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COLLEGE OF PETROLEUM ENGINEERING AND TECHNOLOGY

DEPARTEMENT OF OIL TRANSPORTATION AND RIFINING

DISSERTATIONTITLE: INVISTIGATION OF CO_2 ABSORPTION RATE IN DEAETHANOLAMINEAND POTASSIUM CARBONATE AND PROMOTED POTASSIUM CARBONATE.

تقصي معدل إمتصاص ثاني أكسيد الكربون بواسطة الأمين (DEA)وكربونات البوتاسيوم وكربونات البوتاسيوم المطور (المعزز)

Dissertation submitted in partial fulfillment of the requirement for the Bachelor of engineering (Horns) Degree in transportation and Refining engineering

By:

Hassan HammadIdrisHammad
IbtihalAbdallah Hassan Mursal
Mohamed Omer Mohamed Ali
Mostafa Adam Idris Ibrahim
ZeinabAbdulaziz Mohammed Albashir

Main Supervisor:

Mr.Abdelgadir Bashir Bannaga

Co-Supervisor:

Dr. Omer EisaBabiker

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Prepared by

Hassan HammadIdrisHammad
IbtihalAbdallah Hassan Mursal
Mohamed Omer Mohamed Ali
Mostafa Adam Idris Ibrahim
ZeinabAbdulaziz Mohammed Albashir

Main Supervisor:

Mr.Abdelgadir Bashir Bannaga

Co-Supervisor:

Dr. Omer EisaBabiker

This project approved by college of petroleum engineering and technology to transportation and refining department

Main Supervisor:

Mr.Abdelgadir Bashir Bannaga

Signature …………………………………………………………………………….

Co-Supervisor:

Dr. Omer EisaBabiker

Signature …………………………………………………………………………….

Head of department Dr. Dalia Mammon Bashir

Signature …………………………………………………………………………….

Dean of college: Dr Tagwa Ahmed Musa

Signature …………………………………………………………………………….

Date: October 2017

بسم الله الرحمن الرحيم

قال تعالى:

﴿ شَهِدَ اللَّهُ أَنَّهُ لا إِلَهَ إِلَّا هُوَ وَالْمَلائِكَةُ وَأُولُوا الْعِلْمِ قَائِماً بِالْقِسْطِ لا إِلَهَ إِلَّا
هُوَ الْعَزِيزُ الْحَكِيمُ ﴾

[آلعمران: الآية 18]

Dedication

We would like to dedicate this research to our

Dear parents
To the people who paved our way of science and knowledge
All our teachers Distinguished

To the taste of the most beautiful moments with our friends

Also we dedicate this research to our brothers and sisters

Who spent their life to provide sufficient, Happiness and love

Finally we dedicate this research to our colleagues

In Transportation and Refining department, specially and

To all batch 22th petroleum engineering

Students.

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First of all, we would like to thank Great and Almighty God who gave us the power to fulfill this study. Thanks should be given to our supervisor's Mr. Abdelgadir Bashir Bannaga and Dr. Omer Eisa Babiker for their continuous advice and encouragement throughout the entire course of our study .we would like to express our sincere thanks and gratitude to the Eng. Almogal Abdulgadir.

Thank you all

ABSTRACT

The increase of carbon dioxide (CO_2) emissions to our atmosphere is the major contributor to global climate change. A number of methods for reducing greenhouse gases have been proposed including carbon capture and sequestration (CCS). There are three major approaches for CCS post-combustion capture, pre-combustion capture, and oxyfuel process. Post-combustion capture offers some advantages as existing combustion technologies can still be used without radical changes on them. This makes post-combustion capture easier to implement as a retrofit option (to existing power plants) compared to the other two approaches. Currently, the reactive absorption of CO_2 into amine solvents is the most widely used technology for CO_2 capture. One of the many potential solvent candidates is potassium carbonate (K_2CO_3). Although potassium carbonate is associated with lower cost, less toxicity and is less prone to degradation effects when compared to the current industrial benchmark solvent, monoethanolamine (MEA), it has a low rate of reaction resulting in poor mass transfer performance. Developing a non-toxic and affordable promoter will facilitate the use of potassium carbonate solvent systems for CO_2 capture. Comprehensive flow sheet models have been built for each of the solvent systems, using aspen plus as the modeling tool. Using aspen plus simulation for the reaction kinetics of CO_2 into DEA, unprompted and DEA-promoted potassium carbonate (K_2CO_3) solutions have been studied. The investigation of the CO_2 absorption rate comes out with a clear increase in the CO_2 absorption with the increases of the process pressure. On the other hand, the absorption rate decreases with the increases of the process temperature. the results presented here show that at 80^oC the addition of small amounts of DEA (1%, 2%, and 3%) accelerate the overall absorption process of CO_2 in carbonate solvents by 1.63%, 3.26%, and 4.87% respectively. Furthermore, the investigation of the promoter concentration effects showed a sudden declining in the absorption rate for concentrations greater than 4% for the reason of the involving promoter in the main interaction as an additional solvent. Absorption column has been designed to capture carbon dioxide in this research.

The key words: carbon dioxide capture, diethanolamine, potassium carbonate ,solvent , promotion, and aspen plus.

التجــريد

تعد زيادة إنبعاث ثاني أكسيد الكربون في الغلاف الجوي مساهما رئيسيا" في تغيير المناخ العالمي وهناك عدد من الأساليب لخفض الغازات الدفيئة تشمل احتجاز الكربون ،والطرق الرئيسية هي الاحتجاز قبل الاحتراق ،والاحتجاز بعد الاحتراق والاحتراق الأكسجيني . يقدم الاحتجاز بعد الاحتراق مميزات في ظل تكنولوجيا الاحتراق الموجودة التي يمكن استخدامها من غير احداث تغييرات جذرية كما تعتبر سهلة في التنفيذ والتحديث مقارنة مع غيرها من الطرق . يعتبر تفاعل الامتصاص لثاني أكسيد الكربون بواسطة الامينات أكثر انتشارا،وتعتبر كربونات البوتاسيوم واحدة من أهم المذيبات المرشحة لعمليات الامتصاص ،وترتبط كربونات البوتاسيوم بالميزات التالية فهي غير سامة ،رخيصة الثمن ،أقل عرضة للإهلاك والتدهور مقارنة مع المزيبات القياسيه الصناعيه الحاليه (MEA) وهي ذات معدل تفاعل منخفض مقارنة نتيجة لانخفاض معدل انتقال الكتلة أثناء التفاعل .تم تطويركربونات البوتاسيوم عن طريق محفزات غير سامة تعمل على تسيهل عملية امتصاص ثاني أكسيد الكربون. تم انشاء مخططات سريان شاملة لكل مذيب بإستخدام برنامج(ASPEN PLUS) لوصف حركية تفاعل الـ (CO_2) مع الـ (DEA) (K_2CO_3)و(K_2CO_3-DEA).وأوضحت النتائج التالية عند درجة حراة ($80\ ^oC$) انه عند إضافة كميات قليله من (DEA) بمقدار(0.01%, 0.02% and 0.03%) تزيد معدل تفاعل (CO^2)مع (K_2CO_3) بمعدل(1.63%, 3.26% and 4.87%) على التوالي بالإضافه لانه تم التحقيق في تأثير تركيز المحفزات الذي يظهر انخفاض مفاجئ في معدل الامتصاص للتراكيز أعلى من 4% بسبب أن المحفزات تدخل نفسها في تفاعلات عكسية على انها مذيبات اضافية. كما تم تصميم برج امتصاص ذو حشوات لإحتجاز غاز ثاني اكسيد الكربون.

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ABBREVIATIONS

Abbreviation	Meaning
CO_2	Carbon dioxide
IEA	International Energy Agency
GHG	Greenhouse gases
CCS	CO_2 Capture and storage
H_2O	Water
PCC	Post combustion capture
H_2	Hydrogen gas
CO	Carbon monoxide
MEA	Monoethanolamine
DEA	Diethanolamine
MDEA	Methyldiethanolamine
AMP	2_amino,2_methyl 2_1 propanol
K_2CO_3	Potassium carbonate
M	Molarity
PZ	Piperazine
NO_X	Nitrogen oxides
SO_X	Sulpher oxides
AL_2O_3	Alumina
TEA	Tertiary ethanolamine
CSTR	Continuous stirred tank reactor
$-\Delta H$	The heat of absorption(enthalpy)
DCU	Delay coking unit
NRTL	None Random two Liquid (Property method)
NRTL-RK	Redish Wrong None Random two Liquid (Property method)
ELECNRTL	Electrolyte None Random two Liquid (The most versatile electrolyte property method)
NTU	Number of Transfer Unit
HTU	Height Transfer Unit
HETP	Height of an Equivalent Theoretical Plate

SYMBOLS

Symbols	Description	Unit
D_c	Column diameter.	m
f_1	liquid viscosity correction factor	-
f_2	liquid density correction factor	-
f_3	surface tension correction factor	-
F_p	Packing factor, characteristic of the size and type of packing.	m^-1
G_m	molar gas flow-rate per unit cross-sectional area.	kmol/m2s
H_G	Height of a gas-phase transfer unit.	m
H_L	height of a liquid-phase transfer unit	m
H_{OG}	the height of an overall gas-phase transfer unit.	m
H_{OL}	is the height of an overall liquid-phase transfer unit.	m
K_3	percentage flooding correction factor.	-
K_4	Factor function of (V^*w , Fp, μl,and ρL, ρv)	-
K_g	film mass-transfer coefficient.	m/s
L_m	molar liquid flow-rate per unit cross-sectional area	kmol/m2s.
L^*_w	liquid mass flow-rate per unit area column cross-sectional area.	kg/m2s
N_{OG}	the number of overall gas-phase transfer units	-
P	column operating pressure.	atm ,bar.
$(Sc)v$	gas Schmidt number.	-
$(Sc)_L$	liquid Schmidt number.	-
V^*w	gas mass flow-rate per unit column cross-sectional area.	kg/m2s
X_1 , X_2	the mol fractions of the solute in the liquid at the bottom and top of thecolumn, respectively.	-
Xe	the concentration in the liquid that would be in equilibrium with the gas concentration at any point.	-
Ye	the concentration in the gas that would be in equilibrium with the liquid concentration at any point.	-
$y1$, $y2$	the mol fractions of the solute in the gas at the bottom and top of the column, respectively.	-

Z	column height	m
$\rho L, \rho v$	liquid and vapour densities.	kg/m3
μl	liquid viscosity.	Ns/m2
Ψh	=**H**G factor	-
Φh	=$H_L$factor	-

Chapter 1

INTRODUCTION

1.1 Introduction

Carbon dioxide is one of the greenhouse gases compositions. It is an odorless, colorless gas which is faintly acid and nonflammable, and it has a molecular formula of CO_2[1].

There are two primary sources of CO_2 including the natural CO_2 sources which are representing the majority of CO_2 released to the atmosphere involving the oceans, animal and plant respiration, decomposition of organic matter, forest fires, and emissions from volcanic eruptions. The other sources of CO_2 consist the human activities such as the fuel consumption in power generation, transportation, industries, chemicals manufacturing, petroleum production, and agricultural activities. Many of these source types burn fossil fuels (coal, oil, and natural gas), which are the leading cause of CO_2 emissions [2].

CO_2 makes up the largest share of greenhouse gases (about 60%) which it causes climate change by rising up the planet temperature. Recent international energy agency (IEA) predicted that the CO_2 emissions attributable to the energy sector will increase by 130% by 2050 in the absence of new policies or supply constraints, largely as a result of increased fossil fuel usage see Figure (1). thereby the temperature increase in the range of (4-7)°C, to reduce the emissions of CO_2 by 2050 will increased energy efficiency, increased renewable energies, and nuclear power, and the decarbonization of power generation from fossil fuels. The only technology available to mitigate greenhouse gas (GHG) emissions from large-scale fossil fuel usage is CO_2 capture and storage (CCS) [3].

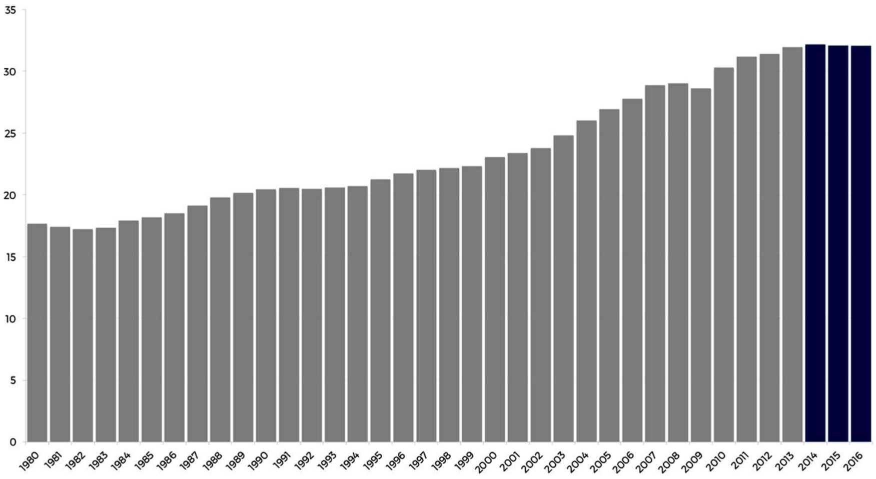

Figure 1-1: Global CO_2 emissions (Giagatonnes) 1989-2016

1.2 Carbon dioxide capture

One of the most promising approaches to tackle the high emission rate of carbon dioxide is the use of Carbon Capture and Storage (CCS) technology. This technology aims at capturing carbon dioxide from power stations and other industrial facilities, compressing, and then transporting it to one of CO_2 storage techniques.Three types of technology have been utilized for carbon capture from power plants comprising the pre-combustion, post-combustion and oxy-combustion [4]. The selection criteria of CO_2 capturing technology typically depend on the gas stream required purity, and the gas stream operating conditions. Post-combustion capture with chemical absorption offers high capture efficiency, high selectivity at low partial pressures, and the lowest energy use and costs when compared with the other separation techniques[8].

1.3 Problem statement

Carbon dioxide is one important greenhouse gases composition when it existed by the normal composition. These gases help protect the Earth from the hazardous radiation by absorbing the redirecting energy back to the Earth's surface.

The increase in the amount of carbon dioxide motivates thescientists to develop several systems to reduce the emission in the atmosphere. The CO_2 capture by aqueous solutions process is one of the effective processes in this field and this process is still on the development track. Furthermore, the investigation of the system will give the potential to understand the enhancement mechansm is.

1.4 Objectives:

1. Investigation on the performance of amines (DEA) and potassium carbonates solvent system.
2. Study the effect of promotion of potassium carbonates by (DEA) on the CO_2 absorption rate.
3. Design of absorption column design for CO_2 absorption.

1.5 The Scope of Study:

Simulation of a chemical absorption process toremoves CO_2 from the feed stream (flue gas) using different solvents: Amines (DEA), potassium carbonates, promoted potassium carbonate, and compare the performance of these solvents to determine the solvents which give the highest absorption rate.

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Chapter 2

LITERATURE REVIEW

2.1 Introduction

Carbon capture and a storage is a range of technologies that hold the promise of trapping up to 90% of carbon dioxide and emissions from the power stations and industrial sites and it involves all the methods that avoid it is escape into the atmosphere and contribute to climate change ,The Capture and sequestration of carbon dioxide could play an important rule in reducing greenhouse gas emissions while enabling low carbon electricity generation from power plants as estimated in (U.S. Inventory of Greenhouse Gas Emissions and Sinks) more than 40% of CO_2 emissions in united states are from electric power generation . CCS technologies are currently available and can dramatically reduce by (80%-90%)CO_2 emissions from power plants that burn fossil fuels applied to 500 MW coal fed power plant which emits roughly 3 million tons of CO_2 per year, the amount of GHG emissions avoided with a 90% reduction efficiency the recent Mandates for CO_2 would be equivalent to planting more than 62 million trees and waiting for them to grow and avoiding annual electricity related emissions from more than 300,000 homes, EPA greenhouse gas reporting program includes facilities that capture CO_2 for the purpose of supplying the CO_2 to the economy or for injecting it underground and is currently occurring at over 120 facilities in the united states . new ways to remove and process CO_2 from their product Streams must be investigated. This chapter reviews and summarizes the previous studies Related to CO_2 capture and what the searchers reached.

2.2 Carbon dioxide emissions

CO_2 is one of the gases in our atmosphere. Both natural processes and human activities Contribute to its presence at a present concentration of about 0.040% [406 parts per Million (ppm) on January 7, 2017], uniformly distributed over the earth. Commercially, CO_2 finds uses as a refrigerant (dry ice is solid CO_2), in beverage carbonation, and in fire Extinguishers. Because the concentration of CO_2 in the atmosphere is low, no practical Process has yet been developed to obtain the gas by extracting it from the air. Most Commercial CO_2 is recovered as a by-product of other processes, such as the production of ethanol by fermentation and the manufacture of ammonia. some CO_2 is obtained From the combustion of coke or other carbon-containing fuels [13].The atmosphere's Concentration of carbon dioxide (CO_2) has increased by more than 30 percent over the Last 250years, largely due to human activity. Two-thirds of that rise has occurred in the Past 50 years Unless there is a change [14].

2.2.1 Effects of the carbon dioxide emissions

Increasing CO_2 emissions in the environmentlead to global warming which is an issue of Great concern today. The climate of the earth is varying continuously due to various Factors, viz., change in the Earth's orbit, change in the Sun's intensity, change in ocean Currents [15].Anthropogenic greenhouse gas emissions have increased since the pre-Industrial era, driven largely by economic and population growth, and are now higher than ever. This has led to atmospheric concentrations of carbon dioxide, methane, and Nitrous oxide that are unprecedented in at least the last 800,000 years. Their effects, Together with those of other anthropogenic drivers, have been detected throughout the Climate system and are extremely likely to have been the dominant cause of the Observed warming since the mid-20th century [16], Carbon dioxide (CO_2), that are thought to cause ''global warming'' – severe increases in Earth's atmospheric and surface temperatures, with disastrous environmental consequences [17].Carbon dioxide capture

Capture is the removal of CO_2 from flue gas, which comes from the thermal power plant Combustion chamber [15]. Carbon capture and storage (CCS) is one of the promising routes to Reduce CO_2 emissions from fossil fuel-fired power plants [18].

They are different technologies for CO_2 capture used before and after combustion, Capture of CO_2 by chemical absorption is the technology that is closest to commercialization. While a number of different solvents for use in chemical absorption Of CO_2 have been proposed, a systematic comparison of the performance of different Solvents has not been performed and claims on the performance of different solvents Vary widely [19].

2.3 Solvent used in carbon dioxide capture

Much research has been done on different types of sorbents that can be used in direct air capture [20], such as (DEA, MEA, K_2CO_3, solid sorbents and other) .and use best one to capture Carbon dioxide.

2.3.1 Primary and Secondary Amines

The capacity for amine solvents to react with carbon dioxide is due to the reactivity of the amine group. The standard absorption process commonly considered for post-combustion CO_2 capture process uses a 30 wt. % or 7 M aqueous solution of MEA. The availability of a lone pair of electrons in the basic amine group of an MEA molecule makes it very reactive towards carbon dioxide [21].

At 50 °C, this reaction proceeds very efficiently releasing a heat load of approximately 72 kJ per mole of CO_2 absorbed (30 wt.% MEA).

The solvent is regenerated by heating the loaded solution to around 120 °C. A thermal energy of 165 kJ per mole of CO_2 desorbed is required for the regeneration.

A significant increase in the thermal energy is required for the desorption of CO_2, when compared to the exothermic heat of absorption, due to the extra energy required to heat water sensibly to approximately 120 °C and to generate steam to drive desorption.

To increase reaction rates, researchers have looked into the use of MEA solvents combined with the use tertiary alkanol amine solvents such as MDEA cyclic diamines such as piperazine (PZ), satirically hindered amines like AMP and blends of various alkanol amines.

Carbon dioxide absorption using primary and secondary amines may encounter many operational issues including high energy consumption. One of the main challenges with the use of amine solvents is its susceptibility to oxidative degradation due to exposure to the solvent to oxygen found in most flue gas streams. Researchers found that primary amines such as MEA degrade faster than their secondary and tertiary counterparts such as DEA and MDEA.

2.3.2 Tertiary Amines

This reaction generates a protonated amine and bicarbonate ion instead of an amine carbamate as observed in the reaction of primary and secondary amines with CO_2.Although the absorption rate is slower and consumes water, this reaction results in high CO_2 loading capacity and has allow heat of absorption.

Unlike primary and secondary amines tertiary amines are not limited to a solvent loading of 0.5 mole CO_2 per mole of amine these solvents readily approach a maximum loading of 1 mole CO2 per mole of amine, significantly increasing the solvent capacity[21].

2.4 Development of solvents

Potassium carbonate (K_2CO_3) is an alternative solvent that may potentially overcome some of the issues associated with amine solvents. The major benefit is the ability to run the absorption process at high temperatures resulting in a more efficient and economical regeneration process. Potassium carbonate is also associated with lower toxicity and better resistance to degradation than commonly seen with amine solvents at high temperatures and in the presence of oxygen and other minor flue gas components such as SOx and NOx. The use of potassium carbonate as an absorption solvent has emerged since the early 20th century in the 1950's, Benson and field established the Benfield process which employed hot potassium carbonate as a CO_2 absorption solvent[21].

. Over time there have been many variations to the process including operating the absorber at higher temperatures and improving the packing systems used in the absorber and regenerator columns [22]. This process was proposed in order to remove CO_2 from synthesis gas manufactured for Fischer-Tropic synthesis. Since the synthesis gas was available at higher pressures, it was beneficial to employ a CO_2 absorption process that operated at higher pressures as well. Hence, it was proposed to use hot, concentrated alkaline solutions of potassium carbonate under pressure [23].for exampleUsedPilot Plant for Capturing CO_2 by using Potassium Carbonate as solvent .and they designed it to capture4 - 10 kg/hr. of co2 from an air/CO_2 feed gas rate of 30 – 55 kg/hr. at 50 °C and it designed else to test the performance of a precipitating potassium carbonate solvent system and to validate Aspen Plus simulations. After ending the study showed that CO_2 recovery results were around five times higher when a promoted K_2CO_3 solvent was used compared to the un-promoted K_2CO_3 solvent.

others develop the Potassium Carbonate and havestudied the effect of blending potassium carbonation (K_2CO_3) with alumina (Al_2O_3) using real flue gas with 8% CO_2 and 12% H_2O at 65 °C and capacity of 66.2 mgCO_2/(gr sorbent). After ending the study showed that The low-cost sorbent and The capture capacity of the sorbent as a function of cycle number and Small changes occurred in the pore size distribution and surface area of the prepared sorbent, else found could be used for industrial CO_2 capture processes with fixed-bed reactors [9](Bongartz 2015)(Bongartz 2015), Potassium carbonate based absorption processes are lower cost, less toxic, and less prone to degradation effects that are commonly seen with MEA at high temperatures and in the presence of oxygen and other minor flue gas components. Potassium carbonate acquires the ability to absorb not only CO_2 but also other polluting gases found in standard flue gases such as sulfur oxides (SO_x) and nitrogen oxides (NO_x). In addition, when compared to amine solvents, potassium carbonate solvents have very low volatility which results in much-reduced solvent loss to the atmosphere.

Diethanolamine (DEA) Used in textile processing, in industrial gas purification, and as a solvent for drugs Administered intravenously [24], DEA which significantly reduced the capital and operating costs of the process and generated higher treated gas purity, and used at normal temperature and pressure, but it not efficient and economical regeneration process with lower resistance to degradation.

This process was further developed by adding a small amount of a rate promoter, The absorption rates of CO_2 in diethanolamine (DEA) promoted potassium carbonate (K_2CO_3) at temperature ranging from 343.2K to 363.2K and normal pressure, with the mass fractions of DEA and K_2CO_3 respectively ranged from 0 to 0.02, and 0.35 to 0.40, after end the investigation appeared that the absorption rate increases when the temperature increase. And absorption rate of CO_2 increases with the increase of the mass Fraction of DEA also very small amount of DEA can significantly enhance the absorption of CO_2 in K_2CO_3 aqueous solution at high temperatures [18].

Some studies work to make comparing between MEA, DEA, TEA, and AMP Solutions at the continuous stirred reactor in 313 to 333 K. and enthalpy for anyone was 88.91, 70.44, 44.72, and 63.95, respectively.

After ending the study appearsdeviation or decrease in Solubilities of CO_2 in the aqueous amine solutions with an increase in temperature. And AMP, DEA, TEA, and MEA respectively had alarge scale of solubility. Also found the Heat of absorption ($-\Delta H$ abs) was high in MEA, DEA, TEA, and AMP, respectively. That means higher CO_2 loadings with lower reaction temperature [25].

Chapter 3

METHODOLOGY

3.1 The main feed steam (flue gas) data: from delay cocking unit (DCU) From the Khartoum refinery, combustion reaction, the total mole of CO_2, H_2O, and SO_2 formed.

Table 3-1: Composition of gas inlet

Component	Moles\hr	Mole fraction
CO_2	140.12	0.09451
H_2O	221.85	0.1496
SO_2	0.0036	2.428×10^{-6}
O_2	39.582	0.02667
N_2	1080.97	0.7291
Total	1482.5236	1.0

Average stack temperature = 298.35 c, =569.03 F

Table 3-2: Simulation Design Data

Absorber	
Diameter	100 mm
Packing Type and Size	SULZER Mellapak 350Y
Packing Height	2568 mm
Stripper	
Diameter	100 mm
Packing Type and Size	SULZER Mellapak 350Y
Packing Height	2568 mm
Feed and Products	
Sour Gas to Absorber	47.58 Nm^3/hr.
Lean KOH solution to Absorber	70.00 l/hr.
Rich KOH solution to Stripper	99.98 l/hr.

3.2 Case study:

Investigate the (DEA), potassiumcarbonates, promoted potassium carbonate systems by develop flow sheet models for chemical absorption process for CO_2 capture from flue gas in ASPEN plus simulator for each solvent system using the ELECNRTL property method and compared the performance of different solvents system to determine the solvents that give the highest absorption rate.

3.3 Potassium Carbonate Solvents

3.3.1 Reaction chemistry

The chemical absorption equilibrium reaction:

$K_2CO_3 + CO_2 + H_2O \leftrightarrow 2KHCO_3$ (3.1)

Dissociation reaction (salt dissociation reaction of carbonate and bicarbonate) :

$K_2CO_3 \rightarrow 2K^+ + CO_3^{-2}$ (3.2)

$KHCO_3 \rightarrow K^+ + HCO_3$ (3.3)

$KOH \rightarrow K^+ + OH$ (3.4)

Hydrolysis of dissolved co_2 to $H_3O^+$and bicarbonate ions (HCO_3^-):

$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$ (3.5)

$CO_2 + OH^- \rightarrow HCO_3^-$ (3.6)

$HCO^-_3 \rightarrow CO_2 + OH^-$ (3.7)

The dissociation of (HCO^-_3) to (H_3O^+) and (CO_3^{-2})

$HCO^-_3 + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$ (3.8)

The ionization of water to hydronium (H_3O^+) and hydroxide (OH^-) ions:

$2H_2O \leftrightarrow H_3O^+ + OH^-$ (3.9)

Hydrolysis of dissolved H_2S to H_3O^+ and HS^-

$H_2O + H_2S \leftrightarrow HS^- + H_3O^+$ (3.10)

$H_2O + HS^- \leftrightarrow S^{-2} + H_3O^+$ (3.11)

3.4 DEA Solvents

3.4.1 Reaction chemistry

The chemical absorption equilibrium reaction:

$DEA + CO_2 + H_2O \rightarrow DEACOO^- + H_3O^+$ (3.12)

Dissociation reaction (salt dissociation reaction of DEA):

$DEACOO^- + H_2ODEA^+ \rightarrow HCO^-_3$ (3.13)

$DEAH^+ + H_2O \leftrightarrow DEA + H_3O^+$ (3.14)

$DEACOO^- + H_3O^+ \rightarrow DEA + H_2O + CO_2$ (3.15)

Hydrolysis of dissolved CO_2 to H_3O^+ and bicarbonate ions (HCO_3^-):

$CO_2 + 2H_2O \rightarrow H_3O^+ + HCO_3^-$ (3.16)

$CO_2 + OH^- \rightarrow HCO_3^-$ (3.17)

$HCO^-{}_3 \rightarrow CO_2 + OH^-$ 3.18)

The dissociation of (HCO_3^-) to (H_3O^+) and (CO_3^{-2})

$HCO^-{}_3 + H_2O \rightarrow H_3O^+ + CO_3^{-2}$ (3.19)

The ionization of water to hydronium (H_3O^+) and hydroxide (OH^-) ions:

$2H_2O \rightarrow H_3O^+ + OH^-$ (3.20)

Hydrolysis of dissolved H_2S to H_3O^+ and HS^-

$H_2O + H_2S \rightarrow HS^- + H_3O^+$ (3.21)

$H_2O + HS^- \rightarrow S^{-2} + H_3O^+$ (3.22)

3.5 Process description

A typical chemical absorption process consists of an absorber and a stripper, in which the absorbent is thermally regenerated. In a chemical absorption process, the flue gas containing CO_2 enters a packed bed absorber from the bottom and contacts counter-currently with a CO_2-lean absorbent. After absorption, the CO_2-rich absorbent flow into a stripper (through heat exchanger exchanges with aCO_2-lean absorbent which come from the stripper) for thermal regeneration. After regeneration, the CO_2-lean absorbent is pumped back to the absorber cyclic use. The pure CO_2 released from the stripper is compressed for the subsequent transportation and storage. The operating pressure is around 1 bar and the temperatures in the absorber and stripper are usually in the range of 40-60ºC and 120-140ºC, respectively. [26]

The outlet streams are:

1- Treated gas stream.
2- CO_2 Captured stream.

3.6 Aspen plus process simulator

ASPEN is a process simulation software package widely used in industry today. Given a process design and an appropriate selection of thermodynamic models, ASPEN uses mathematical models to predict the performance of the process. This information can then be used in an iterative fashion to optimize the design. This accurate modeling of thermodynamic properties is particularly important in the separation of non-ideal mixtures, and ASPEN has large databases of regressed parameters. ASPEN can handle very complex processes, including multiple-column separation systems, chemical reactors, distillation of chemically reactive compounds, and even electrolyte solutions like mineral acids and sodium hydroxide solutions[27].

3.6.1 ELECNRTL

The ELECNRTL property method is the most versatile electrolyte property method. It can handle very low and very high concentrations. It can handle aqueous and mixed solvent systems. The ELECNRTL is fully consistent with the NRTL-RK property method: the molecular interactions are calculated exactly the same way,therefore ELECNRTL can use the databank for binary molecular interaction parameters for the NRTL-RK property method. Many binary and pair parameters and chemical equilibrium constants from the regression of experimental data are included in Aspen Physical Property System databanks.

The electrolyte NRTL model uses the infinite dilution aqueous solution as the reference state for ions. It adopts the born equation to account for the transformation of the reference state of ions from the infinite dilution mixed solvent solution to the infinite dilution aqueous solution.

Water must be present in the electrolyte system in order to compute the transformation of the reference state of ions. Thus, it is necessary to introduce a trace amount of water to use the model for no aqueous electrolyte systems.

The electrolyte NRTL model is more applicable compared with the other models such as Pittermodel; this because the NRTL model includes the general temperature dependence of ion interaction parameters and also the model is conveniently embedded in Aspen Plus software with built-in parameter estimation facility. Furthermore, the NRTL model able to estimate the properties of themedium and high concentration aqueous solutions [10]. The thermodynamic calculation of electrolyte system using NRTL model mainly depends on the ionic force between the individual ionic species. The force changes with the number and the type of the species as well as with the distance between species. Electrolyte NRTL databank contains the non-randomness factors (GMELCN), the energy parameters of (GMELCC, GMELCD, and GMELCE) for several molecule-electrolyte and electrolyte-electrolyte pairs[28].The chemical solvent normally contains (20-40) wt.% potassium carbonate, (1-3) wt.% DEA activator and (0.4-0.7) wt%V_2O_5 corrosion inhibitor. The normal operation conditions of CO_2 absorption process is; pressure range (1- 2 at) and temperature range (70-140) ^oC based on the unit design [28].

3.6.2 Limitations of Electrolytes-I

Restrictions using the True component approach: – Liquid-liquid equilibrium cannot be calculated – The following models may not be used: Equilibrium reactors: Gibbs and REquil, Kinetic reactors: RPlug, RCSTR, and RBatchShortcut distillation: Distl, DSTWU, and SCFrac Rigorous distillation: MultiFrac and Petrobras[29].

3.6.3 Limitations of Electrolytes-II

Restrictions using the Apparent component approach: Chemistry may not contain any volatile species on the right side of the reactions, Chemistry for liquid-liquid equilibrium may not contain dissociation reactions and Input specification cannot be in terms of ions or solid salts[29].

3.7 Process Simulation Procedure

The main basic steps used to run the simulation Program are listed below:

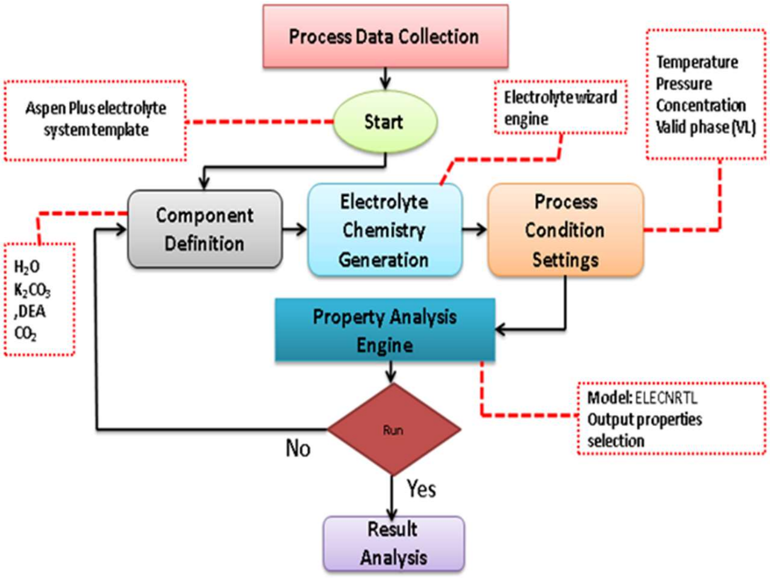


Figure 3-1: Simulation flow diagram

3.8 Material balance of absorption column

Table 3-3: Data of flue of gas absorption column

flue gas component	Moles/hr	Mole.Wt	Mole fraction	g/hr
CO_2	140.12	44	0.09451	6165.28
H_2O	221.85	18	0.1496	3993.3
SO_2	0.0036	64	2.428×10^{-6}	0.2304
O_2	39.58	32	0.02667	1266.56
N_2	1080.97	28	0.7291	30267.16
Total	1482.524		1.0	41692.5304

Amount of DEA = 140.12 $\frac{\textbf{mol}}{\textbf{h}}$ CO_2×DEA $\frac{\textbf{mol/h}}{\textbf{0.3CO2 mol/h}}$ = 467.067 mole/h

Overall material balance:

$$\mathbf{G_{in} + L_{in} = G_{out} + L_{out}} \qquad \textbf{(3.23)}$$

$$\boldsymbol{G_{in}(y_2 - y_1) = L_{in}(x_2 - x_1)} \qquad \textbf{(3.24)}$$

$$\mathbf{1482.524(y_2 - 0.09451) = 467.067(0.3 - 0)}$$

$$y_2 = (y_{co2o} \quad) = 0.189 = 18.9\%$$

$$L_{out} = 467.067 + 140.12 = 607.187 mole/h$$

Amount of exist gas (G_{out}) from overall material balance:

$$\mathbf{G_{out} = G_{in} + L_{in} - L_{out})} \qquad \textbf{(3.25)}$$

$$\boldsymbol{G_{out} = 1482.524 + 467.067 - 607.187 = 1342.4 mole/h}$$

3.9 Packed Column Design

Packed columns are used for distillation, gas absorption, and liquid-liquid extraction,Stripping (desorption) is the reverse of absorption and the same design methods will apply.The gas liquid contact in a packed bed column is continuous, not stage-wise, as in a plate column. The liquid flows down the column over the packing surface and the gasOr vapor, counter-currently, up the column. In some gas-absorption columns co-currentFlow is used. The performance of a packed column is very dependent on the maintenanceof good liquid and gas distribution throughout the packed bed, and this is an importantConsideration in packed-column design.

3.9.1 Types of Packing:

The principal requirements of a packing are that it should: Provide a large surface area: a high interfacial area between the gas and liquid. Have an open structure: low resistance to gas flow. Promote uniform liquid distribution on the packing surface.

Promote uniform vapor gas flow across the column cross-section.Many diverse types and shapes of packing have been developed to satisfy these requirements. They can be divided into two broad classes:

1. Packings with a regular geometry: such as stacked rings, grids and proprietary structured packings.
2. Random packings: rings, saddles and proprietary shapes, which are dumped into the column and take up a random arrangement

3.9.2 Structured packing

The term structured packing refers to packing elements made up from wire mesh or perforated metal sheets. The material is folded and arranged with a regular geometry,to give a high surface area with a high void fraction. Structured packings are produced by a number of manufacturers. The basic constructionAnd performance of the various proprietary types available is similar. They are availableIn metal, plastics and stoneware. The advantage of structured packings over random packing is their low HETP (typically less than 0.5 m) and low pressure drop (around100 Pa/m). They are being increasingly used in the following applications:

1. For difficult separations, requiring many stages: such as the separation of isotopes.
2. High vacuum distillation.
3. For column revamps: to increase capacity and reduce reflux ratio requirements.

3.9.3 Mellapak packing

Mellapak packing is the most widely used structured packing worldwide. It has proven excellent performance in columns with diameters up to 15 m. It is supplied in sheet metal thicknesses from 0.1 mm up.

3.9.4 Special features

1. Pressure drop per theoretical stage 0.3-1.0 mbar
2. Pressure drop at 70-80% flooding about 2 mbar/m.
3. Minimum liquid load approx 0.2 m^3/m^2h.
4. Maximum liquid load up to more than 200 m^3/m^2h (typically in desorption columns).

3.9.5 Preferred applications

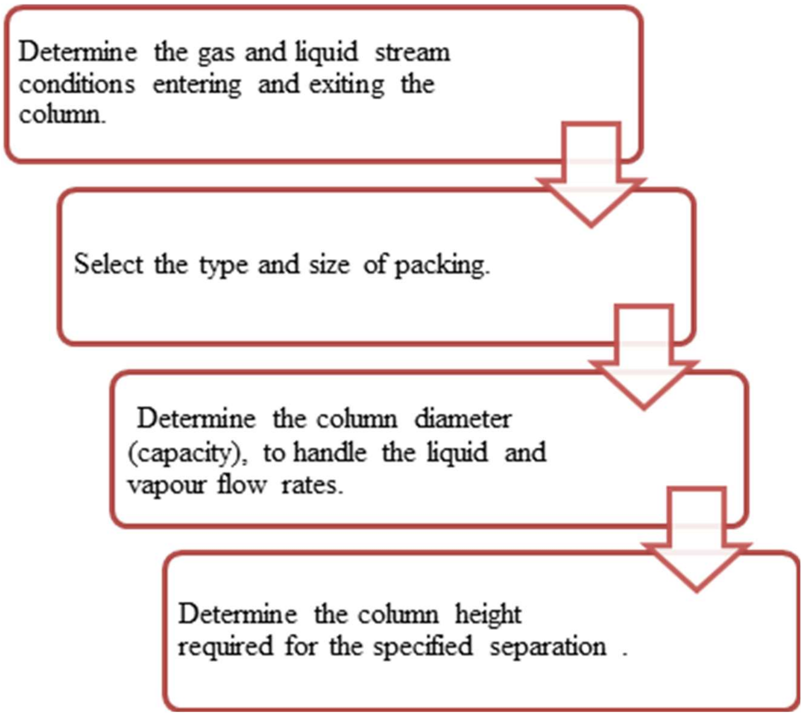
1. Vacuum to moderate pressure.
2. High pressure in selected applications
3. Increasing capacity of existing tray and packed columns

3.9.6 Typical applications

1. Chemical Ethylbenzene/styrene, tall oil, industry: cyclohexonone/-olairseparation.
2. Petrochemical Quench columns, industry: C_3- and C_4- splitters, xylene splitters Refineries Vacuum and atmospheric columns.
3. Absorption: Natural gas drying, CO_2- and H_2S-absorbers and strippers, ethylene oxide absorbers and strippers, acrylonitrile absorbers.

Figure 3.2Mellapak packing

3.9.7 Packed-column design procedures:



Determine the gas and liquid stream conditions entering and exiting the column.

Select the type and size of packing.

Determine the column diameter (capacity), to handle the liquid and vapour flow rates.

Determine the column height required for the specified separation .

Figure 3-3:The design of a packed column will involve the following steps

3.10 Column diameter

The column cross-sectional area and diameter for the selected pressure drop can be determined from the generalized pressure-drop correlation given in Figure (3.4)

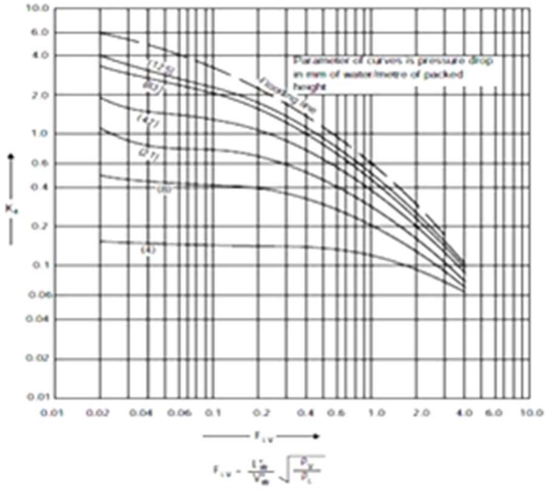


Figure 3-4: Generalized pressure drop correlation, adapted from a figure by the Norton Co. with permission

Figure (3.4) correlates the liquid and vapor flow rates, system physical properties and packing characteristics, with the gas mass flow-rate per unit cross-sectional area;with lines of constant pressure drop as a parameter.

The term K_4 on figure (3.4) is the function:

$$K_4 = \frac{13.1(V_w^*)^2 F_P\left(\frac{\mu_L}{\rho_L}\right)^{0.1}}{\rho_V(\rho_L - \rho_V)} \qquad \textbf{(3.26)}$$

The values of the flow factor FLV given in Figure 11.44 covers the range that will. Generally give satisfactory column performance. The ratio of liquid to gas flow will be fixed by the reflux ratio in distillation; and ingas absorption will be selected to give the required separation with the most economic use of solvent.

$$\textit{Percentage flooding} = \left. \frac{K_4 \textit{ at design pressure drop}}{K_4 \textit{ at flooding}} \right]^{1/2} \qquad \textbf{(3.27)}$$

This can be obtained from Figure(3.4)where a flooding line has been included with the lines of constant pressure drop.

$$V_w^* = \left[\frac{K_4 \rho v(\rho l - \rho v)}{13.1 F_P\left(\frac{\mu l}{\rho l}\right)^{0.1}}\right]^{0.5} \qquad \textbf{(3.28)}$$

$$\textbf{Column area required} = \frac{G_v}{V_w^*} \qquad \textbf{(3.29)}$$

$$\textbf{Diameter}=\sqrt{area\ \ \frac{4}{\pi}} \qquad \textbf{(3.30)}$$

Estimation of H_{OG}:

Cornell's method:

Cornell *et al*. (1960) reviewed the previously published data and presented empirical Equations for predicting the height of the gas and liquid film transfer units. Their correlation Takes into account the physical properties of the system, the gas and liquid flow-rates; and the Column diameter and height.

$$H_G=\frac{0.011\psi_h(Sc)_v^{0.5}\left(\frac{D_C}{0.305}\right)^{1.11}\left(\frac{Z}{3.05}\right)^{0.33}}{\left(L_W^{*}f_1f_2f_3\right)^{0.5}} \qquad \textbf{(3.31)}$$

$$H_L=0.305\phi_h(Sc)_L^{0.5}K_3\left(\frac{Z}{3.05}\right)^{0.15} \qquad \textbf{(3.32)}$$

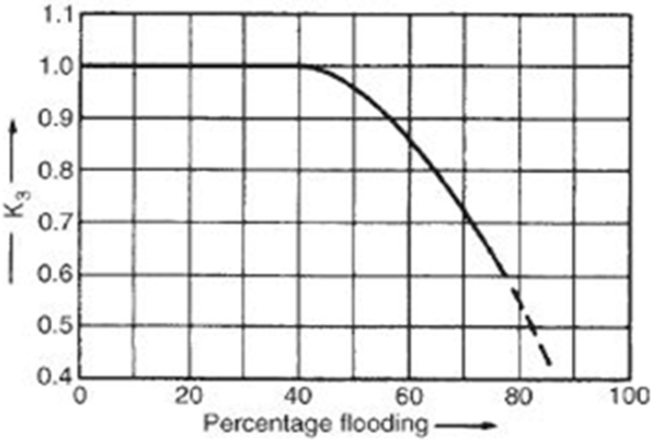


Figure 3-5: Percentage flooding correction factor

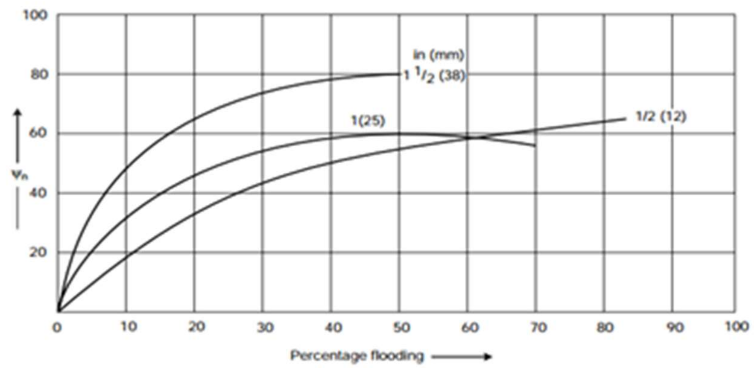


Figure 3-6: Factor for HG

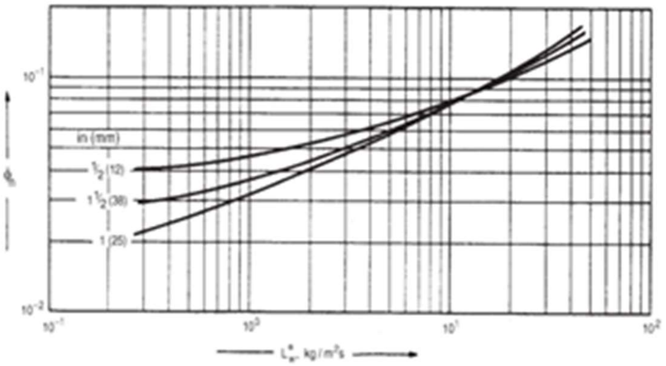


Figure 3-7: factor for H_L

The relationship between the overall height of a transfer unit and the individual film transfer units H_L and H_G, which are based on the concentration driving force across the liquid and gas films, is given by:

$$H_{OG} = H_G + m\frac{G_m}{L_m}H_L \qquad (3.33)$$

$$H_{OL} = H_L + \frac{L_m}{mG_m}H_G \qquad (3.34)$$

The number of transfer units is obtained by graphical or numerical integration ofequations.Where the operating and equilibrium lines are straight, and they can usually be considered to be so for dilute systems, the number of transfer units is given by:

NOG is the number of overall gas-phase transfer units

$$=\int_{y2}^{y1}\frac{dy}{y-ye} \qquad (3.35)$$

NOL is the number of overall liquid-phase transfer units

$$= \int_{x2}^{x1} \frac{dx}{xe-x} \qquad \textbf{(3.36)}$$

The number of overall gas-phase transfer units is often more conveniently expressed in

terms of the partial pressure of the solute gas

$$N_{OG} = \int_{P1}^{P2} \frac{dp}{p-pe} \qquad \textbf{(3.37)}$$

If the equilibrium curve and operating lines can be taken as straight and the solvent feed essentially solute free, the number of transfer units is given by:

$$N_{OG} = \frac{1}{1-\left(\frac{mGm}{Lm}\right)} \ln\left[\left(1-\frac{mGm}{Lm}\right)\frac{y1}{y2}+\frac{mGm}{Lm}\right] \qquad \textbf{(3.38)}$$

This equation is plotted in figure 3.8, which can be used to make a quick estimate of the number of transfer units required for a given separation.

It can be seen from figure 3.8that the number of stages required for a given separation is very dependent on the flow rate Lm. If the solvent rate is not set by:

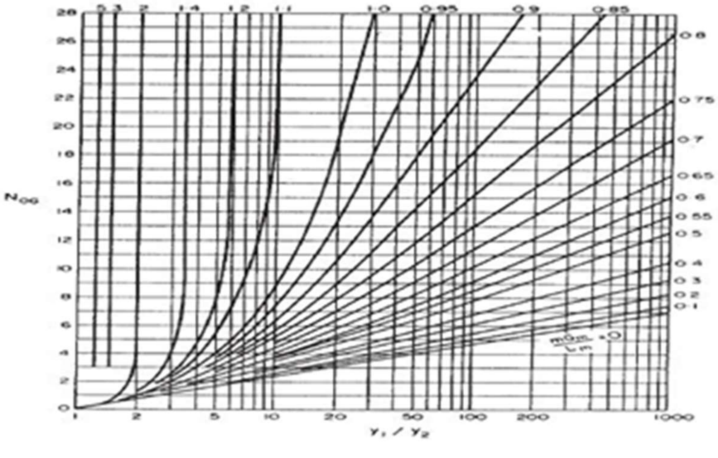


Figure 3-8: number of transfer units NOG as a function of y1/y2 with mGm/Lm as parameter.

Figure 3.9 can be used to make quick estimates of the column height at different flow rates to find the most economic value.

The height of packing required, Z, is given by:

$$\mathbf{Z = H_{OG} N_{O\,G}} \qquad \textbf{(3.39)}$$

$$\mathbf{Z = H_{OL} N_{OL}} \qquad \textbf{(3.40)}$$

Chapter 4

RESULTS AND DISCUSSIONS

4.1 Introduction

In this chapter, we mention all result of each section.

4.2 DEA result

Table (4.1) shows that all the entered solids are dissolved as a result of more than 60% of water feed with the solvent transferred to CO_3^{-2},and hco_3- and the captured CO_2 percentage equals to 67% in addition to other gases in different percentages at normal temperature and pressure .

Table 4-1: Electrolyte DEA simulation results

Substream: MIXED	ACIDGAS	GASIN	GASOUT	LEANIN	LEANOUT	RITCHIN	RITCHOUT
H_2O	0.000347	0.149643	0.002572	0.651359	0.924375	0.90179	0.474391
DEA	1.92E-15	0	8.28E-09	0.032742	0.06312	0.035392	0.010267
CO_2	2.06E-05	0.094515	0.000154	3.26E-09	2.70E-07	0.001204	0.063172
H_3O+	0	0	0	8.25E-13	2.59E-11	1.34E-09	4.23E-11
OH-	0	0	0	8.90E-06	2.09E-05	6.64E-07	1.40E-07
HCO_3^-	0	0	0	0.000183	9.45E-05	0.022813	0.004557
CO_3^{-2}	0	0	0	0.000142	2.55E-06	0.000236	0.000173
$DEAH^+$	0	0	0	0.000519	0.000753	0.026464	0.014247
$DEACOO^-$	0	0	0	7.15E-06	0.000155	0.002171	0.008755
H_2S	0.000539	0.000554	1.01E-06	1.47E-09	2.39E-07	9.04E-06	5.99E-07
HS^-	0	0	0	3.58E-05	0.000477	0.001007	0.000588

4.2.1 Pressure profiles

Figure(4. 1) shows the CO_2 concentration changes during absorption step with change in pressure, The CO_2 concentration was increased with pressure increased. The increase in pressure, decrease the distance between the molecules and so that increase the solubility of gas in the solvents.

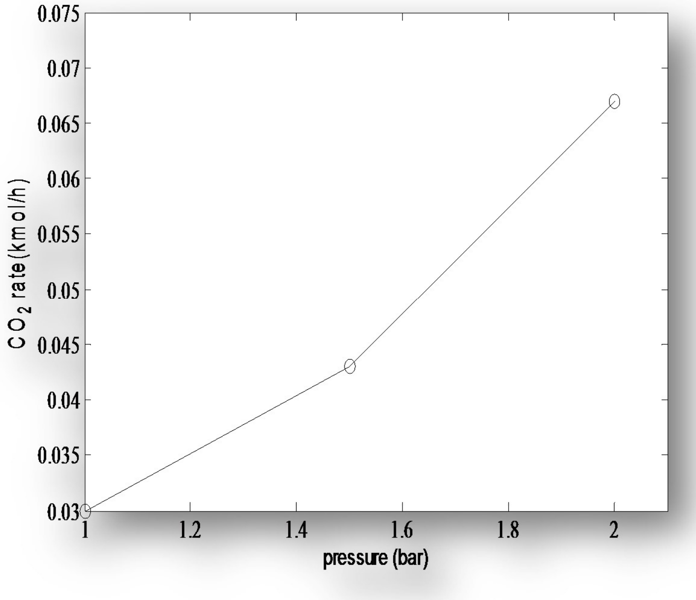


Figure 4-1: Change of the CO_2 concentration with pressure

4.2.2 Temperature profiles

Figure(4.2) shows the CO_2 concentration changes during absorption step with a change in temperature. The CO_2 concentration was decreased when the temperature was increased. The increase in temperature lead to release the gases from the solvents addition to that in the amines solvents the temperature increase cause the solvent degradation.

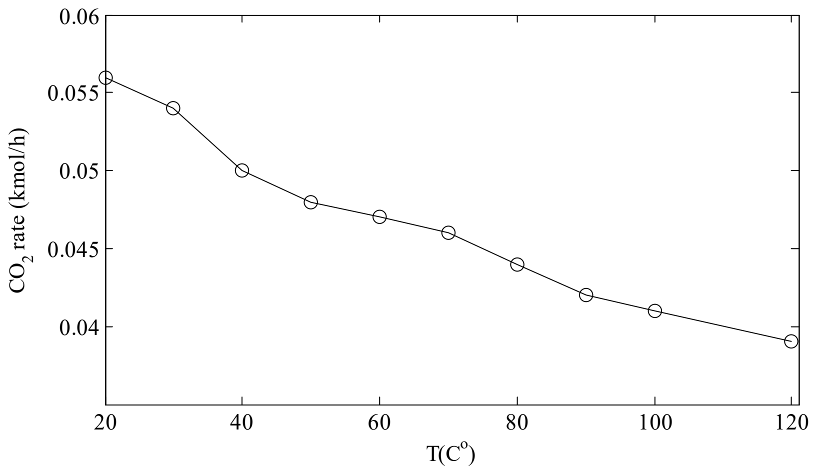


Figure 4-2: Effects of Temperature on CO_2 rate.

4.2.3 Concentration profiles

Figure (4.3) shows the CO_2 concentration changes during absorption step with a change in concentration of DEA. The CO_2 concentration was increased when the concentration was increased because it increased the capacity of the solvent.

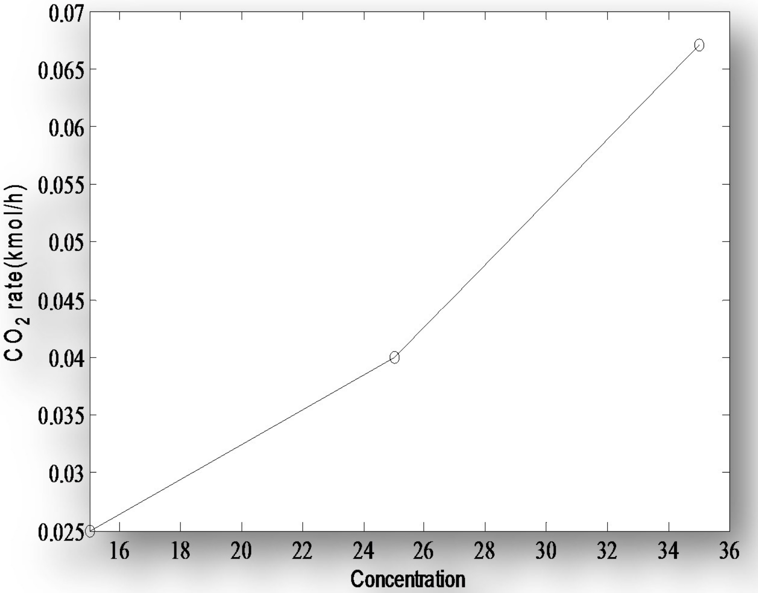


Figure 4-3: Change of the CO_2 rate with solvent concentration

4.3 Potassium carbonate (K_2CO_3) results

Table (4.2) shows that all the entered solids are dissolved as a result of more than 60% of water feed with the solvent transferred to co$_3$-^{2},and hco3- and the captured CO_2 percentage equals to 43% addition to other gases in different percentages at normal temperature and pressure.

Table 4-2: Show the potassium carbonate aspen plus results

Substream: MIXED	ACIDGAS	GASIN	GASOUT	LEANIN	LEANOUT	RITCHIN	RITCHOUT
N_2	0	1.29423	0.360207	0	0	0	1.91E-06
H_2O	0.000347	0.149643	0.002572	0.6528	0.924375	0.90179	
CO_2	1.11E-06	0.094515	0.000154	5.02E-22	9.69E-08	0.000113	0.041565

KOH	0	0	0	0	0	0	0
$H3O^+$	0	7.05E-09	0	1.08E-20	2.08E-12	3.34E-10	8.13E-20
OH^-	0	2.47E-14	0	0.2384	0.000469	1.60E-07	0.330243
HCO_3^-	0	7.00E-09	0	1.95E-10	0.000953	0.013185	0.198499
CO_3^{-2}	0	6.23E-15	0	0.0008	0.006246	0.000365	0.000129
K_2CO_3	0	0	0	0	0	0	0

4.3.1 Pressure profiles

The CO_2 concentration changes during absorption step with the change in pressure. The CO_2 concentration was increased with pressure increased. The CO_2 concentration was increased with pressure increased. The increase in pressure, decrease the distance between the molecules and so that increase the solubility of gas in the solvents.

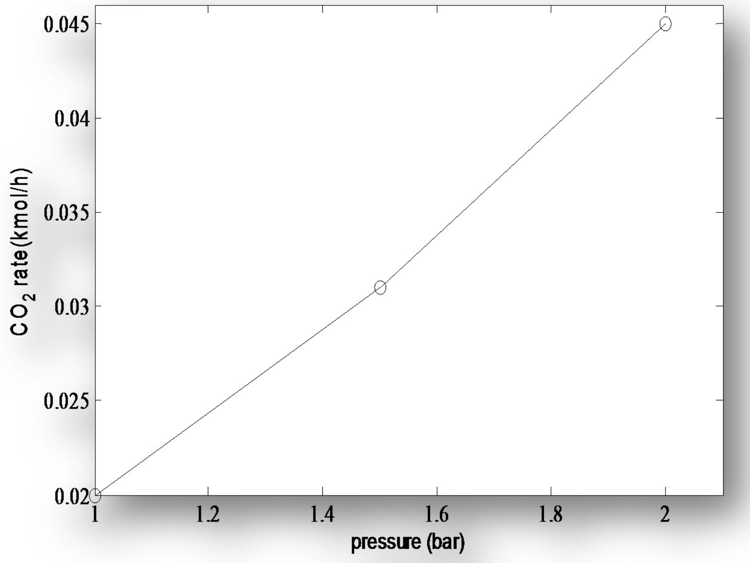


Figure 4-4: Change of the CO_2 concentration with pressure

4.3.2 *Temperature profiles*

Figure(4. 5) shows the CO_2 concentration changes during absorption step with a change in temperature. The CO_2 concentration was increased with temperature increased to specified temperature because the solubility of the potassium carbonate is high.

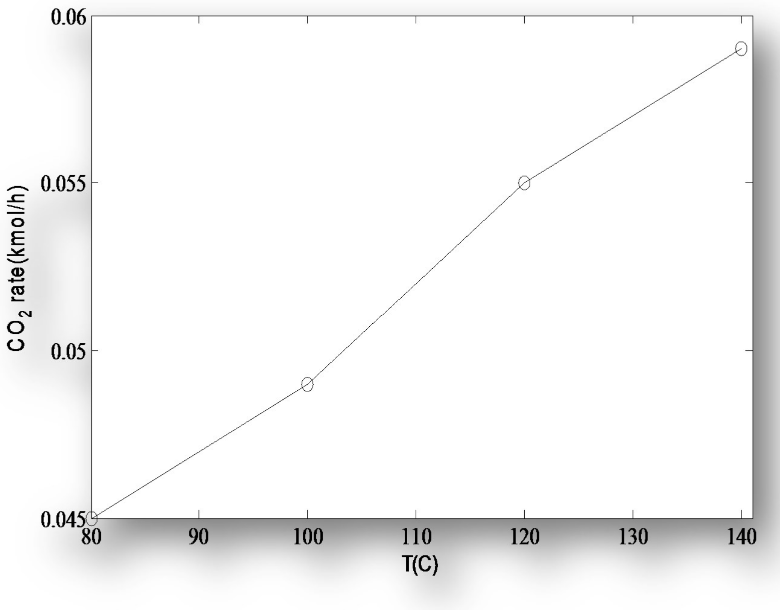


Figure 4-5: Change of the CO_2 concentration with temperature

4.3.3 Concentration profiles

Figure (4.6) shows the CO_2 concentration changes during absorption step with a change in concentration of K_2CO_3. The CO_2 concentration was increased when the concentration was increased because it increased the capacity of the solvent

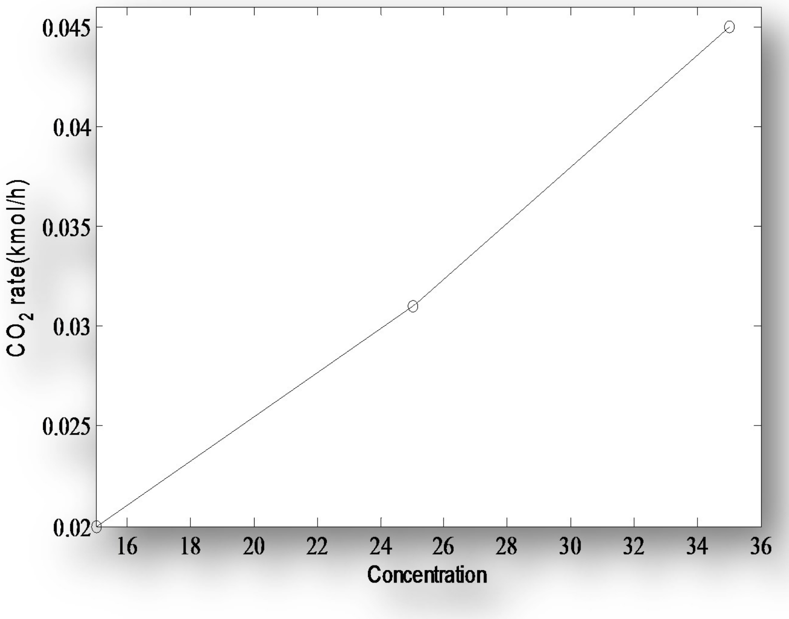


Figure 4-6: Change of the CO_2 concentration with solvent concentration

4.4 Potassium carbonate promoted by DEA results

Table (4.3) shows that all the entered solids are dissolved as a result of more than 60% of water feed with the solvent transferred to co3-2,and Hco3- and the captured co2 percentage equals to 82% in addition to other gases in different percentages at normal temperature and pressure.

Table 4-3: Potassium carbonate promoted aspen plus results

Substream: MIXED	ACIDGAS	GASIN	GASOUT	LEANIN	LEANOUT	RITGHIN	RITCHOUT
CO_2	1.80E-06	0.094515	0.000154	3.08E-06	3.08E-06	3.86E-10	0.078553
H_2O	4.52E-19	0.149643	1.298165	9.24E-06	9.24E-06	2.07E-13	2.07E-13
SO_2	1.80E-10	0.005234	0.065035	2.55E-10	2.55E-10	4.87E-18	4.87E-18
O_2	0	0	0	0	0	0	0
N_2	5.19E-31	1.101928	1.72E-05	1.71E-18	1.71E-18	3.16E-15	3.16E-15
DIETH-01	0	0	0	0	0	0	0
DEA^+	0	0	0	0	0	0	0
$H3O^+$	0	4.57E-05	0	1.35E-06	1.35E-06	2.98E-25	2.98E-25
K^+	0	0	0	0	0	0	0
$K_2SO_3(S)$	0	0	0	0	0	0	0
$DEACOO^-$	0	0	0	0	0	0	0
OH^-	0	3.55E-15	0	6.70E-12	6.70E-12	8.56E-17	8.56E-17
HSO_3^-	0	4.57E-05	0	9.54E-09	9.54E-09	9.62E-10	9.62E-10
HCO_3^-	0	1.16E-09	0	6.22E-10	6.22E-10	1.07E-05	1.07E-05
SO_3^{--}	0	2.86E-10	0	1.28E-15	1.28E-15	8.50E-07	8.50E-07
CO_3^{--}	0	6.71E-18	0	1.09E-06	1.09E-06	3.08E-06	3.08E-06

4.4.1 Pressure profiles

Figure(4. 7) shows the CO_2 concentration changes during absorption step with a change in pressure. The CO_2 concentration was increased with pressure increased. The CO_2 concentration was increased with pressure increased. The increase in pressure, decrease the distance between the molecules and so that increase the solubility of gas in the solvents.

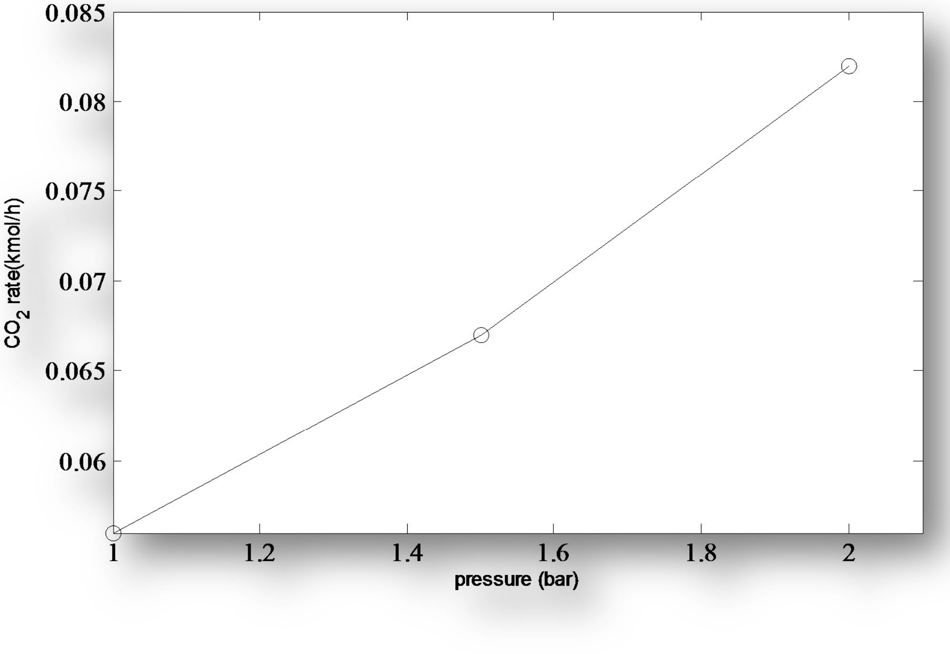


Figure 4-7: Change of the CO_2 concentration with pressure

4.4.2 Temperature profiles

Figure(4. 8) shows the CO_2 concentration changes during absorption step with a change in temperature. The CO_2 concentration was increased with temperature increased. The CO_2 concentration was increased with temperature increased to specified temperature because the solubility of the potassium carbonate is high.

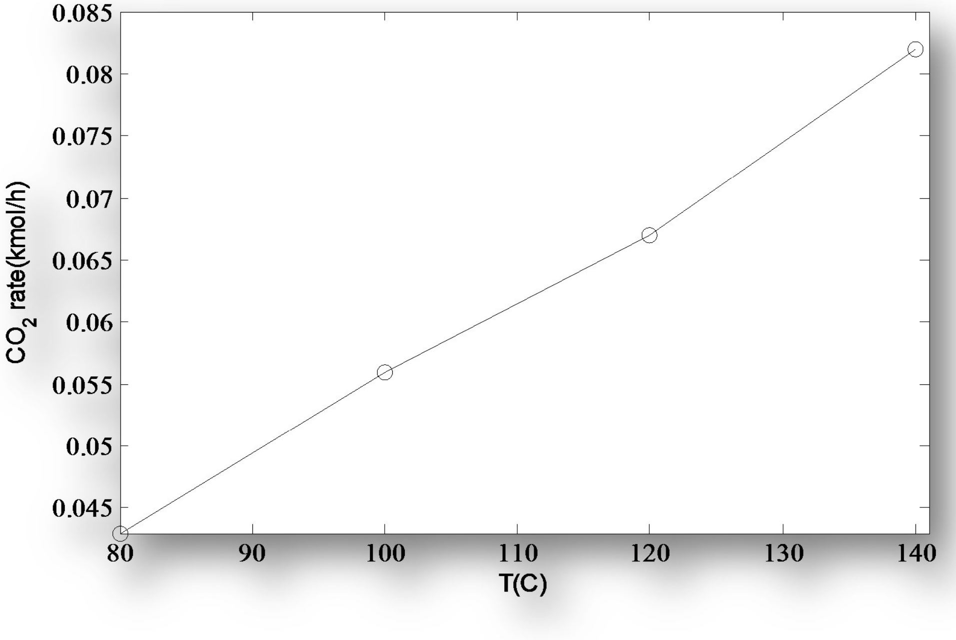


Figure 4-8: Changeof the CO_2 concentration with temperature

4.4.3 Concentration profile

Figure (4.3) shows the CO_2 concentration changes during absorption step with change in concentration of DEA, The CO_2 concentration was increased when potassium carbonate concentration was promoted by little amount of DEA as enhanced, The enhancement rate decreases when the concentration of DEA promoter reached the values greater than 4%.

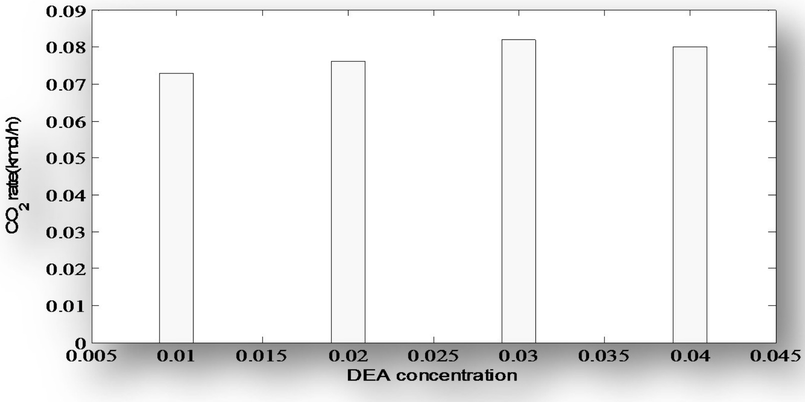


Figure 4-9: Change of the CO_2 concentration with concentration

Table 4-4: Design of Absorption Column: (table data obtained from Raoult's law)

Mole of CO_2 in DEA	0.058	0.06	0.062	0.064	0.066	0.068	0.007
Partial pressure of gas Kpa	5.87	6.08	6.282	6.4848	6.687	6.89	7.092

Assume that P_{total}= 1atm =101.325 Kpa

y_1 = 0.0945

Partial pressure of CO_2 in the feed (P_{CO2}) = 9.5756 Kpa

Number of stage:

Partial pressure in the exist gas at 90 per cent recovery = 9.576 × 0.1 = 0.9576 Kpa

Molecular weights:

$CO_2 = 44$, $N_2 = 28$, O_2=32, H_2O=18 , SO_2 =64 , DEA =105.2

Slope of equilibrium line:

From the data : partial pressure at 0.068 w/w co_2 = 6.89 Kpa

Mole fraction in vapor = $\frac{6.89\text{ Kpa}}{101.325\text{ Kpa}}$ =0.068

Mole fraction in liquid = $\frac{\frac{6.89}{105.2}}{\frac{6.89}{105.2}+\frac{93.11}{18}}$ = 0.0125

Slope (M) = $\frac{0.068}{0.0125}$ = 5.44

Using Figure (3.8)the number of stages required at different water rates will be determined and the "optimum" rate chosen:

$$\frac{y1}{y2} = \frac{p1}{p2} = \frac{9.576}{0.9576} = 10$$

Table 4-5:The optimum rate

$m\frac{Gm}{Lm}$	0.2	0.4	0.55	0.7	0.75	0.8	0.9	0.95	1.0	1.1
N_{OG}	2.3	3	3.7	4.4	4.7	5.6	5.8	7.3	9	18

It can be seen that the “optimum” will be between mG_m/L_m = 0.9 to 1.0, as would be expected. Below 0.9 there is only a small decrease in the number of stages required with increasing liquid rate; and above 1.0the number of stages increases rapidly with decreasing liquid rate. Check the liquid outlet composition at 0.9 and 1.0 :

Material balance:

$L_m x_1 = G_m(y_1 - y_2)$

$x_1 = \frac{Gm}{Lm}(0.0945 \times 0.9) = \frac{Gm}{Lm}(0.08505) \times \frac{m}{5.44}$

at $m\frac{Gm}{Lm}$ =0.9 ,x_1=0.09 mole fraction

at $m\frac{Gm}{Lm}$ = 1.0 ,x_1=0.14 mole fraction

Use 1.0, as the higher concentration will favor the stripper design and operation, without significantly increasing the number of stages needed in the absorber.

N_{OG} =9

4.5 Column diameter:

Gas flow rate =1482.524 mole /h = 41.69 Kg/h

Liquid flow rate =467.067 mole /h=49.135 Kg/h

Select SULZER Mellapak350Y , $F_P = 75\ m^{-1}$

Gas density =2.38174 Kg/m^3

Liquid density=1027.86 Kg/m^3

Liquid viscosity = 8×10^{-3}Ns/m2

F_{LV}= 0.0567

Design for a pressure drop of 20 mm H_2O/m packing

From Figure (3.4)

K_4=0.68

At the flooding K_4= 4

Percentage flooding $=\sqrt{0.68/4}\times 100 = 41.23\ \%$

$V^*_{W=2.34}$ Kg/m^{2}s

Column area required= $5\times10^{-0.6}$ m^2

Diameter = 1.26m

Column area $=\frac{\pi}{4}\times(1.26)^2=1.24$ m^2

Estimation of H_{OG}:

Cornell's method :

$D_L=2.2\times10^{-9} m^2/s$

$D_V=1.5\times10^{-8} m^2/s$

$\mu v=0.013\times10^{-3}$ Ns/m^3

Calculate the Schmidt number:

$(Sc)_v=372$

$(Sc)_L=3537.8$

Calculate the liquid mass flow rate per unit area

$L_W=4671.22$ $Kg/s.m^2$

From figure (3.5), (3.6), (3.7)

$^{K}{}_{3}=0.98$

$\Psi_h=78$

$\Phi_h=0.047$

$H_L=0.833$ m

$H_G=2.255$ m

$H_{og}=3.088$ m

$Z \cong 9m$

Table 4-6: Summary for absorption tower design

Number of transfer unit	9
Column diameter	1.26 m
Height of gas phase transfer unit	2.225 m
Height of liquid phase transfer unit	0.833 m
Over all transfer unit	3.088 m

Height of tower	9 m

Chapter 5

CONCLUSION & RECOMMENDATION

5.1 Conclusion

The best condition for DEA to works high rate of CO_2 capture at normal temperature and pressure, but it not efficient and economical regeneration process with lower resistance to degradation.

Potassium carbonate absorption process at high temperatures resulting in a more efficient and economical regeneration process and better resistance to degradation than commonly seen with amine solvents at high temperatures.

The absorption rates of CO_2 in diethanolamine (DEA) promoted potassium carbonate (K_2CO_3) increases with the increase of the mass Fraction of (DEA),also very small amount of DEA can significantly enhance the absorption of CO_2 in K_2CO_3 aqueous solution at high temperatures which is recorded an absorption rate of 82%.

The enhancement rate decreases when the concentration of DEA promoter reached the values greater than 4%.

5.2 Recommendation

1- To do an experimental work with a series of heterocyclic amine functionalized promoters.
2- To study the energy balance and energy losses around the process units in order to observe .

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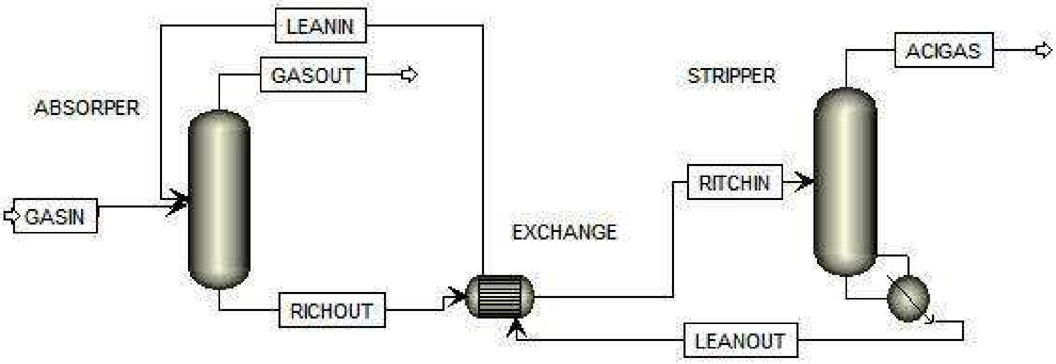
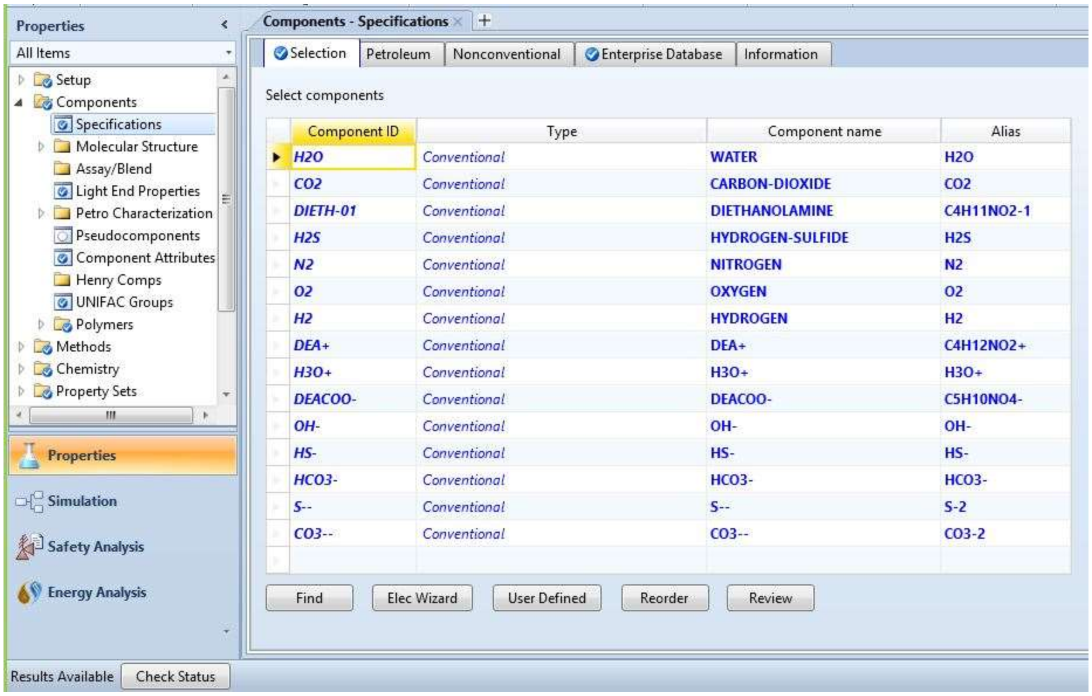
Appendix-A

Model for process simulation



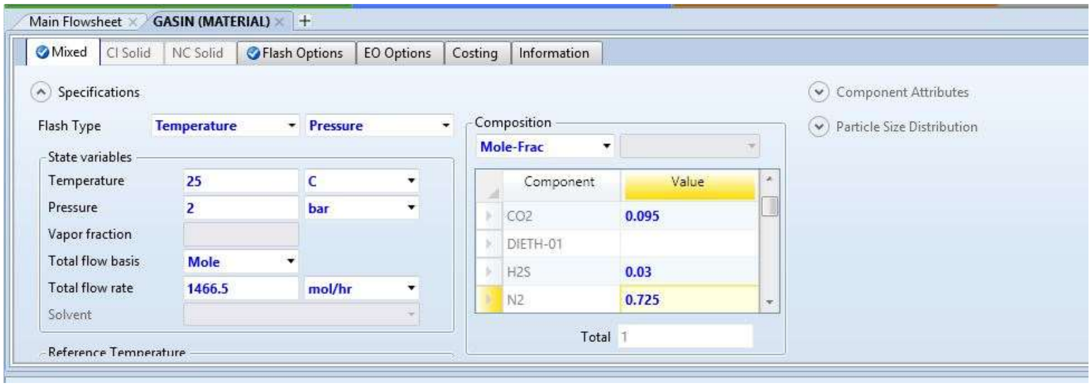
Data input for DEA simulation:-



Select components

Component ID	Type	Component name	Alias
H2O	Conventional	WATER	H2O
CO2	Conventional	CARBON-DIOXIDE	CO2
DIETH-01	Conventional	DIETHANOLAMINE	C4H11NO2-1
H2S	Conventional	HYDROGEN-SULFIDE	H2S
N2	Conventional	NITROGEN	N2
O2	Conventional	OXYGEN	O2
H2	Conventional	HYDROGEN	H2
DEA+	Conventional	DEA+	C4H12NO2+
H3O+	Conventional	H3O+	H3O+
DEACOO-	Conventional	DEACOO-	C5H10NO4-
OH-	Conventional	OH-	OH-
HS-	Conventional	HS-	HS-
HCO3-	Conventional	HCO3-	HCO3-
S--	Conventional	S--	S-2
CO3--	Conventional	CO3--	CO3-2

Operation condition data for DEA flue gas



Flash Type: Temperature, Pressure

State variables

Temperature: 25 C

Pressure: 2 bar

Vapor fraction:

Total flow basis: Mole

Total flow rate: 1466.5 mol/hr

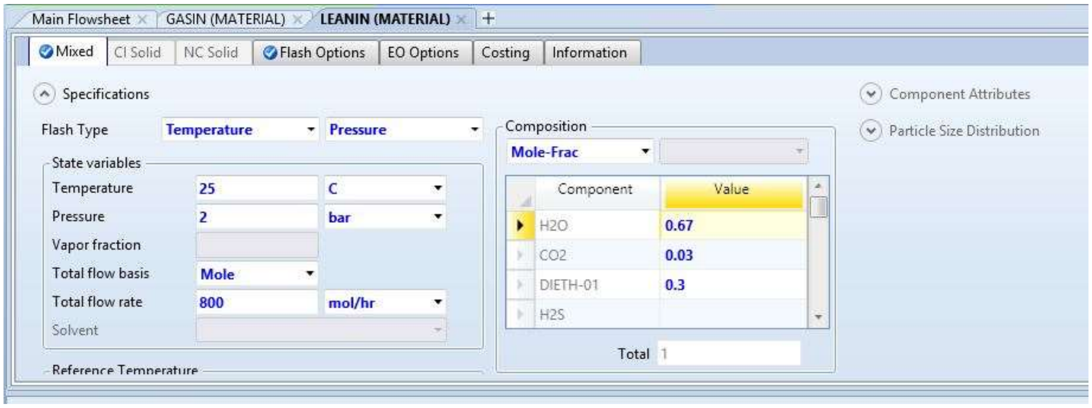
Solvent:

Composition: Mole-Frac

Component	Value
CO2	0.095
DIETH-01	
H2S	0.03
N2	0.725

Total 1

Operation condition data for DEA lean solvents



Flash Type: Temperature, Pressure

State variables

Temperature: 25 C

Pressure: 2 bar

Vapor fraction:

Total flow basis: Mole

Total flow rate: 800 mol/hr

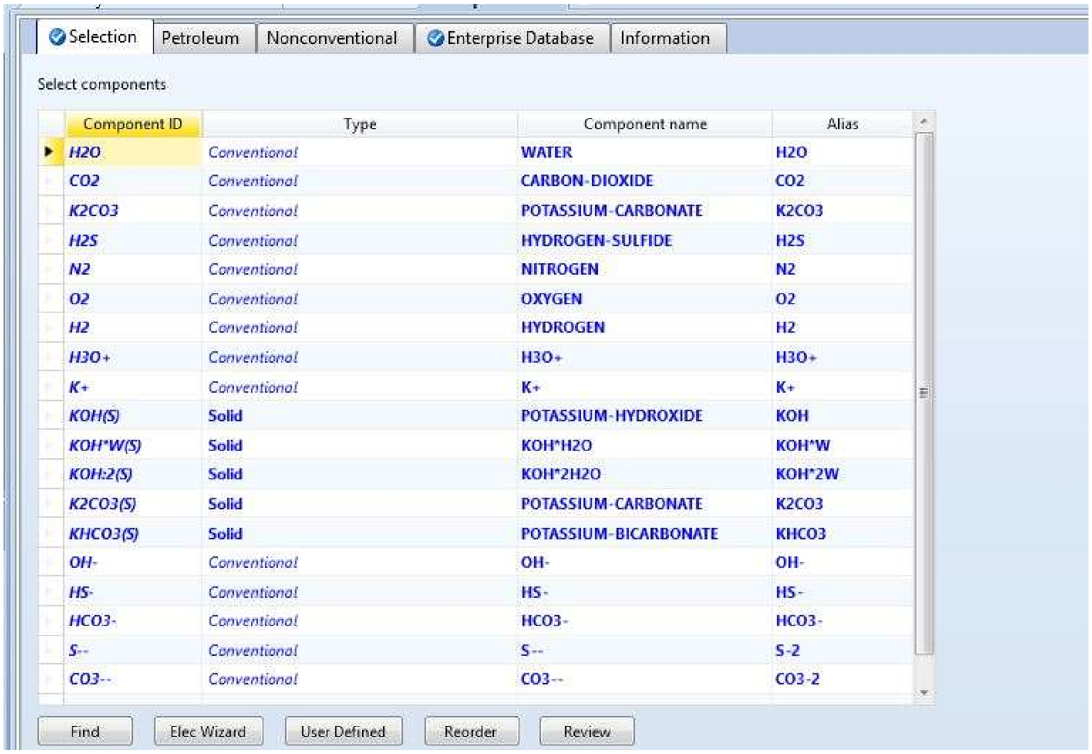
Solvent:

Composition: Mole-Frac

Component	Value
H2O	0.67
CO2	0.03
DIETH-01	0.3
H2S	

Total 1

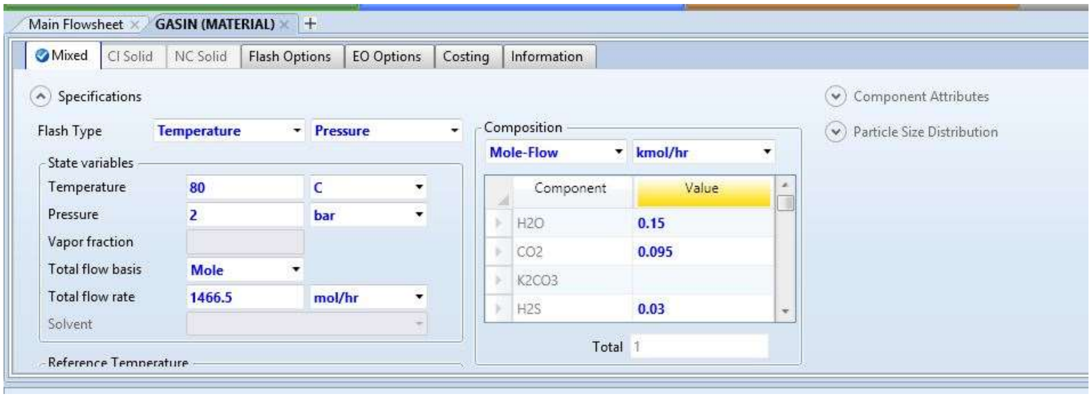
Data input for $k_2co_3$simulation



Select components

Component ID	Type	Component name	Alias
H2O	Conventional	WATER	H2O
CO2	Conventional	CARBON-DIOXIDE	CO2
K2CO3	Conventional	POTASSIUM-CARBONATE	K2CO3
H2S	Conventional	HYDROGEN-SULFIDE	H2S
N2	Conventional	NITROGEN	N2
O2	Conventional	OXYGEN	O2
H2	Conventional	HYDROGEN	H2
H3O+	Conventional	H3O+	H3O+
K+	Conventional	K+	K+
KOH(S)	Solid	POTASSIUM-HYDROXIDE	KOH
KOH*W(S)	Solid	KOH*H2O	KOH*W
KOH:2(S)	Solid	KOH*2H2O	KOH*2W
K2CO3(S)	Solid	POTASSIUM-CARBONATE	K2CO3
KHCO3(S)	Solid	POTASSIUM-BICARBONATE	KHCO3
OH-	Conventional	OH-	OH-
HS-	Conventional	HS-	HS-
HCO3-	Conventional	HCO3-	HCO3-
S--	Conventional	S--	S-2
CO3--	Conventional	CO3--	CO3-2

Operation condition data for k_2co_3 flue gas



Flash Type: Temperature, Pressure

State variables

Temperature: 80 C

Pressure: 2 bar

Vapor fraction:

Total flow basis: Mole

Total flow rate: 1466.5 mol/hr

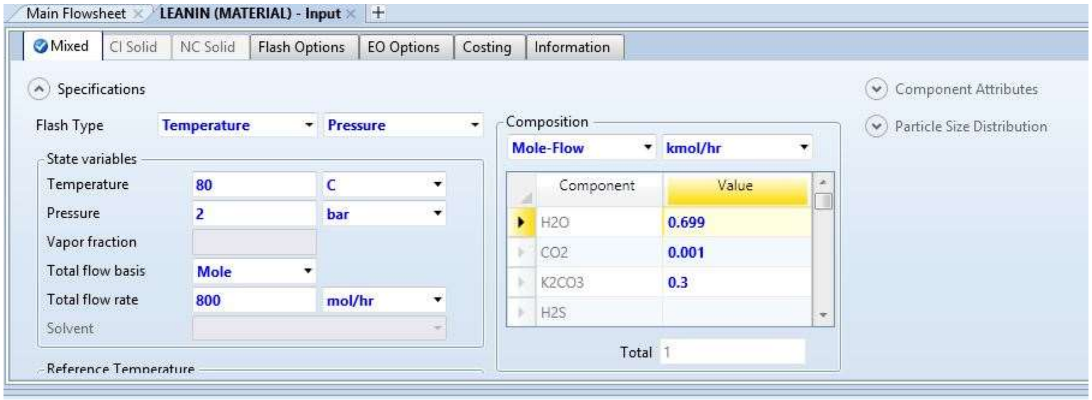
Solvent:

Composition: Mole-Flow, kmol/hr

Component	Value
H2O	0.15
CO2	0.095
K2CO3	
H2S	0.03

Total 1

Operation condition data for k_2co_3 lean solvent:-



Flash Type: Temperature, Pressure

State variables

Temperature: 80 C

Pressure: 2 bar

Vapor fraction:

Total flow basis: Mole

Total flow rate: 800 mol/hr

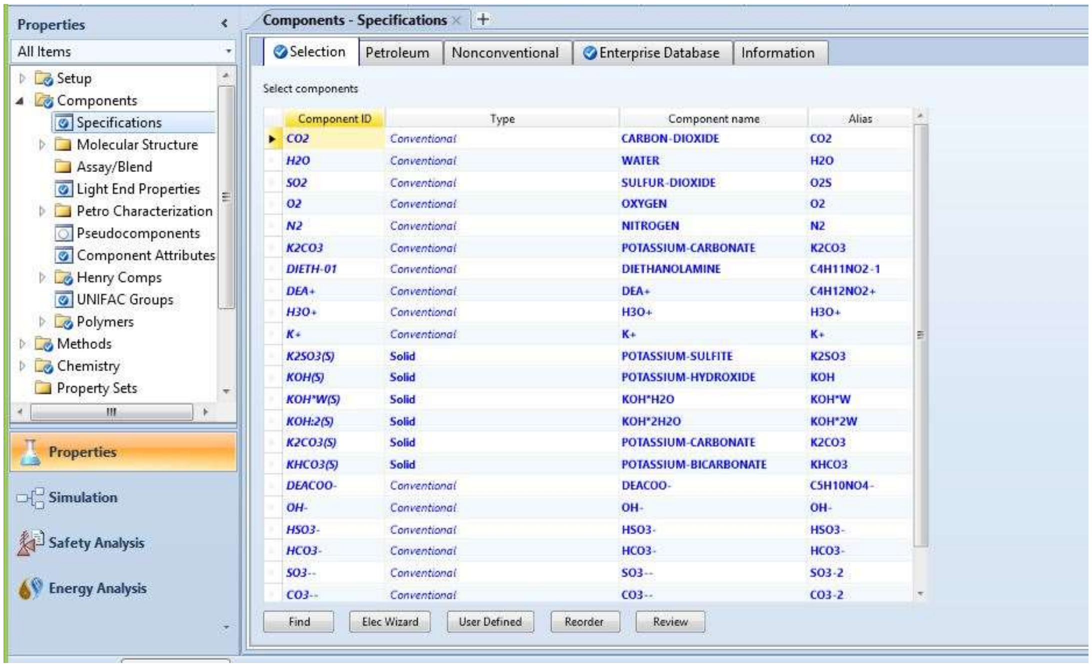
Solvent:

Composition: Mole-Flow, kmol/hr

Component	Value
H2O	0.699
CO2	0.001
K2CO3	0.3
H2S	

Total: 1

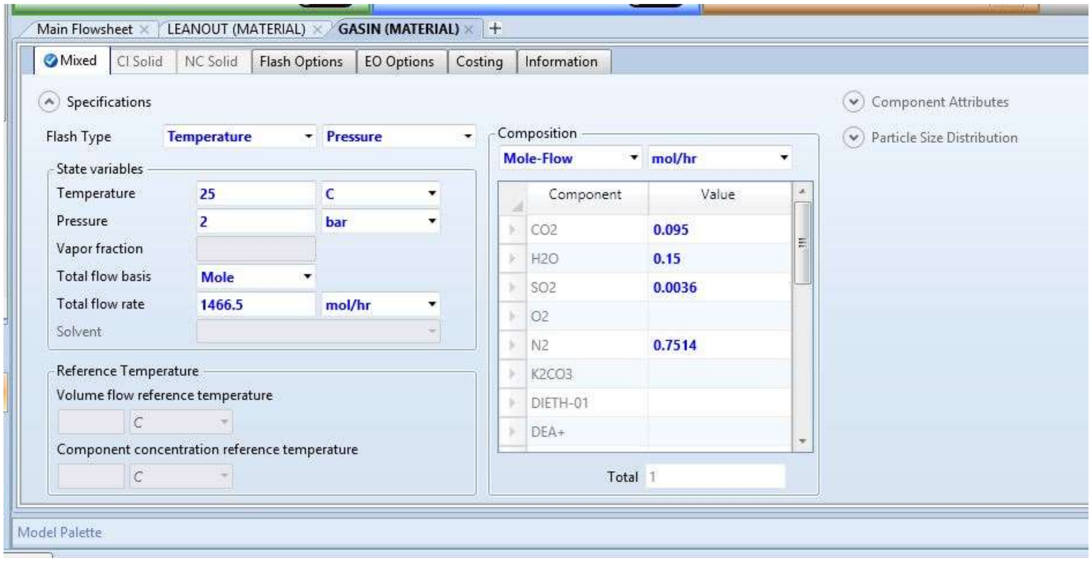
Data input for k_2co_3 promoted by DEA simulation



Select components

Component ID	Type	Component name	Alias
CO2	Conventional	CARBON-DIOXIDE	CO2
H2O	Conventional	WATER	H2O
SO2	Conventional	SULFUR-DIOXIDE	O2S
O2	Conventional	OXYGEN	O2
N2	Conventional	NITROGEN	N2
K2CO3	Conventional	POTASSIUM-CARBONATE	K2CO3
DIETH-01	Conventional	DIETHANOLAMINE	C4H11NO2-1
DEA+	Conventional	DEA+	C4H12NO2+
H3O+	Conventional	H3O+	H3O+
K+	Conventional	K+	K+
K2SO3(S)	Solid	POTASSIUM-SULFITE	K2SO3
KOH(S)	Solid	POTASSIUM-HYDROXIDE	KOH
KOH*W(S)	Solid	KOH*H2O	KOH*W
KOH:2(S)	Solid	KOH*2H2O	KOH*2W
K2CO3(S)	Solid	POTASSIUM-CARBONATE	K2CO3
KHCO3(S)	Solid	POTASSIUM-BICARBONATE	KHCO3
DEACOO-	Conventional	DEACOO-	C5H10NO4-
OH-	Conventional	OH-	OH-
HSO3-	Conventional	HSO3-	HSO3-
HCO3-	Conventional	HCO3-	HCO3-
SO3--	Conventional	SO3--	SO3-2
CO3--	Conventional	CO3--	CO3-2

Operation condition data for k$_2$co$_3$ –DEA flue gas



Flash Type: Temperature, Pressure

State variables

Temperature: 25 C

Pressure: 2 bar

Vapor fraction:

Total flow basis: Mole

Total flow rate: 1466.5 mol/hr

Solvent:

Reference Temperature

Volume flow reference temperature: C

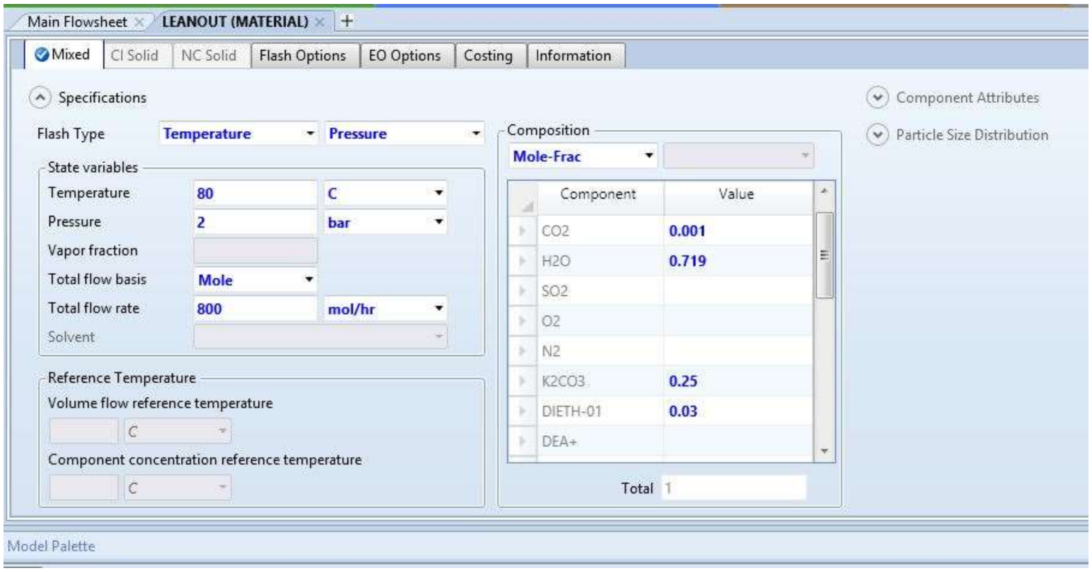
Component concentration reference temperature: C

Composition: Mole-Flow, mol/hr

Component	Value
CO2	0.095
H2O	0.15
SO2	0.0036
O2	
N2	0.7514
K2CO3	
DIETH-01	
DEA+	

Total 1

Operation condition data for k$_2$co$_3$ –DEA lean solvent



Flash Type: Temperature, Pressure

State variables

Temperature: 80 C

Pressure: 2 bar

Vapor fraction:

Total flow basis: Mole

Total flow rate: 800 mol/hr

Solvent:

Reference Temperature

Volume flow reference temperature: C

Component concentration reference temperature: C

Composition: Mole-Frac

Component	Value
CO2	0.001
H2O	0.719
SO2	
O2	
N2	
K2CO3	0.25
DIETH-01	0.03
DEA+	

Total 1