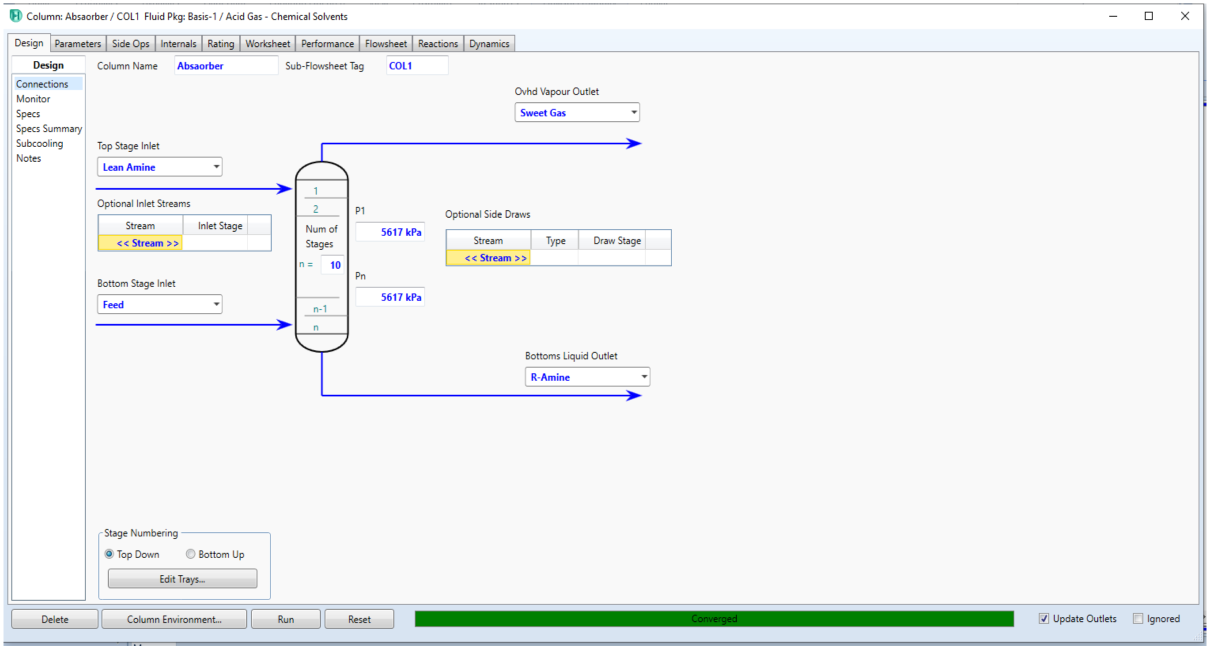
Composition Basis:
- ● Mole Fractions
- ○ Mass Fractions
- ○ Liq Volume Fractions
- ○ Mole Flows
- ○ Mass Flows
- ○ Liq Volume Flows

Total 1.0000



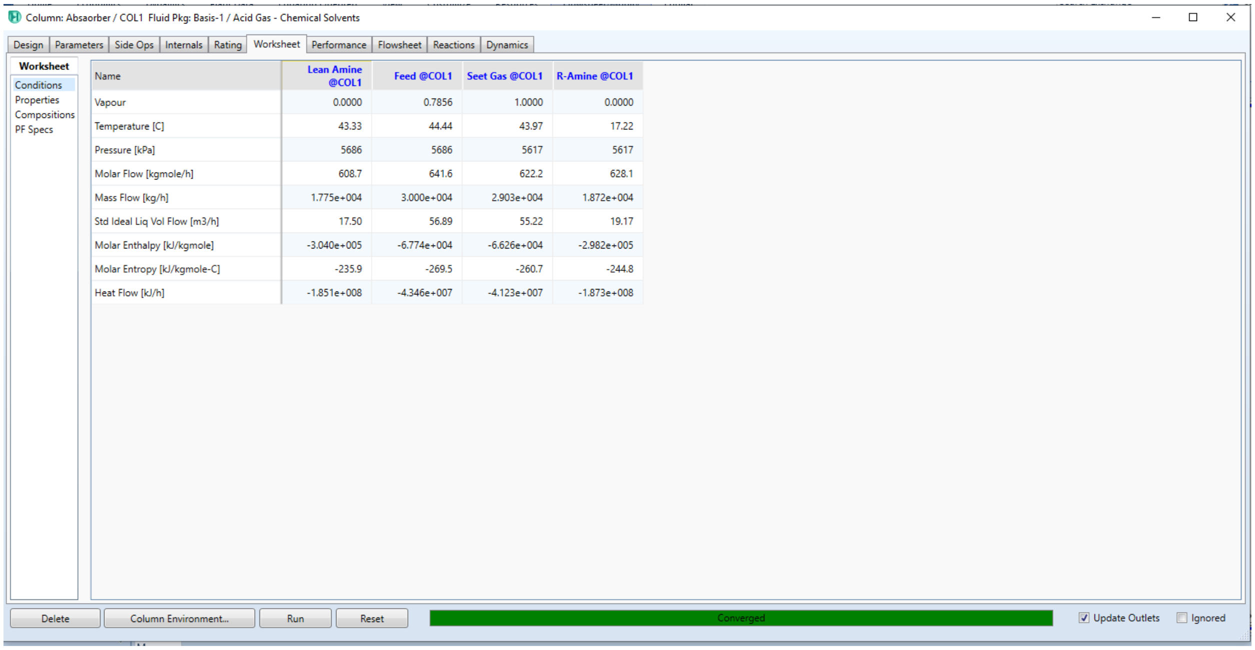
Stream Name	Lean Amine	Aqueous Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	43.33	43.33
Pressure [kPa]	5686	5686
Molar Flow [kgmole/h]	608.7	608.7
Mass Flow [kg/h]	1.775e+004	1.775e+004
Std Ideal Liq Vol Flow [m3/h]	17.50	17.50
Molar Enthalpy [kJ/kgmole]	-3.040e+005	-3.040e+005
Molar Entropy [kJ/kgmole-C]	-235.9	-235.9
Heat Flow [kJ/h]	-1.851e+008	-1.851e+008
Liq Vol Flow @Std Cond [m3/h]	17.03	17.03
Fluid Package	Basis-1	
Utility Type		

Adding the absorber



Column: Absaorber / COL1 Fluid Pkg: Basis-1 / Acid Gas - Chemical Solvents

Column Name: Absaorber
Sub-Flowsheet Tag: COL1
Ovhd Vapour Outlet: Sweet Gas
Top Stage Inlet: Lean Amine
Bottom Stage Inlet: Feed
Bottoms Liquid Outlet: R-Amine
Num of Stages n = 10
P1: 5617 kPa
Pn: 5617 kPa
Stage Numbering: ● Top Down ○ Bottom Up
Converged
☑ Update Outlets ☐ Ignored

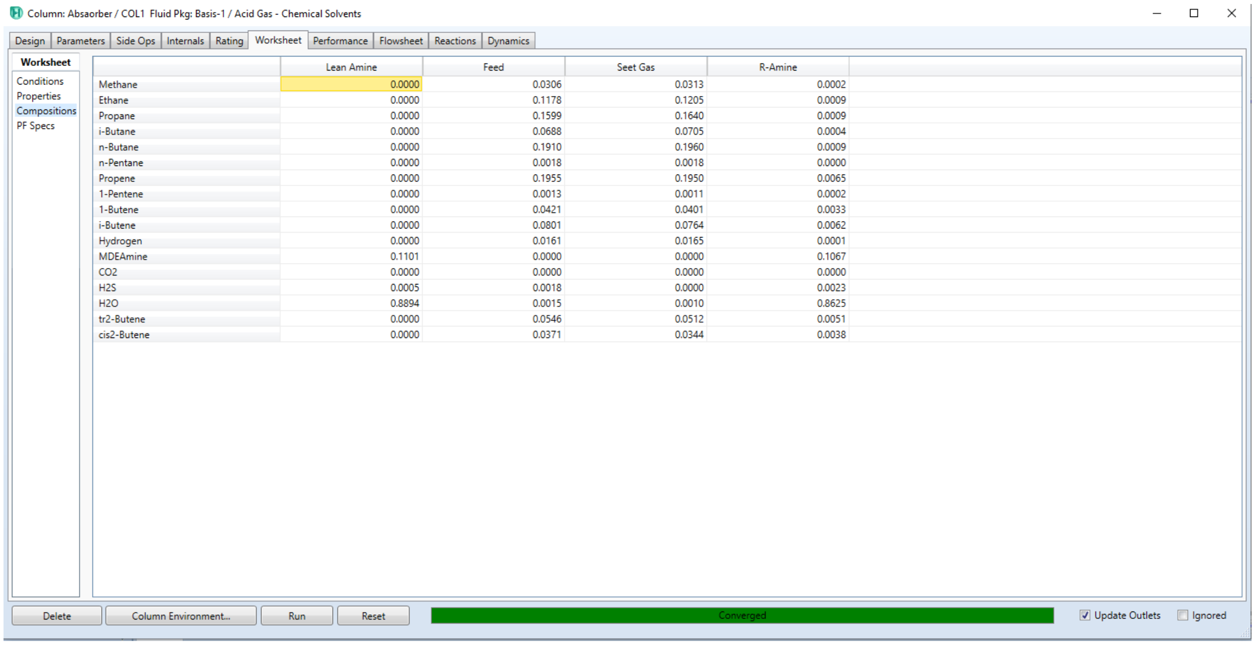


Column: Absaorber / COL1 Fluid Pkg: Basis-1 / Acid Gas - Chemical Solvents

Name	Lean Amine @COL1	Feed @COL1	Seet Gas @COL1	R-Amine @COL1
Vapour	0.0000	0.7856	1.0000	0.0000
Temperature [C]	43.33	44.44	43.97	17.22
Pressure [kPa]	5686	5686	5617	5617
Molar Flow [kgmole/h]	608.7	641.6	622.2	628.1
Mass Flow [kg/h]	1.775e+004	3.000e+004	2.903e+004	1.872e+004
Std Ideal Liq Vol Flow [m3/h]	17.50	56.89	55.22	19.17
Molar Enthalpy [kJ/kgmole]	-3.040e+005	-6.774e+004	-6.626e+004	-2.982e+005
Molar Entropy [kJ/kgmole-C]	-235.9	-269.5	-260.7	-244.8
Heat Flow [kJ/h]	-1.851e+008	-4.346e+007	-4.123e+007	-1.873e+008

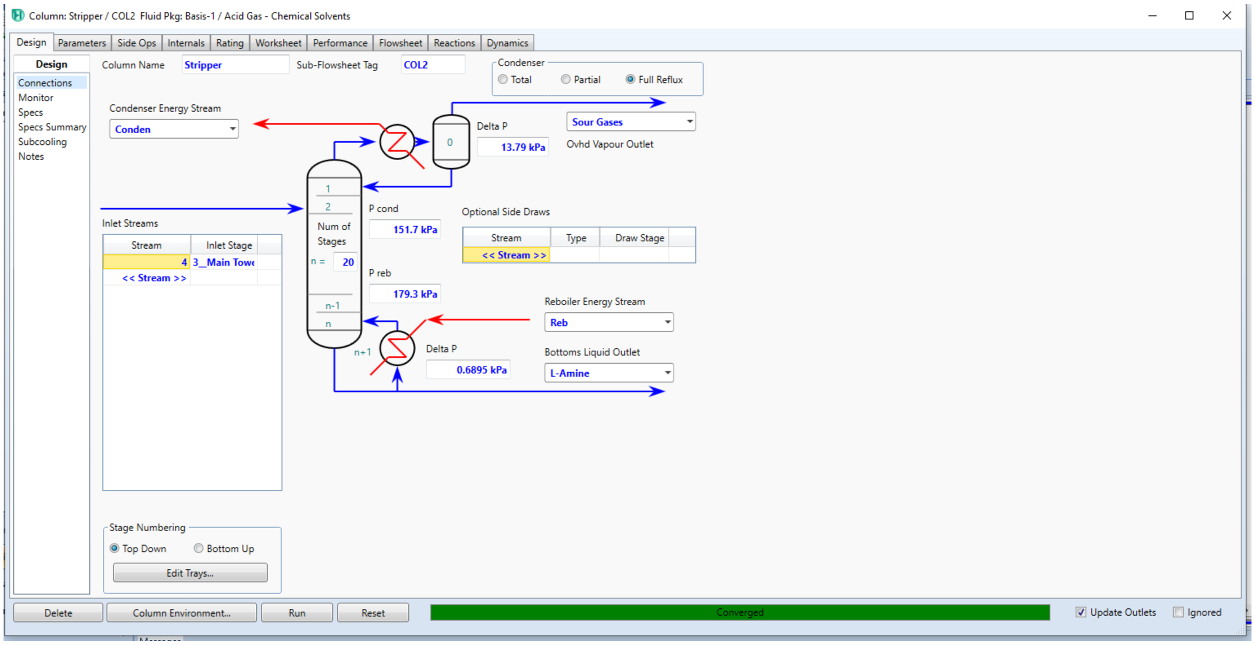
Converged
☑ Update Outlets ☐ Ignored

Absorber work sheet composition



	Lean Amine	Feed	Seet Gas	R-Amine
Methane	0.0000	0.0306	0.0313	0.0002
Ethane	0.0000	0.1178	0.1205	0.0009
Propane	0.0000	0.1599	0.1640	0.0009
i-Butane	0.0000	0.0688	0.0705	0.0004
n-Butane	0.0000	0.1910	0.1960	0.0009
n-Pentane	0.0000	0.0018	0.0018	0.0000
Propene	0.0000	0.1955	0.1950	0.0065
1-Pentene	0.0000	0.0013	0.0011	0.0002
1-Butene	0.0000	0.0421	0.0401	0.0033
i-Butene	0.0000	0.0801	0.0764	0.0062
Hydrogen	0.0000	0.0161	0.0165	0.0001
MDEAmine	0.1101	0.0000	0.0000	0.1067
CO2	0.0000	0.0000	0.0000	0.0000
H2S	0.0005	0.0018	0.0000	0.0023
H2O	0.8894	0.0015	0.0010	0.8625
tr2-Butene	0.0000	0.0546	0.0512	0.0051
cis2-Butene	0.0000	0.0371	0.0344	0.0038

Adding Stripper



Column: Stripper / COL2 Fluid Pkg: Basis-1 / Acid Gas - Chemical Solvents

Column Name: Stripper

Sub-Flowsheet Tag: COL2

Condenser: ○ Total ○ Partial ● Full Reflux

Condenser Energy Stream: Conden

Delta P: 13.79 kPa

Ovhd Vapour Outlet: Sour Gases

Inlet Streams

Stream	Inlet Stage
4	3__Main Towe
<< Stream >>	

Num of Stages n = 20

P cond: 151.7 kPa

P reb: 179.3 kPa

Optional Side Draws

Stream	Type	Draw Stage
<< Stream >>		

Reboiler Energy Stream: Reb

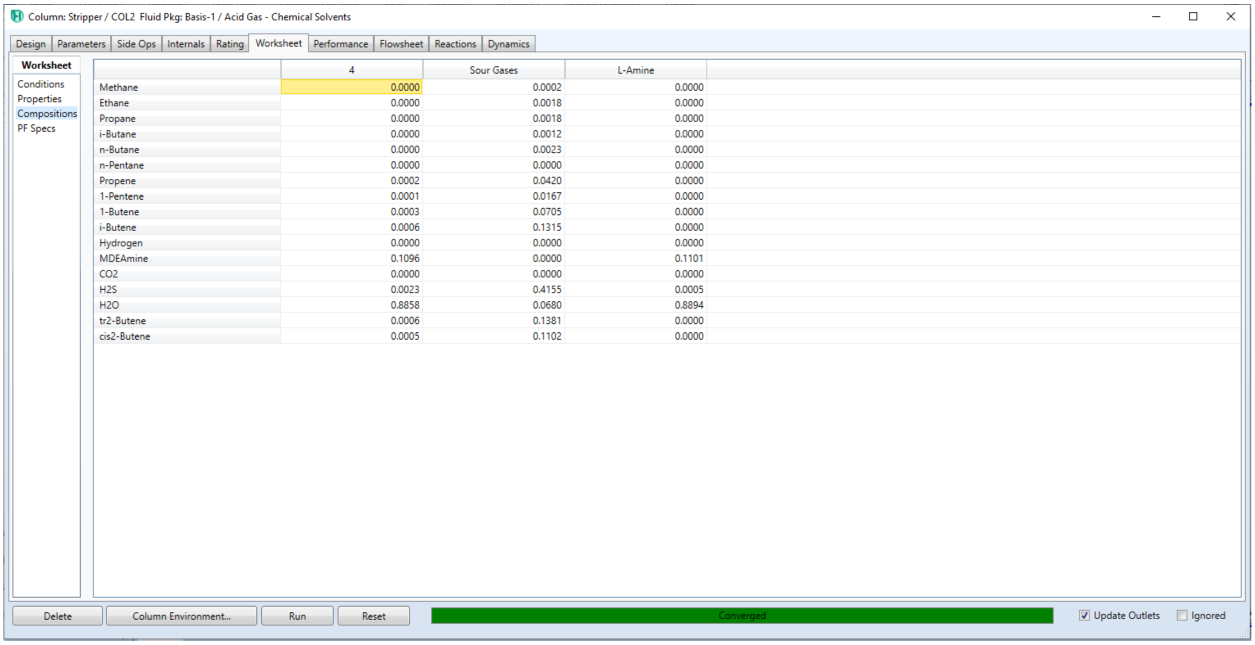
Delta P: 0.6895 kPa

Bottoms Liquid Outlet: L-Amine

Stage Numbering: ● Top Down ○ Bottom Up

Converged

☑ Update Outlets ☐ Ignored



Column: Stripper / COL2 Fluid Pkg: Basis-1 / Acid Gas - Chemical Solvents

	4	Sour Gases	L-Amine
Methane	0.0000	0.0002	0.0000
Ethane	0.0000	0.0018	0.0000
Propane	0.0000	0.0018	0.0000
i-Butane	0.0000	0.0012	0.0000
n-Butane	0.0000	0.0023	0.0000
n-Pentane	0.0000	0.0000	0.0000
Propene	0.0002	0.0420	0.0000
1-Pentene	0.0001	0.0167	0.0000
1-Butene	0.0003	0.0705	0.0000
i-Butene	0.0006	0.1315	0.0000
Hydrogen	0.0000	0.0000	0.0000
MDEAmine	0.1096	0.0000	0.1101
CO2	0.0000	0.0000	0.0000
H2S	0.0023	0.4155	0.0005
H2O	0.8858	0.0680	0.8894
tr2-Butene	0.0006	0.1381	0.0000
cis2-Butene	0.0005	0.1102	0.0000

Converged

☑ Update Outlets ☐ Ignored

Chapter 4

Results and discussion

Chapter 4

Results and discussion

4.1 Material balance results and discussion of absorber

Table (15.4.1) Material balance results and discussion of absorber

Material flow in Stream	**flow by hand calculation kg/hr**	**Flow by hysys simulation**	**Error %=** $(\mathbf{Hand} - \mathbf{hysys}) * \mathbf{100/hand}$
Stream 8 **(sweet gas)**	29100	29030	0.24
Stream 2 **(rich amine)**	18650	18750	0.38

4.2 Material balance results and discussion of separator

Table (16.4.2) Material balance results and discussion of separator

Material flow in stream	**Flow by hand Calculation**	**Flow by Hysys Simulation**	**Error %=** $(\mathbf{Hand} - \mathbf{hysys}) * \mathbf{100/hand}$
Stream 3 **(overhead gas)**	839.25	847.2	0.95
Stream 4 **(rich amine)**	17810.75	17870	0.33

4.3 Material balance results and discussion of stripper

Table (17.4.3) Material balance results and discussion of stripper

Material flow in Stream	**Flow by hand calculation**	**Flow by Hysys Simulation**	**Error %=** $(\mathbf{Hand} - \mathbf{hysys}) * \mathbf{100/hand}$
Stream 14 (Acid gas)	60.75	71.47	17.6
Stream 9 (Lean amine)	17750	17750	0.0

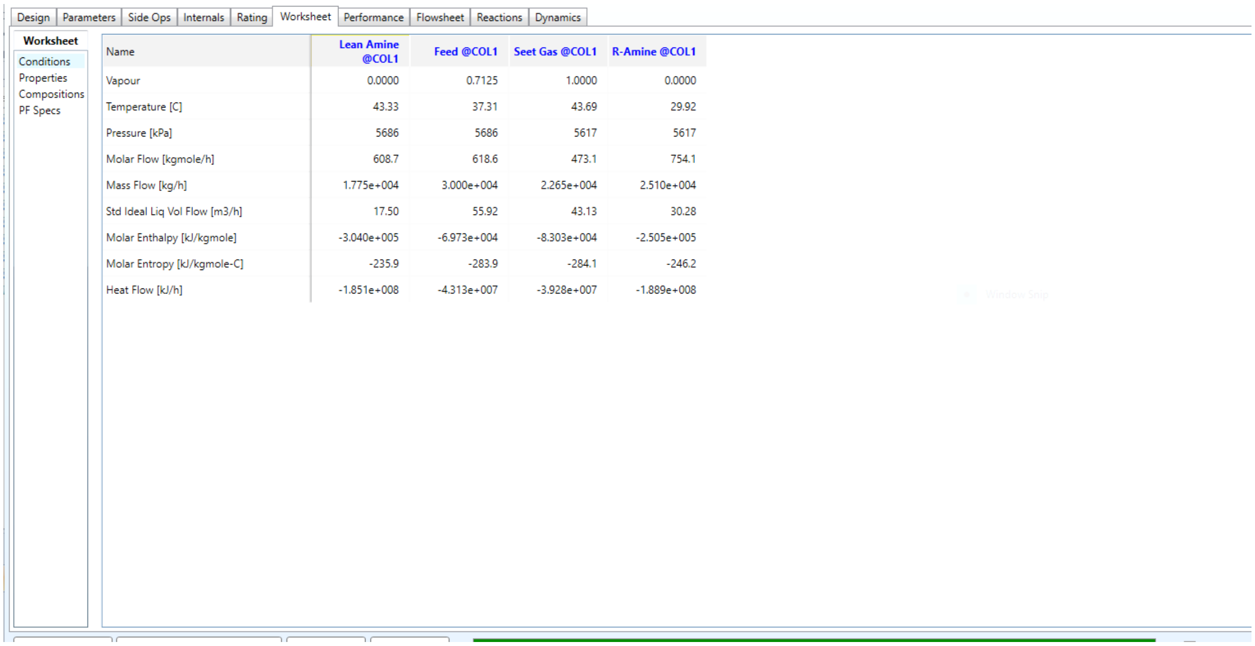
4.4 Effect of feed LPG temperature

Different feed temperature gave same percentage of removed H_2S, but different percentage of sweet LPG recovered

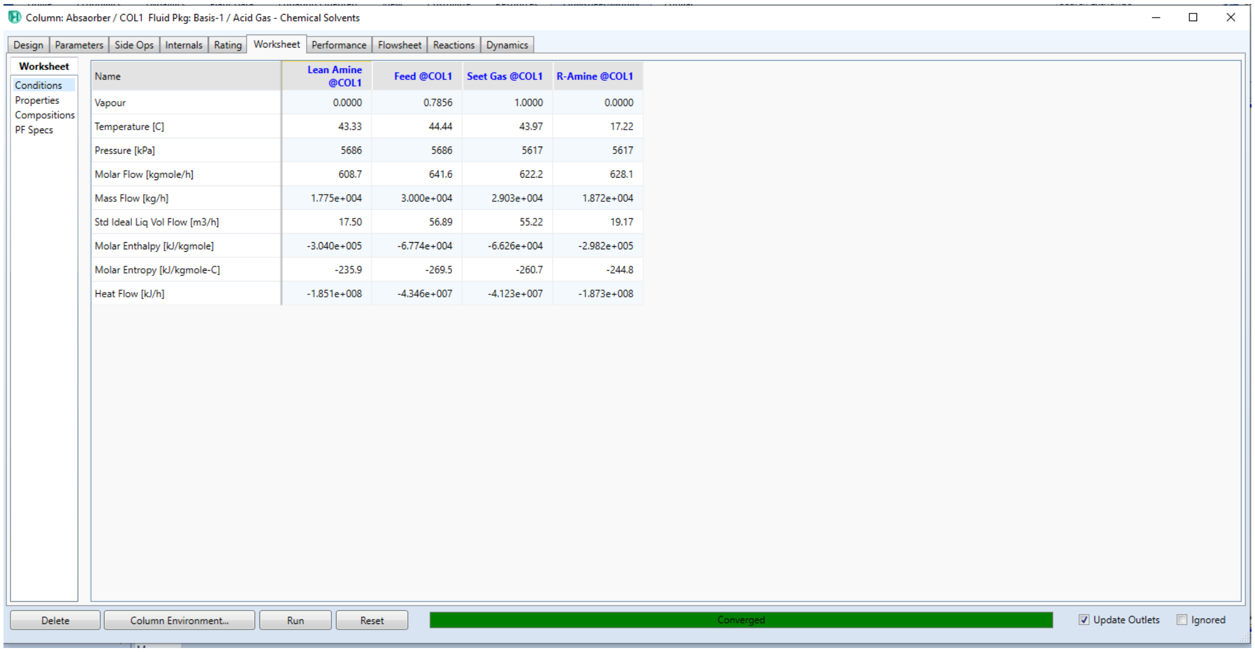
At 37 ℃ we recovered 76% from the feed as sweet LPG

At 45℃ we recovered 96.7% from the as sweet LPG

Absorber work sheet at different feed LPG temperature



Name	Lean Amine @COL1	Feed @COL1	Seet Gas @COL1	R-Amine @COL1
Vapour	0.0000	0.7125	1.0000	0.0000
Temperature [C]	43.33	37.31	43.69	29.92
Pressure [kPa]	5686	5686	5617	5617
Molar Flow [kgmole/h]	608.7	618.6	473.1	754.1
Mass Flow [kg/h]	1.775e+004	3.000e+004	2.265e+004	2.510e+004
Std Ideal Liq Vol Flow [m3/h]	17.50	55.92	43.13	30.28
Molar Enthalpy [kJ/kgmole]	-3.040e+005	-6.973e+004	-8.303e+004	-2.505e+005
Molar Entropy [kJ/kgmole-C]	-235.9	-283.9	-284.1	-246.2
Heat Flow [kJ/h]	-1.851e+008	-4.313e+007	-3.928e+007	-1.889e+008



Name	Lean Amine @COL1	Feed @COL1	Seet Gas @COL1	R-Amine @COL1
Vapour	0.0000	0.7856	1.0000	0.0000
Temperature [C]	43.33	44.44	43.97	17.22
Pressure [kPa]	5686	5686	5617	5617
Molar Flow [kgmole/h]	608.7	641.6	622.2	628.1
Mass Flow [kg/h]	1.775e+004	3.000e+004	2.903e+004	1.872e+004
Std Ideal Liq Vol Flow [m3/h]	17.50	56.89	55.22	19.17
Molar Enthalpy [kJ/kgmole]	-3.040e+005	-6.774e+004	-6.626e+004	-2.982e+005
Molar Entropy [kJ/kgmole-C]	-235.9	-269.5	-260.7	-244.8
Heat Flow [kJ/h]	-1.851e+008	-4.346e+007	-4.123e+007	-1.873e+008

Chapter 5

Conclusion and Recommendations

Chapter 5

Conclusion and Recommendation

5.1 Conclusion

In this project use amine solvent at concentration 45% in water, the LPG treatment process using the software HYSYS, MDEA was the best result in the absorption processes H_2S from the LPG, The simulation result show that, by using of the 609(kg mole /h) MDEA with T=44C were the best result in the absorption processes H_2S (0.0000, mole fraction)

5.2 Recommendation

We recommend to study the process at various parameters to identify the optimum operation condition

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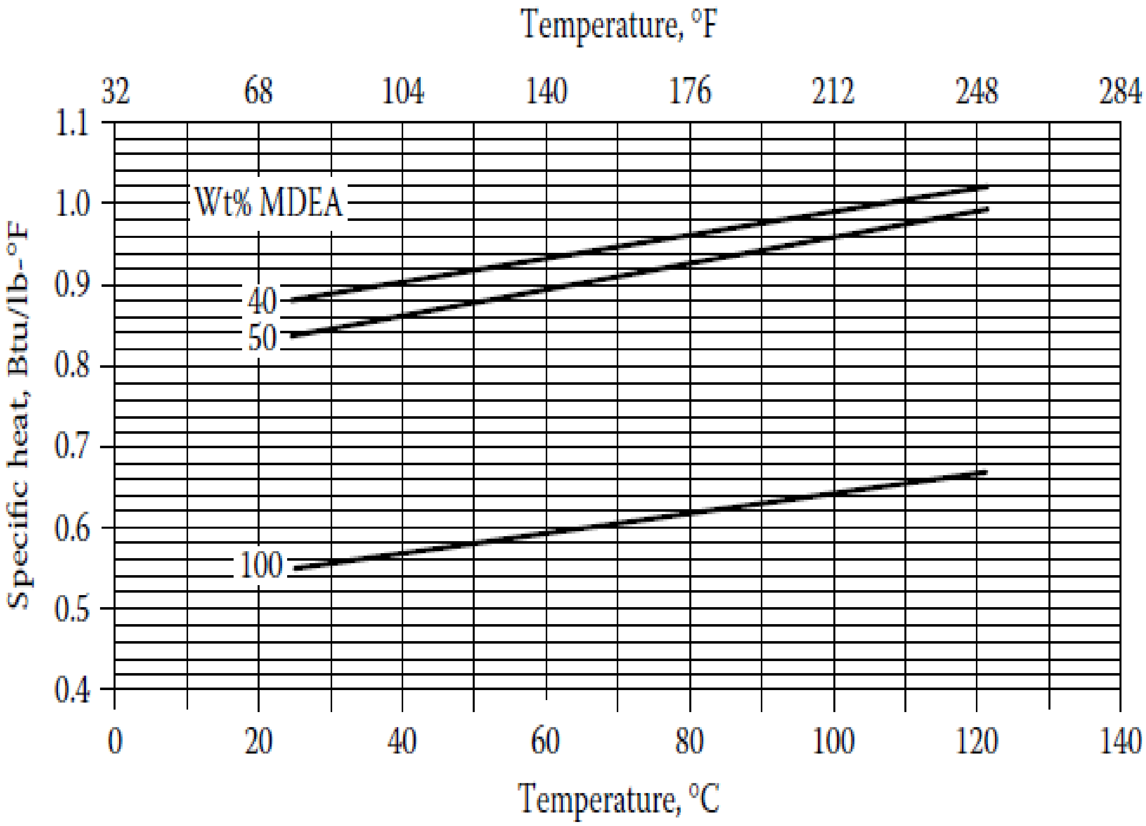
APPENDIX



Heat capacities of methyldiethanolamine (MDEA) – water mixtures as a function of composition and temperature. (Adapted through the courtesy of INEOS Oxide).

TABLE C-4 Heat Capacity of Gas

$C_p = A + BT + CT^2 + DT^3 + ET^4$						(C_p–joule/(mol K), T–K)			
No.	Formula	Substance	A	B	C	D	E	T_{min}	T_{max}
1	$C_2H_3C_{13}$	1,1,1-Trichloroethane	18.674	3.3443E–01	–3.4963E–04	1.8764E–07	–4.0744E–11	100	1500
2	$C_2H_3C_{13}$	1,1,2-Trichloroethane	28.881	2.4893E–01	–1.7639E–04	5.2632E–08	–3.5668E–12	200	1500
3	$C_2H_4C_{12}$	1,1-Dichloroethane	15.730	2.6124E–01	–2.1489E–04	9.5761E–08	–1.8004E–11	200	1500
4	$C_2H_4C_{12}$	1,2-Dichloroethane	37.275	1.4362E–01	1.0378E–05	–7.8305E–08	2.8872E–11	200	1500
5	C_4H_6	1,3-Butadiene	18.835	2.0473E–01	6.2485E–05	–1.7148E–07	6.0858E–11	100	1500
6	$C_4H_8O_2$	1,4-Dioxane	–46.223	5.7263E–01	–3.8800E–04	1.1392E–07	–9.0669E–12	298	1500
7	$C_4H_{10}O$	1-Butanol (*n*-Butanol)	8.157	4.1032E–01	–2.2645E–04	6.0372E–08	–6.2802E–12	200	2980
8	C_4H_8	1-Butene	24.915	2.0648E–01	5.9828E–05	–1.4166E–07	4.7053E–11	200	1500
9	$C_{10}H_{20}$	1-Decene	121.553	2.0974E–01	7.8760E–04	–8.6982E–07	2.6033E–10	150	1500
10	C_9H_{10}	1-Nonane (*n*-Nonane)	29.687	6.6821E–01	–9.6492E–05	–2.0014E–07	8.2200E–11	200	1500
11	C_8H_{16}	1-Octene	56.266	4.0665E–01	1.5805E–04	–3.2277E–07	1.0600E–10	200	1500
12	C_3H_8O	1-Propanol (*n*-Propanol)	31.507	2.3082E–01	–7.8983E–05	6.3696E–09	8.6908E–13	100	2980
13	C_2H_4O	Acetaldehyde	34.140	4.0020E–02	1.5634E–04	–1.6445E–07	4.7248E–11	100	1500
14	$C_2H_4O_2$	Acetic acid	34.850	3.7626E–02	2.8311E–04	–3.0767E–07	9.2646E–11	50	1500
15	$C_4H_6O_3$	Acetic anhydride	9.500	3.4425E–01	–8.6736E–05	–7.6769E–08	3.6721E–11	200	1500
16	C_3H_6O	Acetone	35.918	9.3896E–02	1.8730E–04	–2.1643E–07	6.3174E–11	100	1500
17	$C_3H_4O_2$	Acrylic acid	7.755	2.9386E–01	–2.0878E–04	7.1591E–08	–9.0960E–12	250	1500
18	NH_3	Ammonia	33.573	–1.2581E–02	8.8906E–05	–7.1783E–08	1.8569E–11	100	1500
19	C_6H_7N	Aniline	–22.062	5.7313E–01	–4.5651E–04	1.8410E–07	–2.9867E–11	200	1500
20	C_6H_6	Benzene	–31.368	4.7460E–01	–3.1137E–04	8.5237E–08	–5.0524E–12	200	1500
21	$C_4H_8O_2$	Butyric acid	14.368	3.9591E–01	–1.8906E–04	–7.6462E–09	2.0812E–11	298	1200
22	CS_2	Carbon disulfide	20.461	1.2299E–01	–1.6184E–04	1.0199E–07	–2.4444E–11	100	1500
23	CO_2	Carbon dioxide	27.437	4.2315E–02	–1.9555E–05	3.9968E–09	–2.9872E–13	50	5000
24	CO	Carbon monoxide	29.556	–6.5807E–03	2.0130E–05	–1.2227E–08	2.2617E–12	60	1500
25	CCl_4	Carbon tetrachloride	19.816	3.3311E–01	–5.0511E–04	3.4057E–07	–8.4249E–11	100	1500
26	Cl_2	Chlorine	27.213	3.0426E–02	–3.3353E–05	1.5961E–08	–2.7021E–12	50	1500
27	$CHCl_3$	Chloroform	22.487	1.9823E–01	–2.1676E–04	1.1636E–07	–2.4555E–11	100	1500
28	C_6H_{12}	Cyclohexane	13.783	2.0742E–01	5.3682E–04	–6.3012E–07	1.8988E–10	100	1500
29	$C_6H_{12}O$	Cyclohexanol	17.124	3.3700E–01	2.8176E–04	–4.2713E–07	1.3215E–10	200	1500
30	C_3H_6	Cyclopropane	21.172	6.3106E–02	2.9197E–04	–3.2708E–07	9.9730E–11	100	1500
31	CH_2Cl_2	Dichloromethane	26.694	8.3984E–02	8.9712E–06	–5.0924E–08	1.8726E–11	100	1500
32	$C_4H_{10}O$	Diethyl ether	35.979	2.8444E–01	–1.2673E–06	–1.0128E–07	3.4529E–11	200	1500
33	$C_5H_{10}O$	Diethyl ketone	49.800	2.6897E–01	5.0669E–05	–1.5227E–07	4.9510E–11	200	1500
34	C_2H_7N	Dimethylamine	30.638	1.0737E–01	1.5824E–04	–1.9418E–07	5.8509E–11	200	1500
35	C_2H_6	Ethane	28.146	4.3447E–02	1.8946E–04	–1.9082E–07	5.3349E–11	100	1500
36	C_2H_6O	Ethanol	27.091	1.1055E–01	1.0957E–04	–1.5046E–07	4.6601E–11	100	1500
37	$C_4H_8O_2$	Ethyl acetate	69.848	8.2338E–02	3.7159E–04	–4.1129E–07	1.2369E–10	200	1500
38	C_2H_5Cl	Ethyl chloride	35.946	5.2294E–02	2.0321E–04	–2.2795E–07	6.9123E–11	100	1500
39	C_8H_{10}	Ethylbenzene	–20.527	5.9578E–01	–3.0849E–04	3.5621E–08	1.2409E–11	200	1500
40	C_2H_4	Ethylene	32.083	–1.4831E–02	2.4774E–04	–2.3766E–07	6.8274E–11	60	1500
41	$C_2H_6O_2$	Ethylene glycol	48.218	1.9073E–01	–6.6117E–08	–1.8834E–08	1.2555E–11	200	1500
42	C_2H_4O	Ethylene oxide	30.827	–7.6041E–03	3.2347E–04	–3.2747E–07	9.7271E–11	50	1500
43	F_2	Fluorine	27.408	1.2928E–02	7.0701E–06	–1.6302E–08	5.9789E–12	100	1500
44	$C_3H_8O_3$	Glycerol	9.656	4.2826E–01	–2.6797E–04	3.1794E–08	2.7745E–11	298	1200
45	H_2	Hydrogen	25.399	2.0178E–02	–3.8549E–05	3.1880E–08	–8.7585E–12	250	1500
46	HCl	Hydrogen chloride	29.244	–1.2615E–03	1.1210E–06	4.9676E–09	–2.4963E–12	50	1500
47	CHN	Hydrogen cyanide	25.766	3.7969E–02	–1.2416E–05	–3.2240E–09	2.2610E–12	100	1500
48	H_2O_2	Hydrogen peroxide	36.181	8.2657E–03	6.6420E–05	–6.9944E–08	2.0951E–11	100	1500
49	C_4H_{10}	*i*-Butane (iso-Butane)	6.772	3.1447E–01	–1.0271E–04	–3.6849E–08	2.0429E–11	200	1500
50	CH_4	Methane	34.942	–3.9957E–02	1.9184E–04	–1.5303E–07	3.9321E–11	50	1500
51	CH_4O	Methanol	40.046	–3.8287E–02	2.4529E–04	–2.1679E–07	5.9909E–11	100	1500

TABLE C-4–(continued)

$C_p = A + BT + CT^2 + DT^3 + ET^4$						(C_p–joule/(mol K), T–K)			
No.	Formula	Substance	*A*	*B*	*C*	*D*	*E*	T_{min}	T_{max}
52	CH_3Br	Methyl bromide	29.146	2.4374E–02	1.0655E–04	–1.1324E–07	3.3241E–11	100	1500
53	$C_6H_{12}O$	Methyl isobutyl ketone	2.404	5.8495E–01	–3.7647E–04	1.2418E–07	–1.7051E–11	298	1500
54	CH_5N	Methylamine	40.039	–1.5108E–02	2.5012E–04	–2.3336E–07	6.5582E–11	100	1500
55	C_8H_{10}	*m*-Xylene	–16.725	5.6424E–01	–2.6465E–04	1.3381E–08	1.5869E–11	200	1500
56	$C_{10}H_8$	Naphthalene	67.099	4.3239E–02	9.1740E–04	–1.0019E–06	3.0896E–10	50	1500
57	C_4H_{10}	*n*-Butane	20.056	2.8153E–01	–1.3143E–05	–9.4571E–08	3.4149E–11	200	1500
58	$C_{10}H_{22}$	*n*-Decane	31.780	7.4489E–01	–1.0945E–04	–2.2668E–07	9.3458E–11	200	1500
59	C_7H_{16}	*n*-Heptane	26.984	5.0387E–01	–4.4748E–05	–1.6835E–07	6.5183E–11	200	1500
60	C_6H_{14}	*n*-Hexane	25.924	4.1927E–01	–1.2491E–05	–1.55916E–07	5.8784E–11	200	1500
61	$C_6H_5NO_2$	Nitrobenzene	-16.202	5.6182E–01	–3.9302E–04	1.0043E–07	–1.2252E–12	200	1500
62	N_2	Nitrogen	29.342	–3.5395E–03	1.0076E–05	–4.3116E–09	2.5935E–13	50	1500
63	C_9H_{20}	*n*-Nonane	29.687	6.6821E–01	–9.6492E–05	–2.0014E–07	8.2200E–11	200	1500
64	C_8H_{18}	*n*-Octane	29.053	5.8016E–01	–5.7103E–05	–1.9548E–07	7.6614E–11	200	1500
65	C_5H_{12}	*n*-Pentane	26.671	3.2324E–01	4.2820E–05	–1.6639E–07	5.6036E–11	200	1500
66	O_2	Oxygen	29.526	–8.8999E–03	3.8083E–05	–3.2629E–08	8.8607E–12	50	1500
67	C_8H_{10}	*o*-Xylene	0.182	5.1344E–01	–2.0212E–04	–2.1615E–08	2.3212E–11	200	1500
68	C_6H_6O	Phenol	4.408	3.6338E–01	–6.0417E–05	–1.2794E–07	5.5287E–11	100	1500
69	C_8H_{10}	*p*-Xylene	–17.360	5.6470E–01	–2.6293E–04	1.1217E–08	1.6544E–11	200	1500
70	C_5H_5N	Pyridine	23.262	1.1251E–01	3.7351E–04	–4.5402E–07	1.4286E–10	50	1500
71	C_8H_8	Styrene	71.201	5.4767E–02	6.4793E–04	–6.9875E–07	2.1232E–10	100	1500
72	SO_2	Sulfur dioxide	29.637	3.4735E–02	9.2903E–06	–2.9885E–08	1.0937E–11	100	1500
73	C_7H_8	Toluene	–24.097	5.2187E–01	–2.9827E–04	6.1220E–08	1.2576E–12	200	1500
74	$C_4H_6O_2$	Vinyl acetate	27.664	2.3366E–01	6.2106E–05	–1.6972E–07	5.7917E–11	100	1500
75	H_2O	Water	33.933	–8.4186E–03	2.9906E–05	–1.7825E–08	3.6934E–12	100	1500

C_p – heat capacity of ideal gas, joule/(mol K)

A, *B*, *C*, *D*, and *E* – regression coefficients for chemical compound

T – temperature, K

T_{min} – minimum temperature, K