

Master's Thesis 2013

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Title: Vapor recompression in absorption  
and desorption process for CO<sub>2</sub>  
capture

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## MASTER'S THESIS, COURSE CODE FMH606

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### Abstract:

Due to high emissions of CO<sub>2</sub> and the impact it has on our environment, CO<sub>2</sub> capture from gases is becoming more and more important. There has been performed a lot of work regarding simulation of CO<sub>2</sub> removal at TUC However, little has been done on comparison of different tools.

In this thesis, three different CO<sub>2</sub>-capture configurations have been simulated using two different process simulators, Aspen HYSYS and Aspen Plus. In Aspen HYSYS, Kent-Eisenberg and Li-Mather was used as equilibrium models while eNRTL (electrolyte Non-Random Two-Liquid) was used in Aspen Plus. Both equilibrium and rate-based simulations were performed in Aspen Plus. The configurations simulated were a standard post-combustion process, vapor recompression and vapor recompression combined with split stream.

CO<sub>2</sub> removal efficiency was kept at 85% and Murphree efficiency was kept constant at 0.25. Number of stages in the absorber varied in some cases. The energy consumption was then compared for all the cases.

The energy consumption for the standard post-combustion process was calculated to 3.37 – 4.26 MJ/kg CO<sub>2</sub>. The Aspen Plus equilibrium model calculated the lowest energy consumption while the Aspen Plus rate-based model calculated the highest.

The equivalent energy consumption for vapor recompression was calculated to 2.92 – 3.82 MJ/kg CO<sub>2</sub>. The equivalent energy consumption is reboiler duty + 4 times compressor duty. The Aspen HYSYS Li-Mather model calculated the lowest value while the Aspen Plus rate-based model calculated the highest. The optimum pressure before compression was found to be 1.2 bar for all cases except for the rate-based calculation of vapor recompression combined with split stream.

The equivalent energy consumption for vapor recompression combined with split stream was calculated to 3.0 – 4.1 MJ/kg CO<sub>2</sub>. The Aspen HYSYS Li-Mather model calculated the lowest energy consumption while the Aspen Plus rate-based model calculated the highest. The pressure before compression was kept at 1.2 bar.

The different programs and models calculated an improvement in equivalent energy consumption for the vapor recompression configuration varying from 0.21 – 0.50 MJ/kg CO<sub>2</sub>. The Aspen Plus equilibrium model calculated the lowest improvement while Kent-Eisenberg and Li-Mather calculated the highest. For vapor recompression combined with split stream, the improvement varied from 0.15 – 0.39 MJ/kg CO<sub>2</sub>. Aspen Plus rate-based calculated the lowest value while Aspen HYSYS Li-Mather calculated the highest. This process configuration proved difficult to simulate using the rate-based model.

The results indicate that the vapor recompression configuration is considered to be the most reasonable configuration for reducing the energy consumption. This is in agreement with earlier studies. The most optimum process configuration and most optimum process parameters were calculated to be the same in almost all the simulations.

**Telemark University College accepts no responsibility for results and conclusions presented in this report.**

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# Preface

This thesis has been developed during the 4<sup>th</sup> semester of the master program Process Technology at Telemark University College.

Two different process simulation tools have been used, Aspen HYSYS and Aspen Plus. Knowledge of the simulation tools is not fundamental to the reader.

However, the reader should have knowledge regarding chemical engineering when reading this report

I would like to thank my supervisor, Lars Erik Øi, for his guidance and patience during the development of this thesis.

Porsgrunn, 31. May 2013  
Stian Holst Pedersen Kvam

# Nomenclature

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$\Delta T$	Temperature difference
$\Delta P$	Pressure drop
ADJ	Adjust-operator
eNRTL	Electrolyte Non-Random Two-Liquid
Eq	Equilibrium
K-E	Kent-Eisenberg
L	Lean (Aspen Plus simulations)
L-M	Li-Mather
LNG-exchanger	Multi-stream exchanger
MEA	Monoethanolamine
NRTL	Non-Random Two-Liquid
PFD	Process flow diagram
R	Rich (Aspen Plus simulations)
RB	Rate-based
RCY	Recycle
S	Semilean (Aspen Plus simulations)
Wt%	Weight-%
Q	Duty

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# 1 Introduction

Emission of greenhouse gases, i.e. carbon dioxide, fluorine gases, nitrous oxide and methane, is contributing to one of the largest challenges in the world today. Even though F-gases, nitrous oxide and sulfur hexafluoride have decreased over the last two decades, the CO<sub>2</sub> emissions have increased. According to “Statistisk sentralbyrå” (SSB 2012), CO<sub>2</sub> emissions increased by 28% in the period 1990-2011 and contributed to 84% of the total amount of greenhouse gas emissions.

Due to the climate change and the impact CO<sub>2</sub> has on it, new technologies is under development to keep greenhouse gas emissions under control.

Utvikling i klimagassutslipp 1990-2011. Millioner tonn CO<sub>2</sub>-ekvivalenter

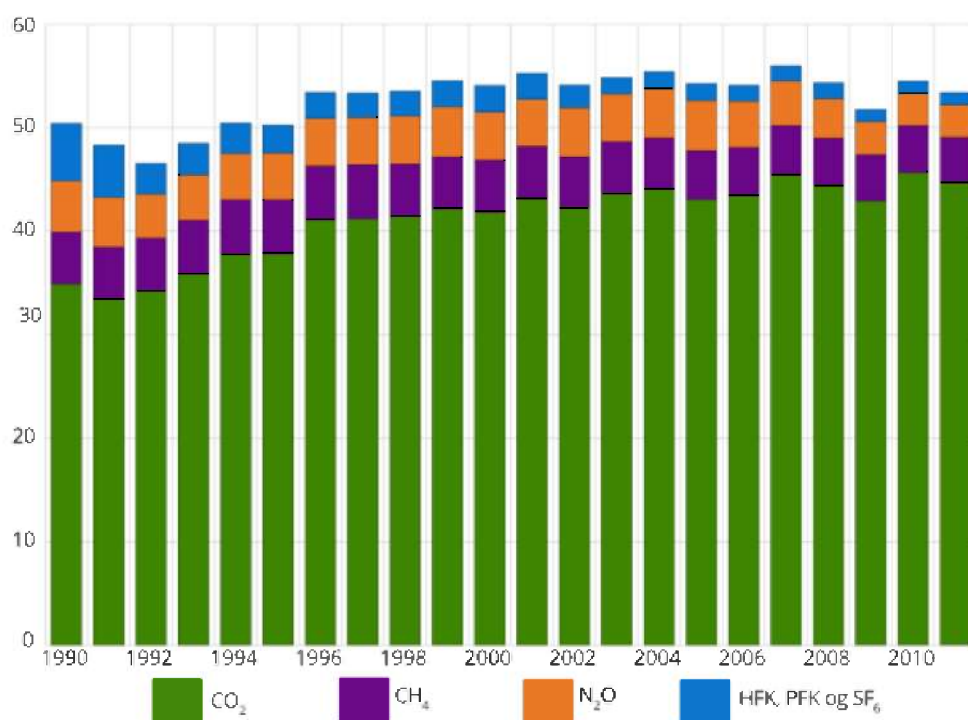


Figure 1-1 Emission of greenhouse gases from 1990-2011 in MTON CO<sub>2</sub>-equivalents(SSB 2012)

## 1.1 Purpose

Purpose of this thesis is to calculate the potential in energy reduction using vapor recompression in CO<sub>2</sub> capture using monoethanolamine. Another aim of this thesis is to compare Aspen HYSYS and Aspen Plus. At Telemark University College, there has been performed a lot of work regarding simulation of CO<sub>2</sub> capture but most of this work has been performed by focusing on one simulation software at the time.

## 1.2 Previous work

For most of the work performed at Telemark University College, the focus has primarily been on one process simulator at the time, but there are a couple of theses that compares different process simulators.

Kumara Munasinghe(Munasinghe 2009) compared Aspen HYSYS and ProMax for the absorption process. He compared the effects of different models such as Li-Mather, Kent-Eisenberg, Wilson, NRTL and eNRTL.

It was concluded that ProMax gives better results; almost 66% lower compared to Aspen Hysys, when it comes to MEA concentration in the exhaust gas. Munasinghe still concluded that Aspen HYSYS with either Li-Mather or Kent-Eisenberg was better to use and that Wilson or NRTL was better to use for the water wash section.

Espen Hansen(Hansen 2011) performed simulation of a general CO<sub>2</sub> capture process using three different process simulators; Aspen HYSYS, Aspen Plus and ProMax. The removal efficiencies varied from 77.22 – 88.60% and the reboiler duties varied from 3.53 – 4.43 MJ/kg CO<sub>2</sub>. It was found that Aspen Plus rate-based model calculated the largest reboiler duty while Aspen HYSYS Li-Mather model calculated the lowest reboiler duty. The differences in removal efficiencies are due to variation of circulation rate, variation of stages and variation of Murphree efficiencies.

Jostein Bergstrøm(Bergstrøm 2012) compared Aspen HYSYS and Aspen Plus regarding split-stream configuration. In Aspen HYSYS, both Kent-Eisenberg and Li-Mather were used and equilibrium- and rate-based model was used in Aspen Plus.

Li-Mather gave the highest reduction in reboiler duty with 0.2-0.25 MJ/kg CO<sub>2</sub>. Kent-Eisenberg and the equilibrium model in Aspen Plus gave a reduction of approximately 0.15 MJ/kg CO<sub>2</sub>.

The rate-based model in Aspen Plus gave the lowest reduction of approximately 0.05-0.10 MJ/kg CO<sub>2</sub>.

In a bachelor thesis(Berg et. al 2012), the aim was to compare four different flow sheet configurations; standard post-combustion process, split stream, vapor recompression and a combination of vapor recompression and split stream. The energy consumption was respectively found to be 3,3-, 3,2-, 2,9- and 3,0 MJ/kg CO<sub>2</sub> removed. The standard post combustion process was simulated using Kent-Eisenberg model while Li-Mather model was used for the other configurations.

## 1.3 Objectives

Thesis description can be found in Appendix A.



## 2 Process descriptions

Due to high operational costs involved running a post combustion process, finding alternative configurations in order to reduce reboiler duty have become more applicable. In this section, different configurations will be described.

### 2.1 Standard post combustion process

The exhaust gas enters the bottom of the absorber where the gas meets the absorption liquid, MEA and water, which enter at the top of the absorber.

The counter-current flow of the flue gas and the absorption liquid makes sure that the MEA reacts with CO<sub>2</sub>. The gas leaving the top of the absorber contains mostly water and nitrogen but also some MEA and CO<sub>2</sub>. The bottom product is a CO<sub>2</sub>-rich stream.

The rich stream is being pumped through the main heat exchanger where it is heated by the bottom product of the distillation column. The heated rich stream enters the distillation column where the MEA is stripped of the absorption liquid so it can be reused. The top product, distillate, contains mostly CO<sub>2</sub> and H<sub>2</sub>O.

The bottom product is a lean mixture and is pumped through the main heat exchanger where it exchanges heat with the rich stream. The lean stream is further cooled by a cooler and is recirculated back to the absorber.

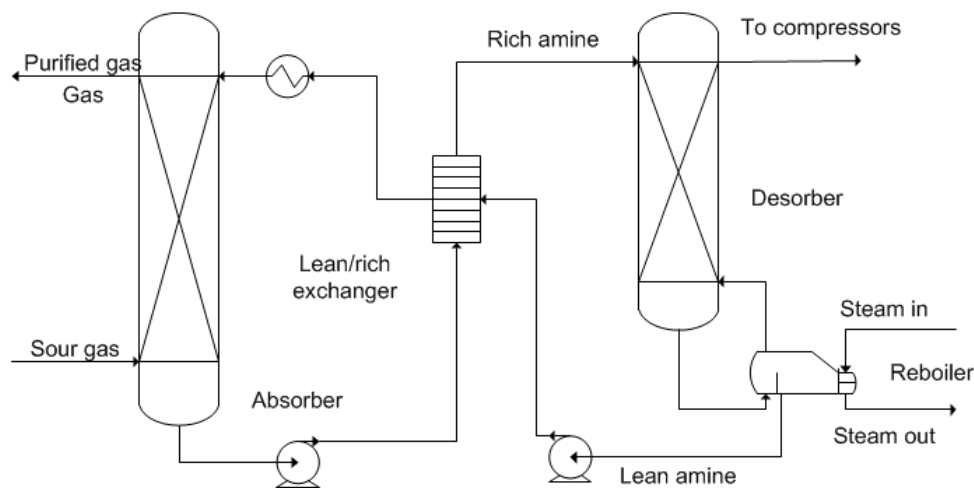


Figure 2–1 Flow chart of a standard post combustion configuration (Berg et. al 2012)

### 2.2 Inter-stage temperature control

CO<sub>2</sub> removal by chemical absorption from a flue gas is performed at temperatures around 40-60°C. This is because the absorption rate is highest in this temperature range when using a

30-wt% amine solution. The absorption process is an exothermic process, which leads to a temperature increase of the solvent. A part of the temperature increase is offset by evaporation of water to the flue gas stream, but there is still an overall increase in temperature. The driving forces for the absorption will be limited by this temperature increase, which will lead to lower absorption capacity of the MEA solvent. Low temperature is favored by thermodynamically CO<sub>2</sub> absorption reaction and higher temperature is favored by reaction kinetics. Improved viscosities and diffusion coefficients is a result from higher temperature that will lead to a higher mass transfer coefficients. Adjusting the temperature and flow of the flue gas and lean solvent can control the absorber temperature at the top and bottom. Temperature variations still occurs within the column (Cousins 2011).

A process for controlling the temperature profile in the absorber was suggested by Aroonwilas and Veawab (Aroonwilas 2007). Because of the temperature control, Aroonwilas and Veawab claims that a higher CO<sub>2</sub> loading is achieved compared to the base case. This process uses heat from the top of the absorber to enhance the kinetically limited mass transfer. In the lower stages, inter-stage cooling is used in order to provide thermodynamically driven mass transfer by maintaining a higher CO<sub>2</sub> loading in the solvent.

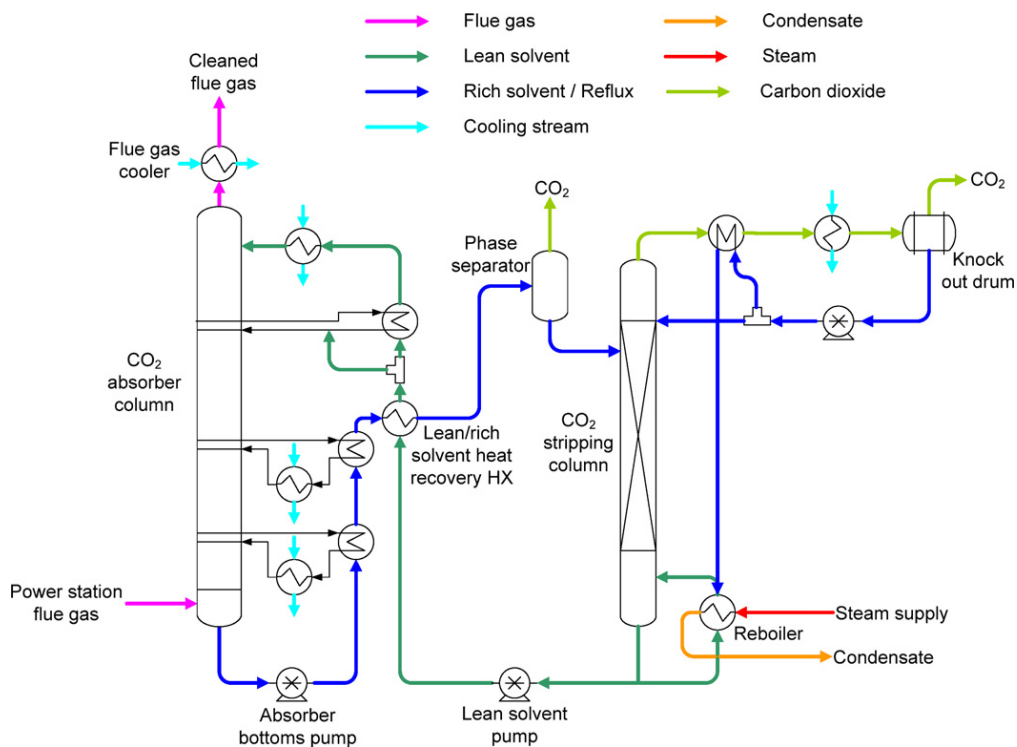


Figure 2–2 Flow chart of inter-stage temperature control configuration(Cousins 2011)

Using a part of the condensate removed from the CO<sub>2</sub> leaving the stripper cools the vapor upstream of the separator. The heated condensate is used as feed to the reboiler, reducing the steam demand in the reboiler. A 56% energy saving in reboiler duty was claimed compared to the base case. This is due to the higher CO<sub>2</sub> loading in the rich solvent, which leads to a

higher percentage of flashed CO<sub>2</sub> before the stripper and lower circulation rate of the absorbent.

## 2.3 Heat-integrated stripping column

It was suggested by (Leites 2003) to use a heat-integrated stripping column in order to reduce the energy penalty associated with the regeneration of the amine solution. In this process the rich/lean heat exchanger is fully integrated into the stripping column. By doing this, the operation and equilibrium conditions are brought closer together along the height of the column, lowering the exergy<sup>1</sup> expenditure.

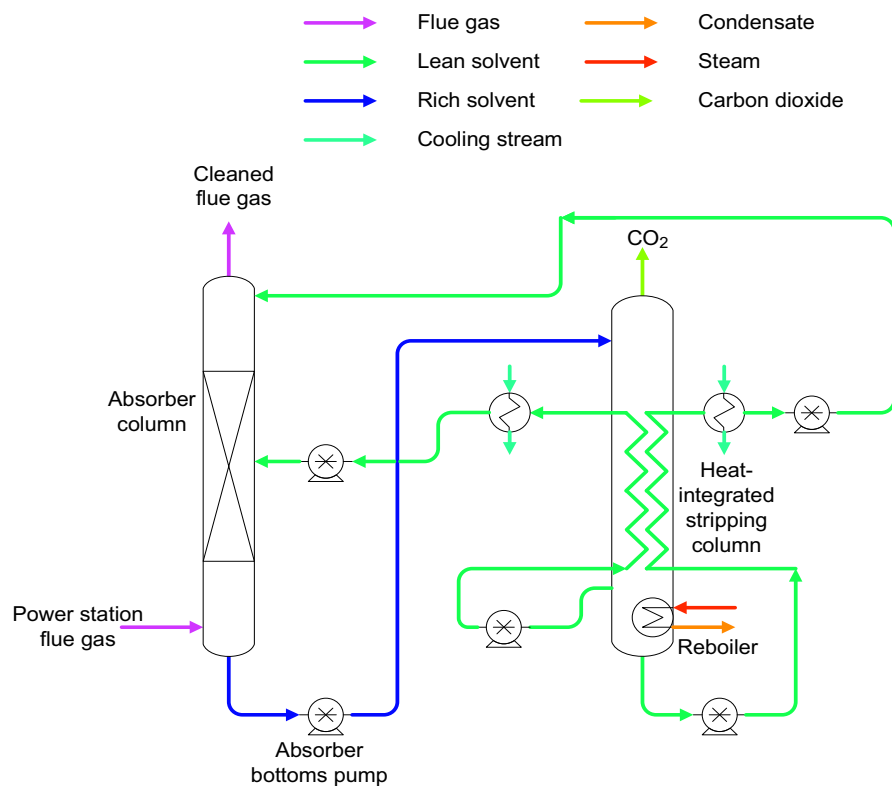


Figure 2–3 Flow chart of heat-integrated stripping column configuration(Cousins 2011)

Leites et al. claims that by introducing this modified configuration into a newly built ammonia plant, the heat requirement has been reduced by 55-66% compared to the base case.

<sup>1</sup> Exergy: "Maximum useful work possible during a process that brings the system into equilibrium with a heat reservoir" Wikipedia (2004). "Exergy." from <http://en.wikipedia.org/wiki/Exergy>.

Oyenekan and Rochelle(Oyenekan 2006a) developed such a model in Aspen Plus custom modeller. They found that the total work of the internal exchange stripper (including CO<sub>2</sub> compression) is 17% lower compared to a conventional stripper.

## 2.4 Multi-pressure stripper

Multi-pressure stripping is a design developed by G. Rochelle(Rochelle 2004). The stripper is divided into separate stages with different pressure at each stage. The vapor from a lower pressure stage is compressed and returned to a stage with a higher pressure. The liquid solvent will flash when moving down through the stripper. This design allows for recovery of the latent heat of water, which contributes to reducing the reboiler duty. The CO<sub>2</sub> product will have a higher pressure than it would have with a conventional stripper, leading to a lower energy requirement for the final compression.

The total energy requirement for compression will be slightly higher than that of a vapor recompression concept. Depending on the rich CO<sub>2</sub> partial pressure, Oyenekan and Rochelle(Oyenekan 2006b) claims that the reboiler duty has been reduced by 20-27%. They also claim an 8% saving in equivalent work for the multi-stage stripper compared to a conventional base case stripper.

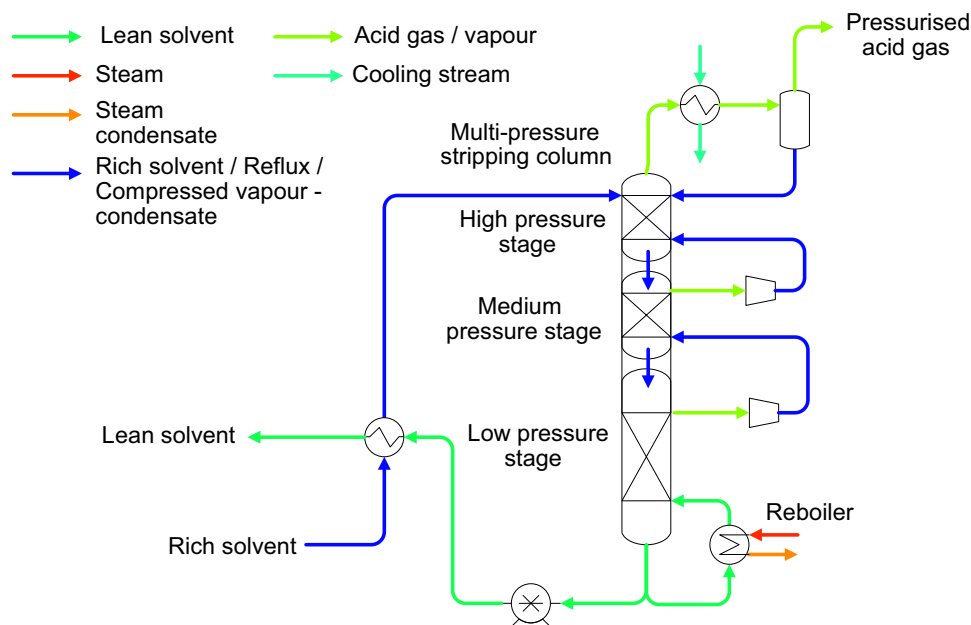


Figure 2–4 Flow chart of multi-pressure stripper configuration(Cousins 2011)

## 2.5 Compressor integration

The top product of the distillation column contains mostly CO<sub>2</sub>. The gas has to be compressed before it can be transported and stored. During the compression of the gas, heat is being

produced. The principle of compressor integration is that the heat produced during compression is used in the regeneration process in order to reduce steam demand for the reboiler.

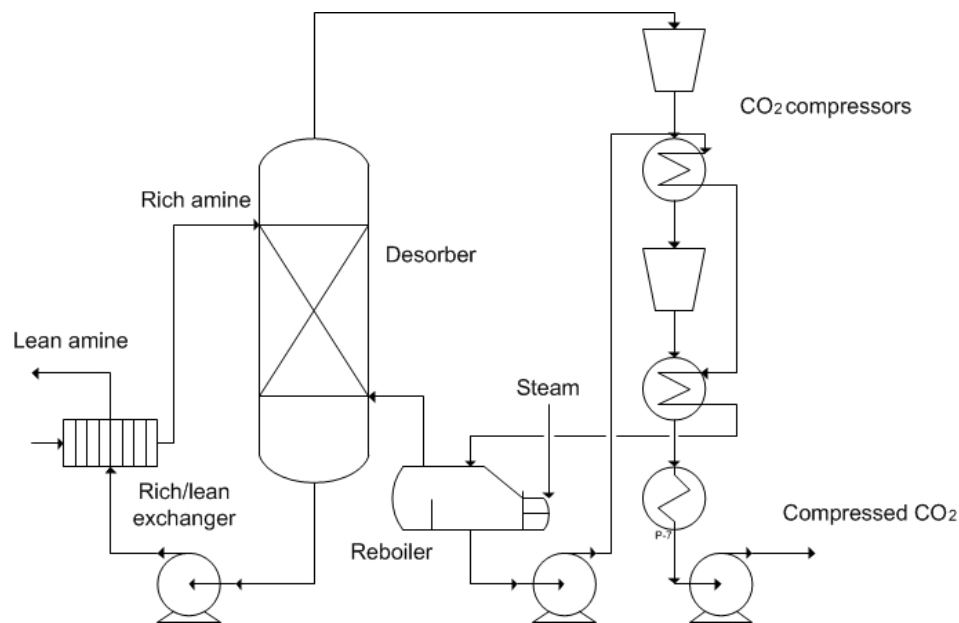


Figure 2–5 Flow chart of compressor integration configuration(Berg et. al 2012)

You can choose to have a condenser at the top of the desorber. If a condenser is used, you can't use the heat produced from the first compressor stage because the temperature is not high enough. If a condenser is not chosen, the heat produced from first compressor stage can be utilized. If a condenser is not used, the main challenge is the high fraction of water in the steam going into the compressor due to high exit temperature from the desorber. This may lead to high compressor work(Berg et. al 2012).

## 2.6 Vapor recompression

The exhaust gas enters the bottom of the absorption column where it comes in contact with the absorption liquid, MEA and water. The absorption liquid enters at the top of the column. There are two exiting streams from the absorber, one at the top and one from the bottom. The top product is sweet gas containing mostly water and nitrogen but also some CO<sub>2</sub> and MEA. The bottom product is a CO<sub>2</sub>-rich stream.

The rich stream is pumped through the main heat exchanger where it is heated by the bottom product of the distillation column before entering the distillation column. The CO<sub>2</sub> is stripped from the absorption liquid, which leaves the bottom of the column as a CO<sub>2</sub>-lean stream. The distillate contains mostly CO<sub>2</sub> and water. The bottom product goes through a valve where pressure is reduced and vapor flashes off. The stream enters a two-phase separator where the top product is vapor and bottom product is liquid. The vapor product is compressed, where pressure and temperature increases, and is entering the reboiler.

The bottom product of the two-phase separator is pumped through the main heat exchanger where it exchanges heat with the rich stream. The lean stream is further cooled before it is re-circulated back to the absorber.

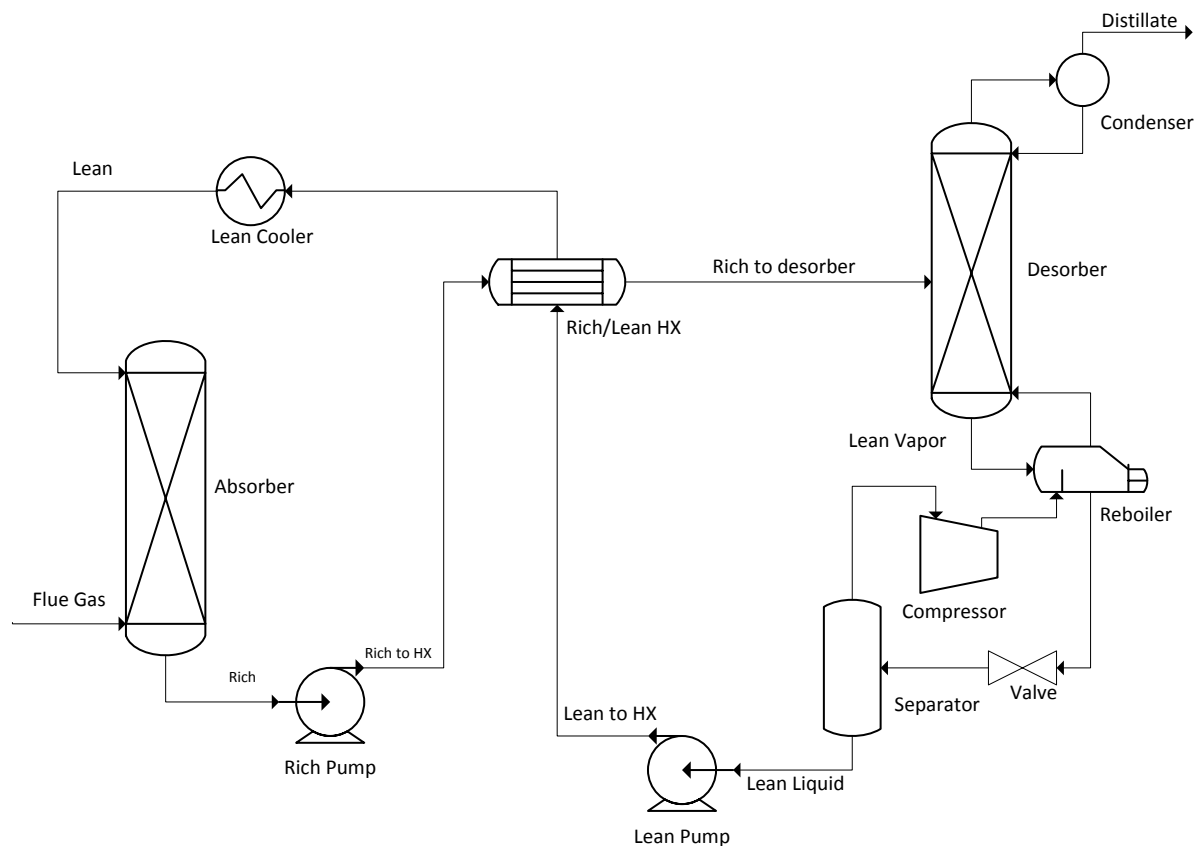


Figure 2–6 Flow chart of vapor recompression configuration(Cousins 2011)

## 2.7 Vapor recompression + split stream

The exhaust gas enters the bottom of the absorption column where it comes in contact with the absorption liquid, MEA and water. The absorption liquid enters at the top of the column. There are two exiting streams from the absorber, one at the top and one at the bottom. The top product is sweet gas containing mostly water and nitrogen but also some CO<sub>2</sub> and MEA. The bottom product is a CO<sub>2</sub>-rich stream.

The rich stream is pumped through the main heat exchanger where it is heated before entering the distillation column. The CO<sub>2</sub> is stripped from the absorption liquid, which leaves the bottom of the column as a CO<sub>2</sub>-lean stream. The distillate contains mostly CO<sub>2</sub> and water.

The bottom product is split into two streams, semilean and lean. The semilean stream goes through the main heat exchanger, where it heats up the CO<sub>2</sub>-rich stream. The semilean outlet is further cooled by a cooler and enters the absorber at the middle of the column.

The lean stream goes through a valve where pressure is reduced and vapor flashes off. The stream enters a two-phase separator where the top product is vapor and bottom product is liquid. The vapor product is compressed, where pressure and temperature increases, and returned to the reboiler.

The bottom product of the two-phase separator is pumped through the main heat exchanger where it exchanges heat with the CO<sub>2</sub>-rich stream. The lean stream is further cooled by a cooler before it is re-circulated back to the top of the absorber.

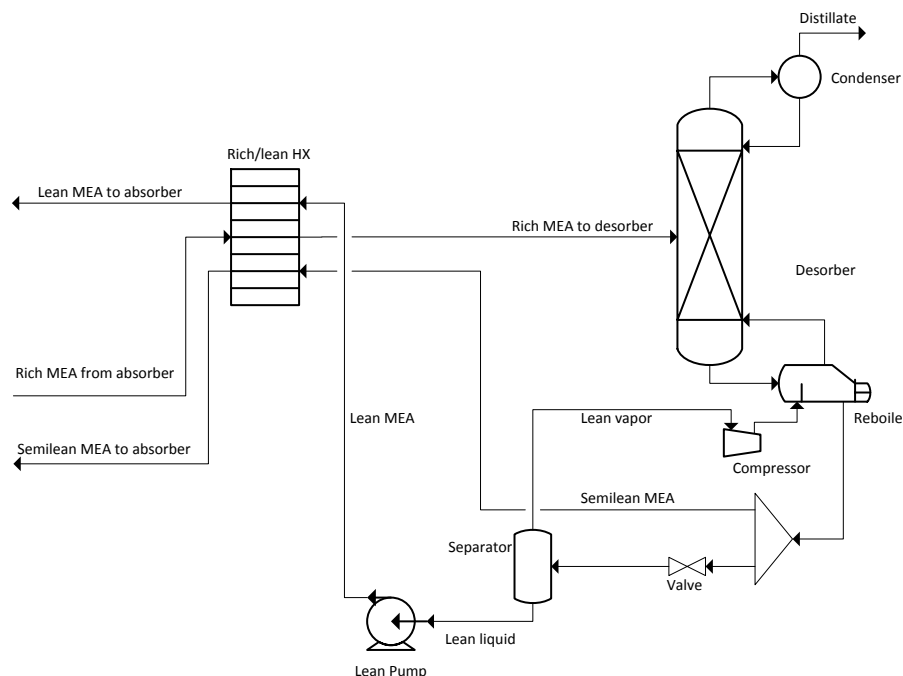


Figure 2-7 Flow chart of vapor recompression + split stream configuration

### 3 Process simulations

This thesis includes simulations of three different configurations using Aspen HYSYS and Aspen Plus. These configurations are a base case, vapor recompression and vapor recompression combined with split stream. The simulations in Aspen HYSYS were simulated using Kent-Eisenberg and Li-Mather equilibrium models; non-ideal gas phase was chosen. In Aspen Plus, the eNRTL model were used for the equilibrium and rate-based simulations.

The CO<sub>2</sub> removal efficiency was set to be 85% and was kept constant. For the absorption column, it means that 85% of the CO<sub>2</sub> in the flue gas is removed and the remaining 15% exits through the top of the column.

The user has the option to specify Murphree efficiency (tray efficiency) in the simulation software. For Kent-Eisenberg, Li-Mather and equilibrium eNRTL, Murphree efficiency was specified to 0.25 in the absorber and 1.0 in the desorber. For the rate-based model in Aspen Plus “true component approach” was used, meaning that the user will not be able to specify Murphree efficiency due to the presence of ionic species in the system.

The minimum temperature approach in the rich/lean heat exchanger was set to be 5°C.

The pressure in the absorber was kept constant at 1.1 bar. The pressure in the desorber was kept constant at 2 bar. The reflux ratio in the desorber was specified to 0.3 and reboiler temperature was specified to 120°C.

An article presented at the SIMS2007 conference in Gothenburg(Øi 2007) has been used regarding the initial set of parameters for the base case. Values from this article can be viewed in (Øi 2007) with minor changes from.

In this thesis, the simulations do not contain the water wash section, pre-treatment of the flue gas or post-treatment of the distillate. This has been decided in corporation with the supervisor, as it will not have any effect on the energy reduction potential.



*Table 3–1 Stream specifications for simulations in Aspen HYSYS and Aspen Plus*

<b>Sour Gas:</b>	<b>Specifications:</b>
Sour gas temperature	40 °C
Sour gas pressure	1.1 bar (a)
Sour gas flow	85 000 kmole/h
Mole fractions:	
CO <sub>2</sub>	0.0373
H <sub>2</sub> O	0.0671
<b>Lean MEA:</b>	
Lean MEA temperature	40 °C
Lean MEA pressure	1.1 bar (a)
Lean MEA flow	120 000 kmole/h
Mass fractions <sup>2</sup> :	
MEA	0.29
CO <sub>2</sub>	0.055
Number of stages absorber <sup>3</sup>	10
Murphree efficiency absorber <sup>4</sup>	0.25
Rich pump pressure	2 bar
Rich MEA to desorber temperature <sup>5</sup>	104.5 °C
Number of stages desorber	6
Murphree efficiency desorber	1.0
Reflux ratio desorber	0.3
Reboiler temperature	120°C
Lean pump pressure	4 bar
Minimum $\Delta T$ Rich/Lean HX	5°C

<sup>2</sup> Initial values for mass fractions of the absorption liquid

<sup>3</sup> Initial value for number of stages in the absorber. This value will be changed later in the simulations

<sup>4</sup> Murphree efficiency is used in the simulations for the CO<sub>2</sub> component

<sup>5</sup> Rich/lean HX initial value for cold outlet. This value gives  $\Delta T = 10^\circ\text{C}$ . Later adjusted by using an ADJUST-operator

## 3.1 Base Case (standard post combustion)

### 3.1.1 Aspen HYSYS

Kent-Eisenberg and Li-Mather equilibrium models have been used for the base case simulations.

Number of stages was specified to be 10 with Murphree efficiency of 0.25 on all stages. The Murphree efficiency was kept constant through the entire simulation.

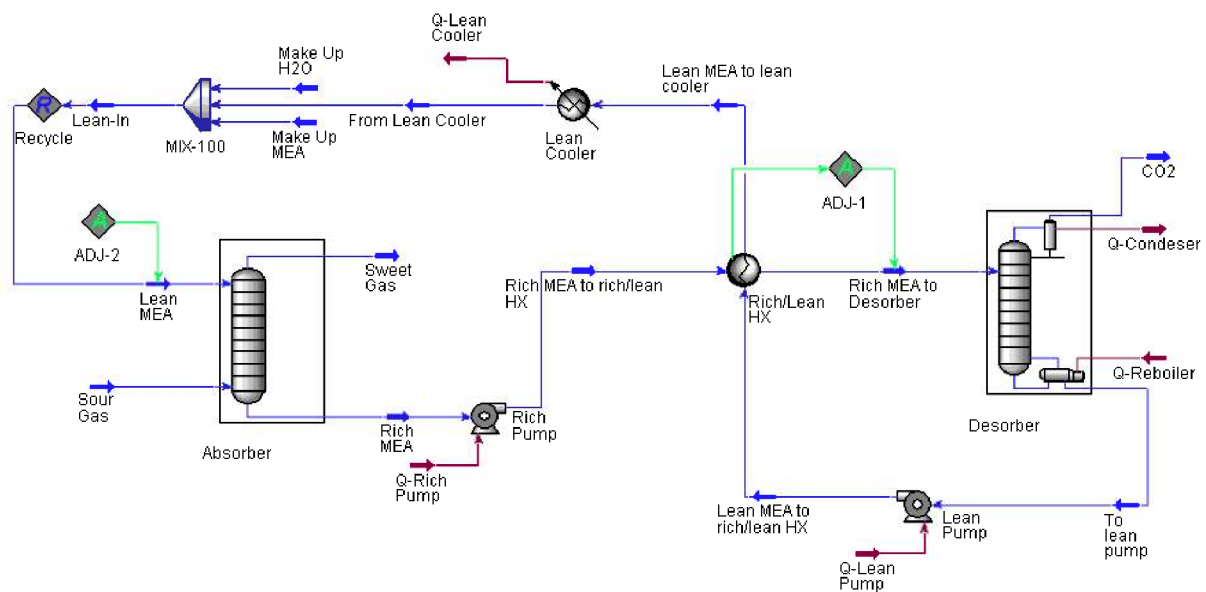


Figure 3–1 PFD of base case in Aspen HYSYS

The sour gas, with values from Table 3–1, enters at the bottom of the absorber while the lean MEA, with values from Table 3–1, enters at the top of the absorber.

The  $\text{CO}_2$ -rich stream is pumped to the rich/lean heat exchanger at 2 bar. The pressure drop was specified to be  $\Delta = 0$  kPa on both cold side and hot side of the heat exchanger. The cold outlet temperature was initially specified to be  $104,5^\circ\text{C}$  but was at a later point adjusted by the ADJUST-operator in order to obtain a  $\Delta T = 5^\circ\text{C}$  across the heat exchanger. The rich stream enters the desorber at stage 2 where numbers of trays was specified to 6. Pressure across the column was kept constant at 2 bar with a reflux ratio of 0.3 and a reboiler temperature of  $120^\circ\text{C}$ . The regenerated amine solution exits the bottom of the desorber and is pumped through the heat exchanger at 4 bar where it exchanges heat with the rich stream. The hot outlet temperature is further cooled down to  $40^\circ\text{C}$  by a lean cooler with a pressure drop of 2,9 bar. It was necessary to account for water and MEA loss in the absorber and desorber in order to maintain mass balance across the system. By using a spreadsheet, the total loss of water and MEA was calculated and exported to respective streams in the PFD. A recycle block was inserted in order to transfer calculated values to the lean absorber feed. The removal efficiency of  $\text{CO}_2$  was calculated in the spreadsheet and an ADJUST-operator was, at the end

of the simulation, connected to the lean MEA stream in order to achieve 85% removal efficiency. Spreadsheet of the simulation can be viewed in appendix B.

*Table 3–2 Results from base case simulation using Aspen HYSYS K-E & L-M*

	Kent-Eisenberg	Li-Mather
<b>Lean:</b>		
Molar flow [kmole/hr]	117874 kmole/hr	122226 kmole/hr
Mass fractions:		
H <sub>2</sub> O	0.6557	0.6557
CO <sub>2</sub>	0.0549	0.0545
MEA	0.2894	0.2899
Rich MEA to desorber temperature [°C]	106.8°C	106.2°C
<b>Energy consumption:</b>		
	3.48 MJ/kg CO <sub>2</sub>	3.42 MJ/kg CO <sub>2</sub>

### 3.1.2 Aspen Plus/Equilibrium

From previous projects at TUC<sup>6</sup> when Aspen Plus has been used, the students have used the rate-based example file found in the AspenTech folder. The students have then changed some input parameters so the simulation will run as an equilibrium model instead of a rate-based model.

In this thesis, an electrolyte insert file has been used instead. This file shows an empty PFD but the specifications for an amine system has already been set up. The difference is that the electrolyte insert file uses new binary interactions -and electrolyte pair parameters. A theory study has not been compiled on the subject.

The description of the electrolyte insert says following: *“This is a modified insert, which includes new parameters and Henry’s constant for CO<sub>2</sub> in MEA to improve the calculation of heat duty. Parameters have been tested against real life plant data for few cases. The old parameters for this system are still available in the KMEA.BKP file in the elecins folder”*.

In the mea electrolyte insert file, the user will have to add the N<sub>2</sub>-molecule to the components list, which for some reason has been left out. In the properties section, ELECNRTL (eNRTL) model has already been chosen so the user can continue to the streams section.

<sup>6</sup> TUC: Telemark University College



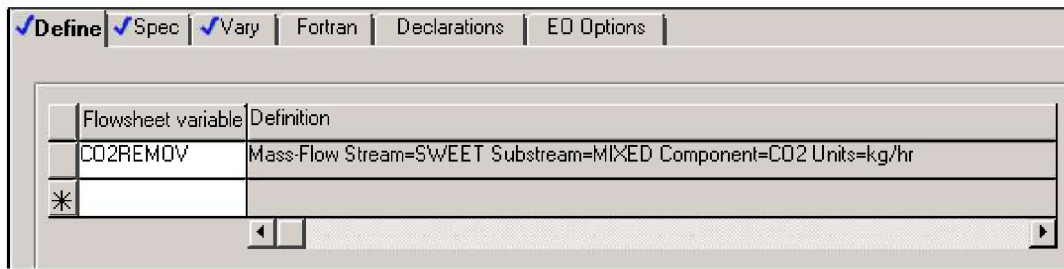


Figure 3–3 Define tab for the absorber removal efficiency in the Design-Spec block

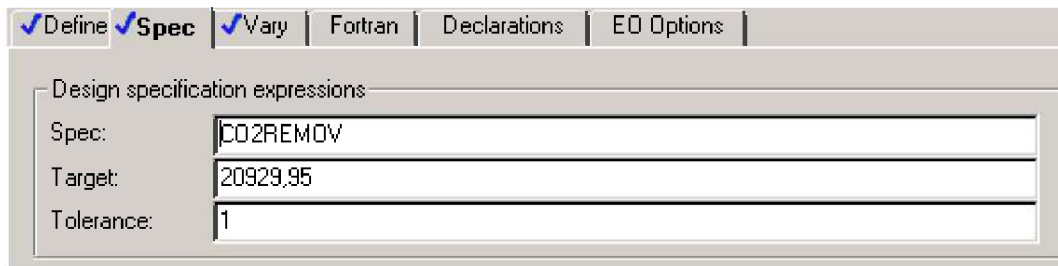


Figure 3–4 Spec tab for the absorber removal efficiency in the Design-Spec block

Target is the value of the mass flow of CO<sub>2</sub> in the sweet stream that the Design-Spec block is to approach.

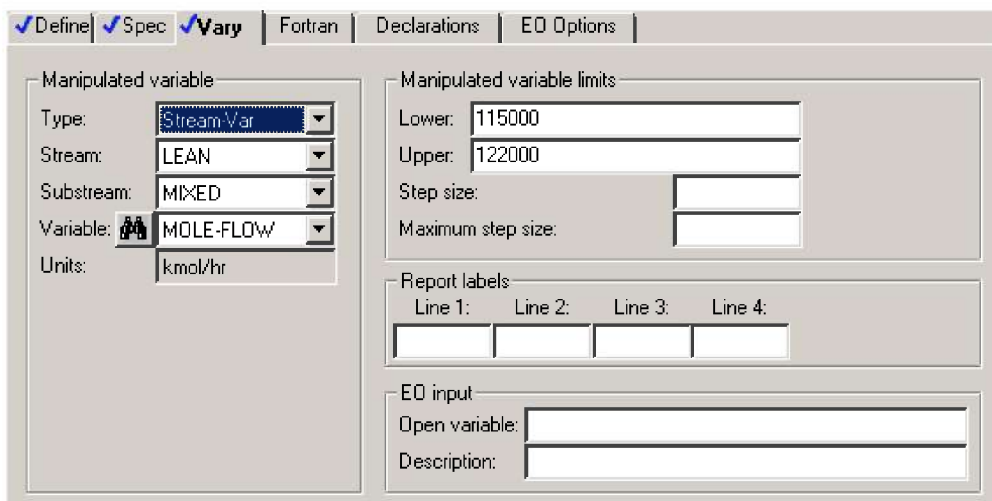


Figure 3–5 Vary tab for the absorber removal efficiency Design-Spec block

Now the user can press  which runs the simulations.

A pump is inserted into the PFD with discharge pressure of 2 bar and pump efficiency of 0.75. Now the user can press the run button. It is a good idea to run the simulation between each time new equipment is added to the simulation to make sure if any warnings and/or errors occur. If several units are added before running the simulation, it can be difficult and time consuming to locate the error and make the necessary changes. From this point it is assumed that the user runs the simulation after a new unit is added.

A simple heater was now selected, which will be replaced with a HeatX model at a later point in the simulation. An outlet temperature of 104.5°C and a pressure of 2 bar was specified.

A RadFrac model was used for the desorber. Calculation type was set to equilibrium with 8 stages, which includes condenser and reboiler. Partial-Vapor condenser type was selected, which gives us only vapor in the distillate. Kettle reboiler type was selected. Two extra specifications need to be added for the desorber configuration. Distillate rate was set to 4400 kmole/hr and reflux ratio was set to 0.3 on mole basis. Numbers of iterations was set to 150 to avoid any problems.

In order to achieve a reboiler temperature of 120°C, a Design-Spec block was used to vary the mole flow rate of the distillate. The temperature of the bottom product is the same as the reboiler temperature. Procedure can be seen in Figure 3–6 to Figure 3–8.

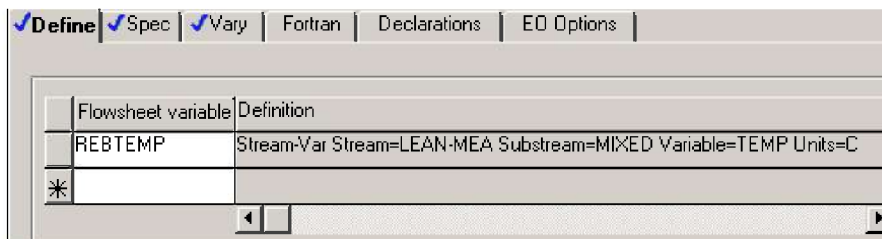


Figure 3–6 Define tab for the reboiler temperature Design-Spec block

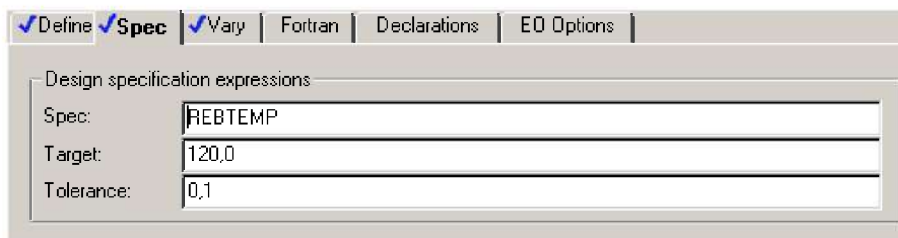


Figure 3–7 Spec tab for the reboiler temperature Design-Spec block

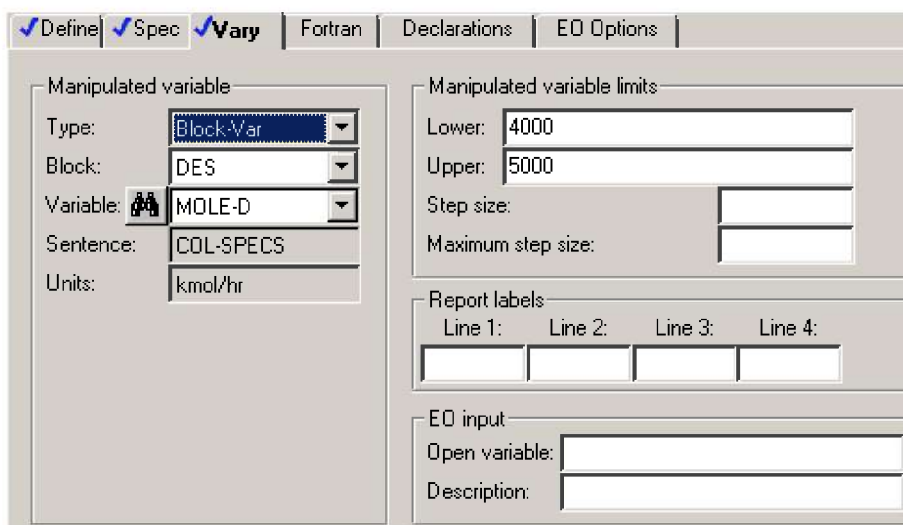


Figure 3–8 Vary tab for the reboiler temperature Design-Spec block

A pump is added with a discharge pressure of 4 bar and a pump efficiency of 0.75. At this point, the simple heater was replaced with a HeatX model. Shortcut was selected as

calculation type with a counter-current flow. Hot outlet-cold inlet temperature difference was specified to 5°C.  $\Delta P = 0$  bar was assumed across the exchanger on both cold and hot side. A heater was inserted and used as a cooler in order to get the regenerated amine solution down to 40°C. Outlet temperature was set to 40°C and outlet pressure was set to 1.1 bar. In order to maintain the material balances through the system, water loss and MEA loss was accounted for by mixing the regenerated amine solution with makeup streams of water and MEA. In Aspen HYSYS, the water loss and MEA loss was calculated using a spreadsheet and exported to their respective streams. In Aspen Plus, spreadsheet does not exist. Two calculator blocks were used instead. The calculator is based on Fortran coding and can be seen in Figure 3–9 to Figure 3–11.

Variable name	Info. flow	Definition
H2OSOUR	Import	Mole-Flow Stream=SOUR Substream=MIXED Component=H2O Units=
H2OSWEET	Import	Mole-Flow Stream=SWEET Substream=MIXED Component=H2O Units=
H2OCO2	Import	Mole-Flow Stream=CO2 Substream=MIXED Component=H2O Units=
MKUPH2O	Export	Stream-Var Stream=MKUP-H2O Substream=MIXED Variable=MOLE-F
*		

Figure 3–9 Define tab of makeup H<sub>2</sub>O calculator block

Calculation method:  
 Fortran  Excel Fortran Declarations

Enter executable Fortran statements:

```
MKUPH2O=H2OSWEET+H2OCO2-H2OSOUR
```

Figure 3–10 Calculate tab of makeup H<sub>2</sub>O calculator block

Calculator block execution sequence

Execute: Before Block type: Unit operation Block name: MIX

List variables as import or export

Import variables: H2OSOUR H2OSWEE H2OCO2  

Export variables: MKUPH2O  

Figure 3–11 Sequence tab of makeup H<sub>2</sub>O calculator block

The same procedure is repeated for makeup MEA. Regarding the Fortran coding, the first column is used for descriptions marked by a *c* at column 1. The equation starts at column 8. If the equation doesn't start at column 8, the simulation will not be able to run.

The Lean stream and Lean-In stream will have slightly different values. The mass fractions of the components in the lean feed stream were slightly adjusted to match the values of the recycle stream. Due to the complexity and time consumption running this software, it was decided not to connect the recycled amine solution to the absorber. It was tried several times in different ways but error messages were always shown.

*Table 3–3 Results from base case using Aspen Plus Equilibrium*

---

<b>Lean:</b>	
Molar flow [kmole/hr]	119265 kmole/hr
Mass fractions:	
H <sub>2</sub> O	0.657
CO <sub>2</sub>	0.29
MEA	0.053
<b>Lean-In:</b>	
Molar flow [kmole/hr]	119331 kmole/hr
Mass fractions:	
H <sub>2</sub> O	0.656
CO <sub>2</sub>	0.054
MEA	0.29
Rich to desorber temperature [°C]	103.6°C

---

<b>Energy consumption:</b>	3.365 MJ/kg CO <sub>2</sub>
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---

### 3.1.3 Aspen Plus/Rate-based

For the rate-based simulation, the example file found in the AspenTech folder was used.

The reason for not using the electrolyte insert file used in the base case is due to the complexity of the different parameter settings. The electrolyte insert file led to divergence.

In the rate-based simulation, ELECNRTL model was used with true components. This means that ionic species will be present in the system. Therefore the user will not have the option of running simulations with Murphree efficiency.



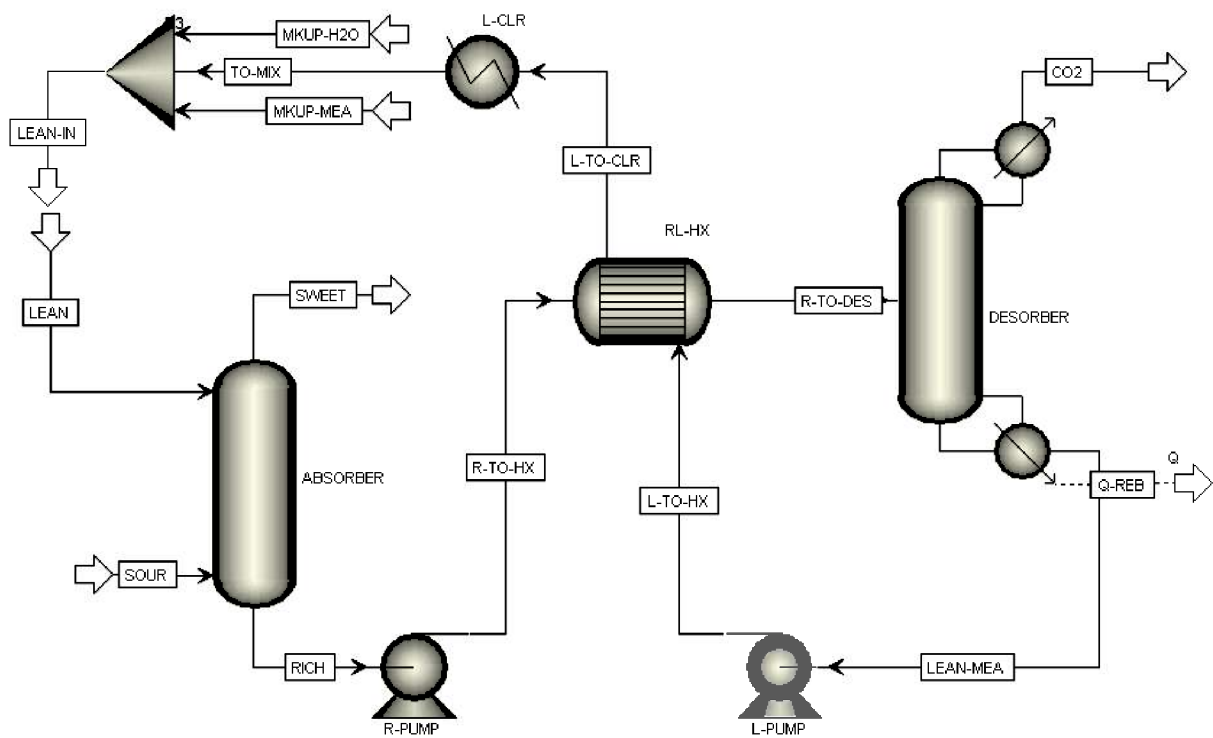


Figure 3–12 PFD of base case rate-based model in Aspen Plus

The sour-, lean-, sweet- and rich stream was added with values from Table 3–1. The absorber was selected from RadFrac using the ABSBR1 icon. Rate-based was selected as calculation type with 10 stages where condenser and reboiler were set to none.

Lean stream enters On-Stage 1 and sour stream enters On-Stage 10. Even though this is different from the equilibrium model of the base case in Aspen Plus, the setup of the absorber in the two cases is the same. Above-Stage 11 is the same as On-Stage 10.

Stage 1/condenser pressure was set to 1.1 bar. With nothing else specified, stage 1 pressure was kept constant across the whole column.

In “*Comparison of Aspen HYSYS and Aspen Plus simulation of CO<sub>2</sub> absorption into MEA from atmospheric gas*”(Øi 2012), a rate-based simulation of the absorber was performed.

The reaction condition factor was changed from 0.9 in the example file to 0.5. The interfacial area factor was changed from 1.2 in the example file to 1.0 and height of one stage was kept at 2.0 meter.

In the rate-based simulations in this thesis, standard AspenTech values were used.

In the reaction tab, the reaction was set to start at stage 1 and end at stage 10 with a liquid holdup of 0.0015 m<sup>3</sup> from stage 1 to stage 10. The parameters used for the rate-based calculations can be seen in Table 3–4. A design-spec block was used in order to obtain 85% removal of CO<sub>2</sub>.

*Table 3–4 Parameters used for rate-based calculations in the absorber and desorber*

	Absorber	Desorber
Reaction condition factor	0.9	0.9
Packing material	Sulzer Mellapak 250Y	Sulzer Mellapak 250Y
Packing stages	1 – 10	2 – 7
Section diameter	17 meter	7 meter
Section height	12 meter	12 meter
Flow model	Mixed	Mixed
Interfacial area factor	1.2	1.0
Liquid film resistance phase	Discrxn	Discrxn
Vapor film resistance phase	Film	Film
Liquid film discretization points	5	5

A rich pump was added with a discharge pressure of 2 bar and pump efficiency of 0.75. A regular heater was first used and later replaced by a HeatX model. The cold outlet stream temperature was set to 105°C. Espen Hansen (Hansen 2011) had problems in his thesis regarding the main heat exchanger. He therefore used two regular heaters and adjusted temperatures manually to get approximately the same duty on cold and hot side. The same problems occurred in this simulation. The solution was to increase the diameter of the distillation column until the HeatX model converged.

The heated rich stream enters the desorber On-Stage 3, which has 8 stages including condenser and reboiler. Partial-vapor was selected as condenser type. The distillate rate and reflux ratio was specified to 6400 kmole/hr and 0.3, respectively. The column was set to operate at 2 bar. In the reactions tab, the reactions was set to start on stage 2 and end at stage 7 with a liquid holdup of 0.0015 m<sup>3</sup>. The distillate stream was adjusted by using a design spec block, in order to obtain 85% removal of CO<sub>2</sub> in the desorber. The procedure for design-spec can be seen in Figure 3–3 to Figure 3–5.

In the rate-based simulations, the reboiler temperature is not affected by changing the distillate rate as it was in the Aspen Plus equilibrium model. Due to the complexity and difficulties running rate-based simulations, the reboiler temperature was kept at the value calculated by Aspen Plus. The discharge pressure of the lean pump was set to 4 bar with a pump efficiency of 0.75. At this point, the heater was replaced by a HeatX unit where hot outlet/cold inlet temperature difference was set to 5°C.  $\Delta P$  across the both sides of the heat exchanger was assumed to be zero. The outlet temperature of the cooler was set to 40°C and the pressure to 1.1 bar.

To account for the water and MEA loss in the system, makeup streams was used in order to maintain material balances. Two calculator blocks were used. The procedure can be seen in Figure 3–9 to Figure 3–11.

*Table 3–5 Results from base case using Aspen Plus Rate-Based*

---

<b>Lean/Lean-In:</b>	
Molar flow [kmole/hr]	106138/106189 kmole/hr
Mass fractions:	
H <sub>2</sub> O	0.654/0.654
CO <sub>2</sub>	4.36E <sup>-8</sup> /4.37E <sup>-8</sup>
MEA	0.138/0.138
H <sub>3</sub> O <sup>+</sup>	2.74E <sup>-12</sup> /2.74E <sup>-12</sup>
OH <sup>-</sup>	6.65E <sup>-6</sup> /6.65E <sup>-6</sup>
HCO <sub>3</sub> <sup>-</sup>	5.60E <sup>-4</sup> /5.61E <sup>-4</sup>
CO <sub>3</sub> <sup>-2</sup>	2.04E <sup>-3</sup> /2.04E <sup>-3</sup>
MEA <sup>+</sup>	0.08/0.08
MEACOO <sup>-</sup>	0.126/0.126
Rich to desorber temperature [°C]	110.3°C
<hr/>	
<b>Energy consumption:</b>	4.259 MJ/kg CO <sub>2</sub>
<hr/>	

### 3.1.4 Temperature profiles

In this subchapter, the temperature profiles of the absorber and desorber will be shown. The temperature profiles will start at stage 1 which is the top stage.

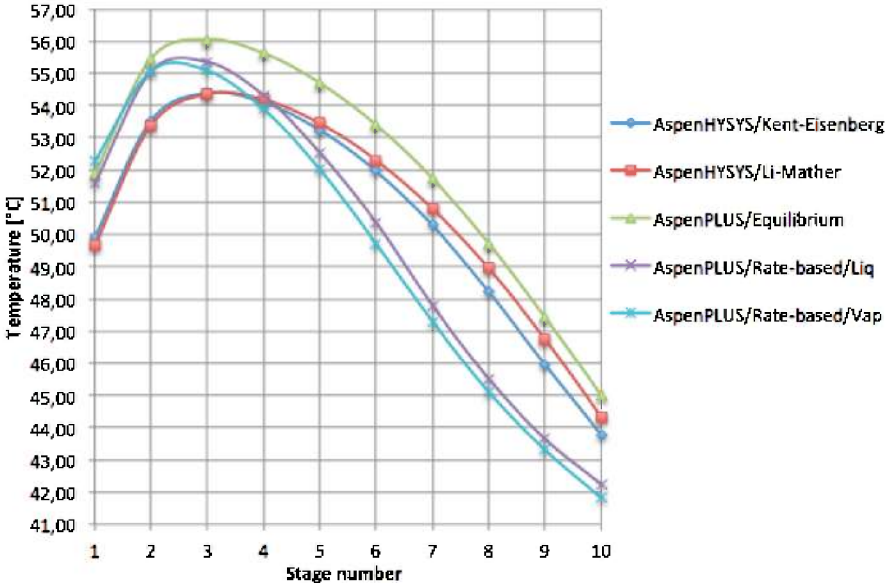


Figure 3–13 Temperature profiles in the absorber

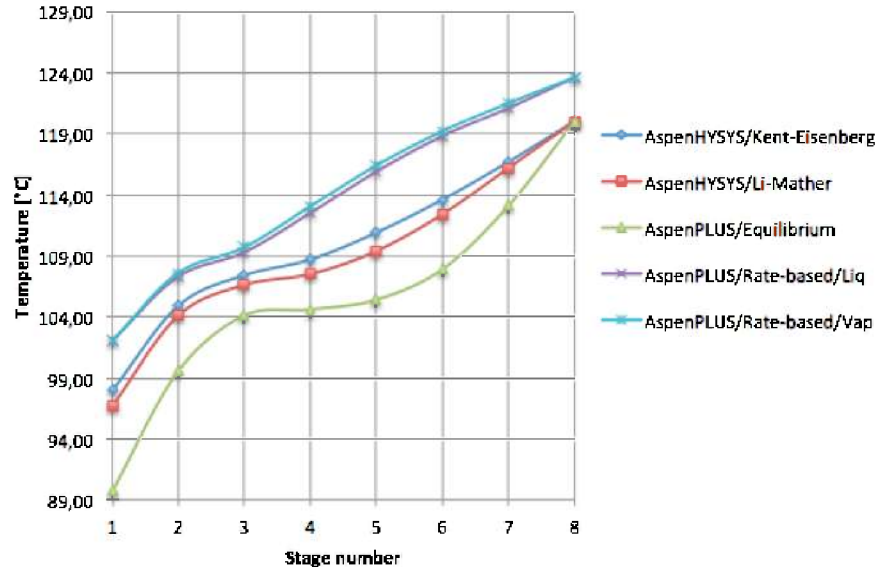


Figure 3–14 Temperature profiles in the desorber

## 3.2 Vapor recompression

The vapor recompression configuration, also known as lean vapor compression in some published articles, is the configuration that shows most potential reducing the energy consumption. Even though the compressor increases the electrical consumption, the reduction in reboiler duty is more than the increase in compressor duty. The compressor duty is converted to equivalent steam duty by multiplying with 4 to get a better understanding of the reduction potential.

### 3.2.1 Aspen HYSYS

In the vapor recompression configuration, the number of stages was maximized in order to reduce the equivalent energy consumption as much as possible.

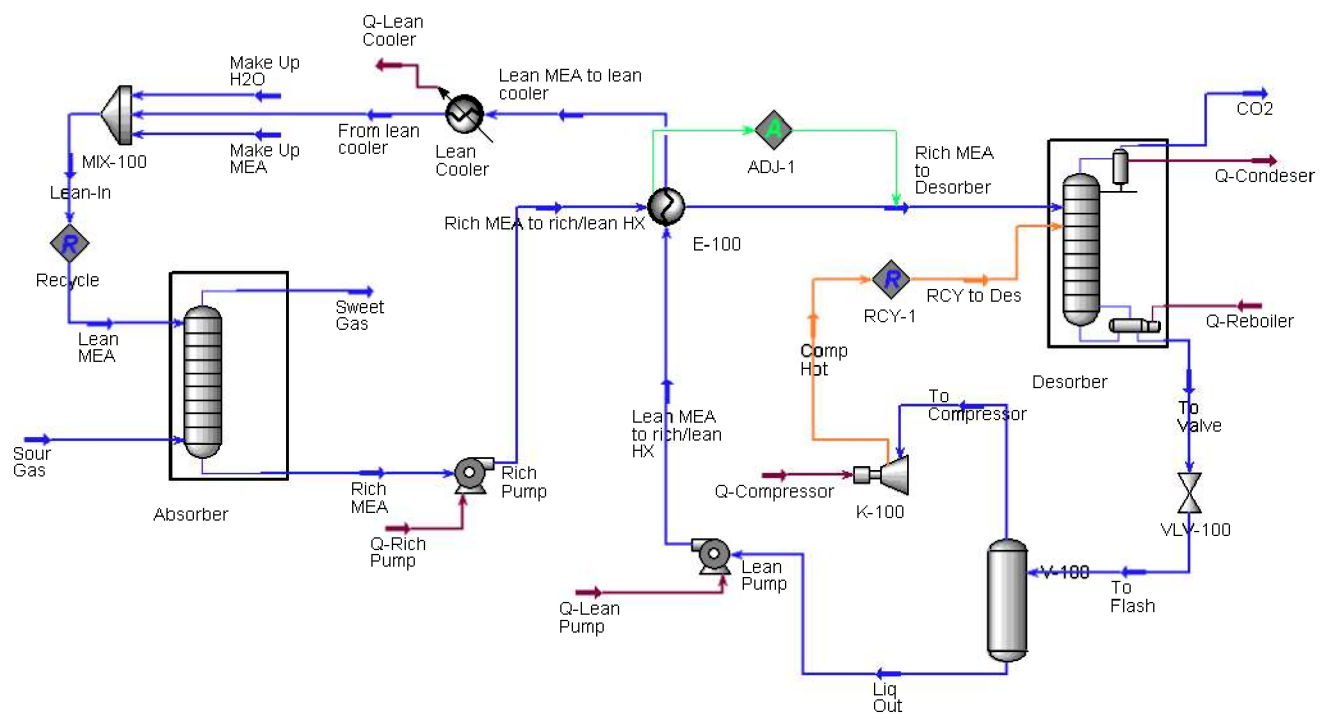


Figure 3–15 PFD of vapor recompression in Aspen HYSYS

The sour gas and lean stream was added with the values from table 3-1.

Number of stages in the absorber was set to 15 with Murphree efficiency of 0.25. Operating pressure of the column was 1.1 bar. The modified HYSIM Inside-Out solver was selected with adaptive damping factor.

A pump was added with a discharge pressure of 2 bar and a pump efficiency of 0.75 and goes through the rich/lean heat exchanger where the cold outlet temperature was specified to 104.5°C.  $\Delta P$  across both sides was assumed to be zero. Number of stages in the desorber was set to 6, which do not include condenser and reboiler. Murphree efficiency was set to 1.0. The heated rich stream enters the desorber on stage 2. The condenser is a full reflux condenser, where the product is vapor only. Operating pressure of the column was set to 2 bar with a

reboiler temperature of 120°C. Reflux ratio was set to 0.3. The modified HYSIM inside-out method was chosen as solver for this column. Damping factor was set to adaptive. The bottom product enters a valve where pressure is reduced to 1.2 bar.

Vapor is flashed off the liquid and is separated by a two-phase separator. The separator is operating at the conditions of the valve outlet stream, which are transferred automatically.

The bottom product, which is liquid, is pumped to the rich/lean heat exchanger by a lean pump at 4 bar with a pump efficiency of 0.75. The lean stream goes through the rich/lean heat exchanger where it exchanges heat with the rich stream. The heated rich stream is adjusted by an ADJUST-operator in order to maintain a  $\Delta T = 5^\circ\text{C}$  in the heat exchanger. The hot outlet is cooled down to 40°C by a cooler with a specified pressure drop of 2.9 bar.

The top product, which is vapor, is compressed up to 2 bar. The yellow line from the compressor indicates that the temperature is out of temperature range. The compressed vapor is returned to the reboiler. A solution to handle the high temperature of the compressed stream has not been addressed in this thesis.

It was necessary to account for water and MEA loss in the absorber and desorber in order to maintain material balances across the system. By using a spreadsheet, the total loss of water and MEA was calculated and exported to the respective streams in the PFD. A recycle block was inserted in order to transfer calculated values to the lean absorber feed. The removal efficiency of CO<sub>2</sub> was calculated in the spreadsheet and an ADJUST-operator was, at the end of the simulation, connected to the lean MEA stream in order to achieve 85% removal efficiency. Spreadsheet of the simulation can be viewed in appendix C.

*Table 3–6 Results from vapor recompression using Aspen HYSYS K-E & L-M*

	Kent-Eisenberg	Li-Mather
<b>Lean:</b>		
Molar flow [kmole/hr]	104933 kmole/hr	104394 kmole/hr
Mass fractions:		
H <sub>2</sub> O	0.657	0.6595
CO <sub>2</sub>	0.0518	0.0509
MEA	0.2912	0.2896
Rich MEA to desorber temperature [°C]	98.54°C	97.83°C
Outlet compressor temperature [°C]	170.8°C	170.7°C
<b>Equivalent energy consumption:</b>	2.98 MJ/kg CO <sub>2</sub>	2.92 MJ/kg CO <sub>2</sub>

### 3.2.2 Aspen Plus/Equilibrium

The electrolyte insert file used in the base case was also used for the vapor recompression configuration. The sour-, lean-, sweet- and rich streams were added with the values from Table 3–1. Number of stages in the absorber was set to 10 with a Murphree efficiency of 0.25 on all stages. Operating pressure was set to 1.1 bar. A pump is added with a discharge pressure of 2 bar and a pump efficiency of 0.75.

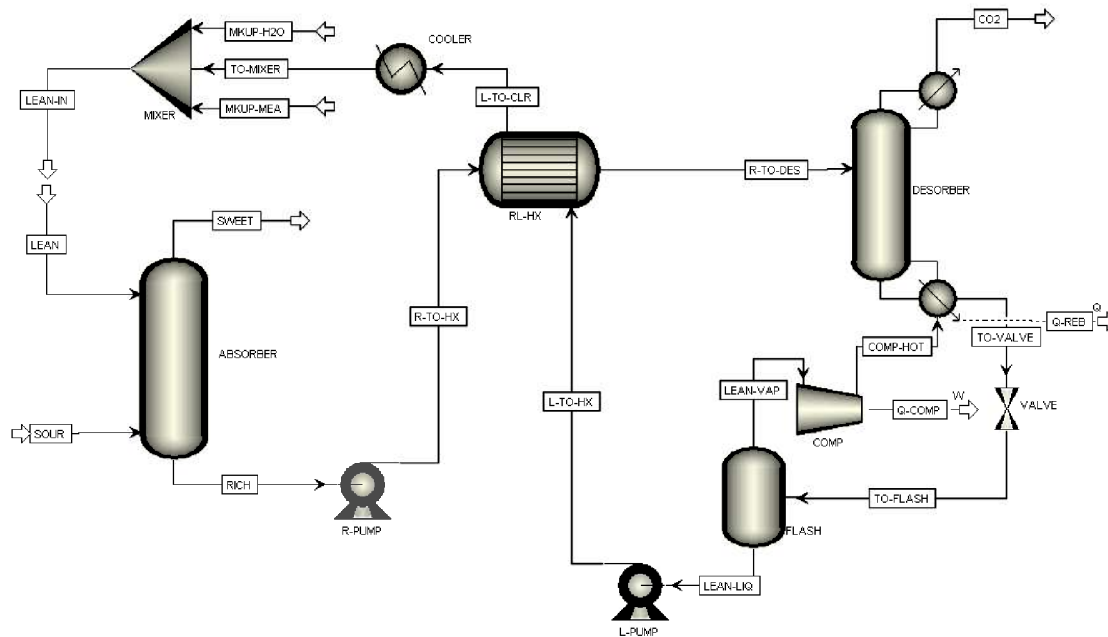


Figure 3–16 PFD of vapor recompression using Aspen Plus Equilibrium

At this point, a heater was used instead of a HeatX model. The heater was at a later point replaced by a HeatX model. The outlet temperature of the heater was specified to 104.5°C. Numbers of stages in the desorber was set to 8, including condenser and reboiler. The distillate rate was set to 4500 kmole/hr with a reflux ratio of 0.3. The heated rich stream enters the desorber On-Stage 3, and the operating pressure was set to 2 bar. Murphree efficiency was set to 1.0 on all stages.

In order to achieve a reboiler temperature of 120°C, a design-spec block was used. The procedure for setting up the design-block can be found in Figure 3–6 to Figure 3–8.

The bottom product of the desorber goes through a valve where the outlet pressure is 1.2 bar. Vapor flashes off and the stream enter a separator. In Aspen HYSYS, the separator retrieves parameters automatically. This is not the case in Aspen Plus. The separator was provided with pressure and temperature values from the valve outlet stream. Two transfer blocks was used, one for valve outlet temperature and one for valve outlet pressure. These values were transferred to the separator. The transfer blocks will come in handy if the user wants to perform sensitivity analysis of various parameters. By using the transfer blocks, the user won't have to change the temperature and pressure specifications for the separator manually.

The setup for the pressure transfer block can be seen in Figure 3–17 to Figure 3–19. The setup for the temperature transfer block is the same.

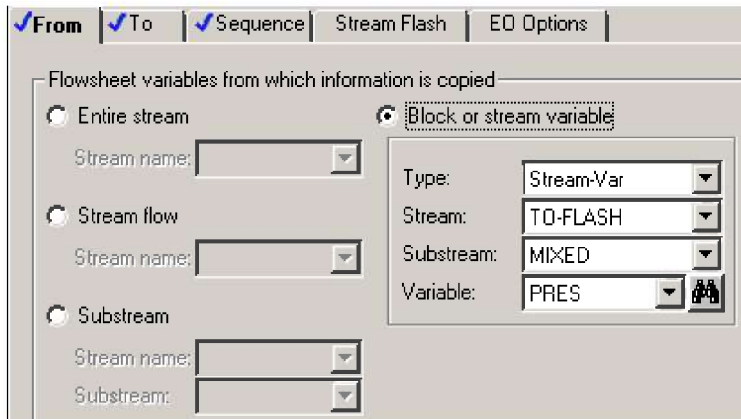


Figure 3–17 “From” tab of pressure transfer block

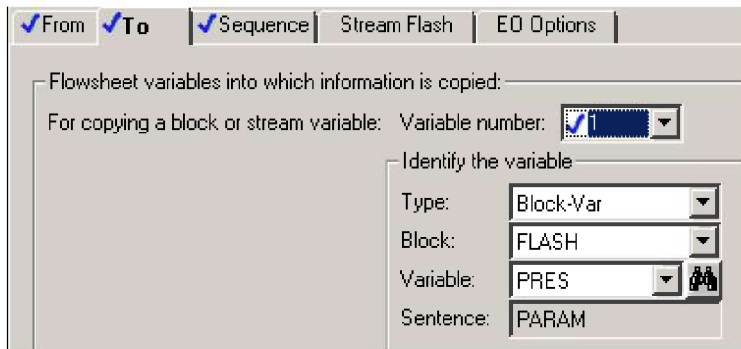


Figure 3–18 “To” tab of pressure transfer block

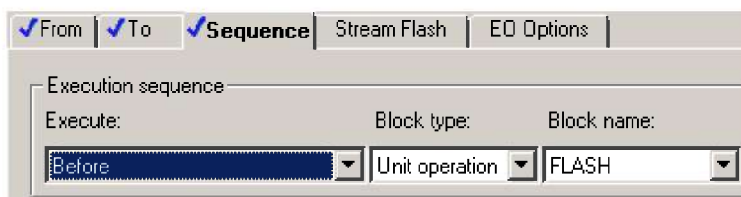


Figure 3–19 “Sequence” tab of pressure transfer block

The top product of the separator goes through a compressor. “*Isentropic using ASME method*” was selected as compressor type. An isentropic efficiency of 0.75 was selected.

The compressor outlet was selected to enter the desorber On-Stage 10, which is the reboiler. The bottom product from the separator is pumped at 4 bar with a pump efficiency of 0.75 and goes through the rich/lean heat exchanger.  $\Delta P = 0$  bar was assumed across the heat exchanger on both cold- and hot side. Hot outlet/cold inlet temperature difference was specified to 5°C. A shortcut model was used for the heat exchanger.

The hot outlet stream was cooled down to 40°C by a cooler with a pressure drop of 2.9 bar.



In order to maintain the material balances through the system, the water loss and MEA loss was accounted for by mixing the regenerated amine solution with makeup streams of water and MEA. Two calculator blocks were used to calculate the exact amount of water and MEA loss. The calculator is based on Fortran coding and can be seen in Figure 3–9 to Figure 3–11. Initial values have to be used for the makeup streams in order for the simulation to start iterating. At this point, values of mass fraction in the lean stream entering the absorber were adjusted to match outlet stream of the mixer to try and get similar values.

*Table 3–7 Results of vapor recompression using Aspen Plus Equilibrium*

<b>Lean/Lean-In:</b>	
Molar flow [kmole/hr]	111717/110850 kmole/hr
Mass fractions:	
H <sub>2</sub> O	0.658/0.656
CO <sub>2</sub>	0.051/0.051
MEA	0.291/0.293
Rich to desorber temperature [°C]	96.9°C
Compressor outlet temperature [°C]	172.5°C
<b>Equivalent energy consumption:</b>	3.16 MJ/kg CO <sub>2</sub>

### 3.2.3 Aspen Plus/Rate-based

The sour-, lean-, sweet- and rich stream was added with values from Table 3–1. Number of stages in the absorber was set to 10. The lean stream enters the absorber On-Stage 1 and the sour stream enters On-Stage 10. Operating pressure was set to 1.1 bar. A design-spec block was used to obtain 85% removal of CO<sub>2</sub> in the absorber. Procedure for design-block setup can be seen in Figure 3–3 to Figure 3–5.

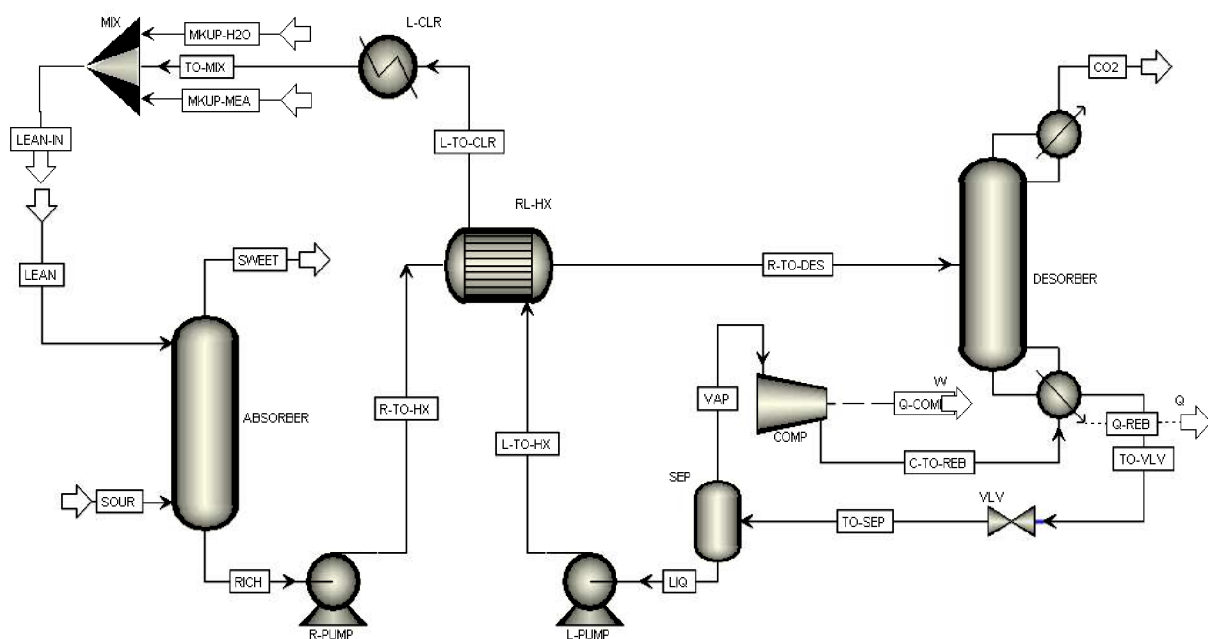


Figure 3–20 PFD of vapor recompression using Aspen Plus Rate-Based

Regarding the packing material and such, the values remained the same for the absorber as for the base case. These values can be seen in Table 3–4.

A rich pump was added with discharge pressure of 2 bar and a pump efficiency of 0.75. A regular heater was used with a specified outlet temperature of 104.5°C.  $\Delta P$  was assumed to be zero. Numbers of stages in the desorber was set to 8, including condenser and reboiler.

Partial-vapor was selected as condenser type. Distillate rate was set to 4500 kmole/hr with a reflux ratio of 0.3. The heated rich stream enters the desorber On-Stage 3. The operating pressure was set to 2 bar and kept constant across the whole column. A design-spec block was used to maintain 85% removal of CO<sub>2</sub> in the desorber. The user may experience convergence problems regarding flooding in the column. By increasing the diameter of the packing material, in this case from 7 meter to 7.5 meter, flooding was avoided. The diameter was reduced to initial value at a later point.

Since the reboiler temperature does not depend on the distillate flow rate, the reboiler temperature was kept as calculated by Aspen Plus.

The bottom product of the desorber goes through a valve reducing pressure down to 1.2 bar. Vapor is flashed off and the stream flows into a separator. As explained previously, the separator in Aspen Plus does not retrieve values automatically. Temperature and pressure from the valve outlet stream was added manually at first. Two transfer blocks was added, one for temperature and one for pressure. By using the transfer blocks, the user won't have to change the temperature and pressure specifications for the separator manually. Procedure for setup of transfer blocks can be seen in Figure 3–17 to Figure 3–19. The top product of the separator goes through a compressor. "Isentropic using ASME method" was selected as compressor type. An isentropic efficiency of 0.75 was used.

The compressor outlet stream enters the desorber on-stage 8. The bottom product is pumped at 4 bar with a pump efficiency of 0.75. At this point, the regular heater was replaced by a HeatX unit. The HeatX model had problems with convergence in rate-based simulation as previously mentioned. The solution regarding HeatX unit in rate-based simulations can be found in chapter 3.1.3.  $\Delta P$  was assumed to be zero on both sides.

Hot outlet/cold inlet was specified to 5°C. The hot outlet was further cooled by a lean cooler down to 40°C with a pressure drop of 2.9 bar.

In order to maintain the material balances through the system, the water loss and MEA loss was accounted for by mixing the regenerated amine solution with makeup streams of water and MEA. Two calculator blocks were used for this purpose. The calculator is based on Fortran coding and can be seen in Figure 3–9 to Figure 3–11. Initial values have to be used for the makeup streams in order for the simulation to start iterating. At this point, values of mass fraction in the lean stream entering the absorber were adjusted to match outlet stream of the mixer to try and get similar values.

*Table 3–8 Results of vapor recompression using Aspen Plus Rate-based*

<b>Lean/Lean-In:</b>	
Molar flow [kmole/hr]	106125/106125 kmole/hr
Mass fractions:	
H <sub>2</sub> O	0.654/0.654
CO <sub>2</sub>	4.36E <sup>-8</sup> /437.E <sup>-8</sup>
MEA	0.138/0.138
H <sub>3</sub> O <sup>+</sup>	2.74E <sup>-12</sup> /2.74E <sup>-12</sup>
OH <sup>-</sup>	6.65E <sup>-6</sup> /6.66E <sup>-6</sup>
HCO <sub>3</sub> <sup>-</sup>	5.6E <sup>-4</sup> /5.6E <sup>-4</sup>
CO <sub>3</sub> <sup>-2</sup>	2.04E <sup>-3</sup> /2.04E <sup>-3</sup>
MEA <sup>+</sup>	0.08/0.08
MEACOO <sup>-</sup>	0.126/0.126
Rich to desorber temperature [°C]	102.9°C
Compressor outlet temperature [°C]	173.3°C
<b>Energy consumption:</b>	3.82 MJ/kg CO <sub>2</sub>

### 3.2.4 Temperature profiles

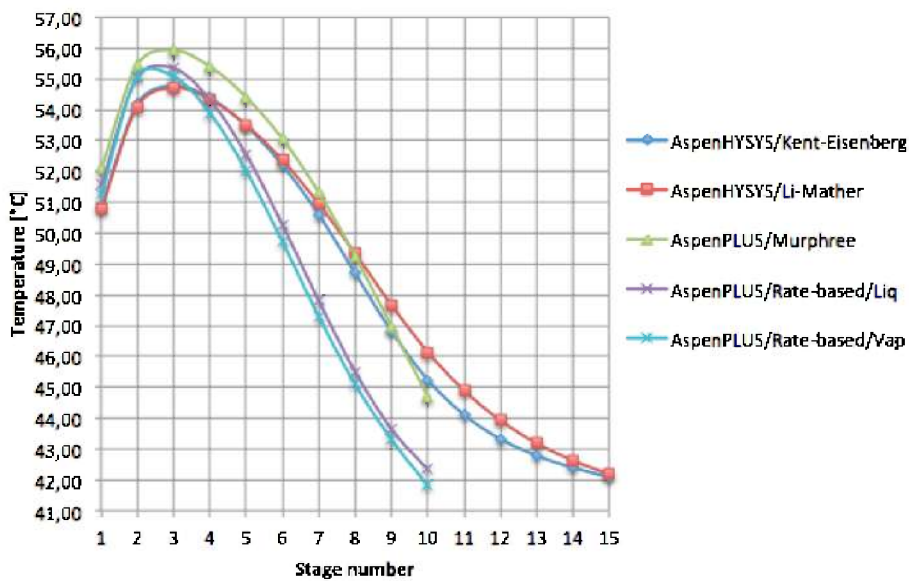


Figure 3–21 Temperature profiles in the absorber

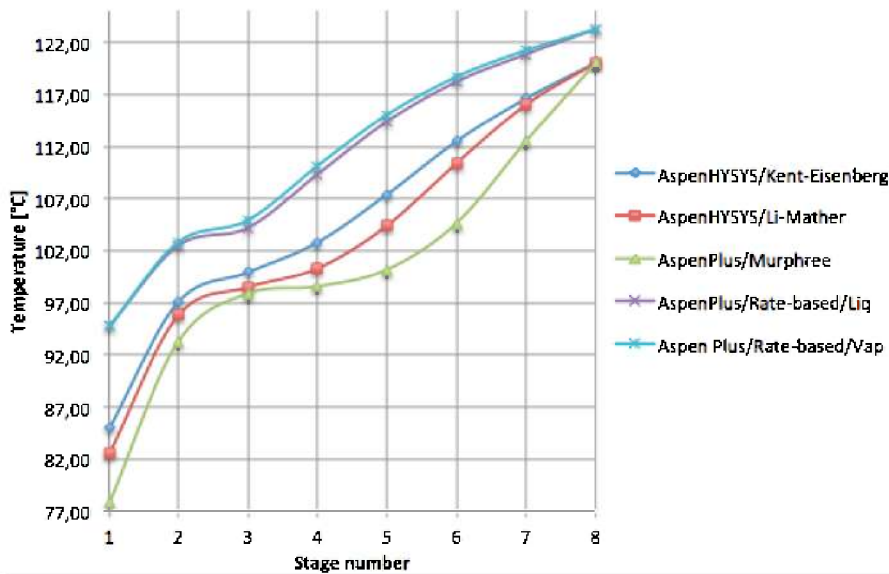


Figure 3–22 Temperature profiles in the desorber

### 3.3 Vapor recompression + split stream

In several theses', regarding CO<sub>2</sub> capture, simulations of split stream configuration have shown a fairly good reduction in energy consumption. Vladyslav shchuchenko(Shchuchenko 2011) calculated a reduction in 1.13 MJ/kg CO<sub>2</sub> removed comparing standard CO<sub>2</sub> removal process with standard split-stream configuration.

Christian Berg(Berg et. al 2012) calculated a reduction of 0.65 MJ/kg CO<sub>2</sub> removed comparing the same configurations. Christian Berg et al. changed the  $\Delta T$  in the heat



to 0.3. Reboiler temperature was specified to 120°C in the “*specs*” tab. “*Modified HYSIM Inside-Out*” solver was selected with damping factor set to adaptive.

The bottom product is split into two streams, semilean- and lean stream.

The split fraction is 0.39 and 0.61, respectively. The lean stream goes through a valve where the pressure is reduced to 1.2 bar. The valve outlet goes into a separator operating at valve outlet conditions. The top product, which is vapor, is compressed up to 2 bar and returned to the reboiler. The yellow line from the compressor indicates that the temperature is out of temperature range. The bottom product is pumped at 4 bar with a pump efficiency of 0.75 through the LNG exchanger. The outlet temperature of the lean stream is reduced to 40°C by a cooler with a pressure drop of 2.9 bar. It was necessary to account for water and MEA loss in the absorber and desorber in order to maintain material balances across the system. By using a spreadsheet, the total loss of water and MEA was calculated and exported to the respective streams in the PFD. A recycle block was inserted in order to transfer new calculated values to the lean absorber feed. The semilean stream is pumped at 3 bar with a pump efficiency of 0.75 through the LNG exchanger. A SET-operator was used between the cold inlet stream and the semilean outlet stream. This was done to ensure a  $\Delta T = 5^\circ\text{C}$  between the two streams. In the spreadsheet, a  $\Delta T$  was calculated between the hot lean outlet stream and the cold inlet stream. An ADJUST-operator was then connected to the cold outlet stream to adjust its temperature, so the  $\Delta T$  calculated in the spreadsheet would maintain 5°C.

The semilean outlet stream was further cooled by a semilean cooler down to 40°C with a pressure drop of 1.9 bar. A recycle block was added and connected to the semilean stream to make sure that no problems occurred. Before connecting the semilean stream to the absorber, the simulation was put in holding mode. The semilean stream was connected and the molar flow of the lean feed was adjusted down 75000 kmole/hr. Holding mode was then switched off. After the simulation had found a solution, number of stages was increased by one stage at the time. The user must remember to specify Murphree efficiency of 0.25 on the added stages. To achieve an 85% removal of CO<sub>2</sub>, the lean molar flow rate was adjusted down to 66800 kmole/hr and number of stages was increased to 15. By adding more stages the column could not converge. The yellow lines before the separator and on the lean liquid stream indicates a higher wt-% of MEA than 30 wt-%. The wt-% warning has been assumed to be negligible. Spreadsheets can be seen in appendix D.

Table 3–9 Results of vapor recompression + split stream using Aspen HYSYS K-E & L-M

	Kent-Eisenberg	Li-Mather
<b>Lean:</b>		
Molar flow [kmole/hr]	66800 kmole/hr	66400 kmole/hr
Mass fractions:		
H <sub>2</sub> O	0.659	0.66
CO <sub>2</sub>	0.052	0.051
MEA	0.289	0.289
<b>Semilean:</b>		
Stage entry	7	9
Molar flow [kmole/hr]	40938.5 kmole/hr	40820.3 kmole/hr
Mass fractions:		
H <sub>2</sub> O	0.646	0.648
CO <sub>2</sub>	0.056	0.055
MEA	0.298	0.297
Rich MEA to desorber temperature [°C]	101.8°C	101°C
Outlet compressor temperature [°C]	170.8°C	170.7°C
<b>Equivalent energy consumption:</b>	3.12 MJ/kg CO <sub>2</sub>	3.03 MJ/kg CO <sub>2</sub>

### 3.3.2 Aspen Plus/Equilibrium

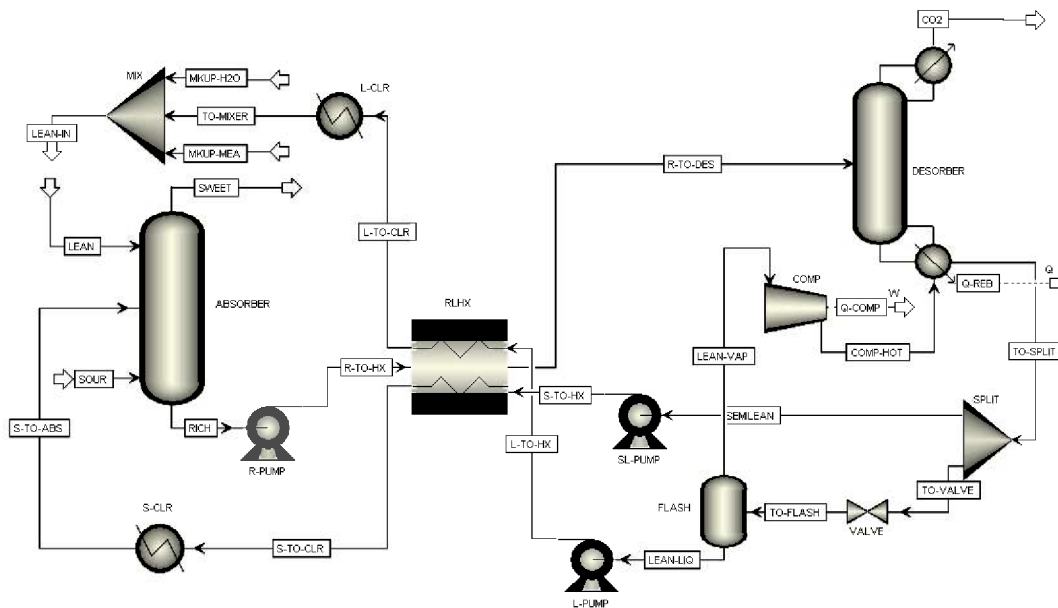


Figure 3–24 PFD of vapor recompression + split stream in Aspen Plus

The sour-, lean-, sweet- and rich stream was added with values from Table 3–1. Number of stages in the absorber was set to 10 with Murphree efficiency of 0.25 on all stages. Operating pressure of the column was 1.1 bar. Maximum iterations were set to 100 to make sure the column would converge. A pump was added with a discharge pressure of 2 bar and a pump efficiency of 0.75. A simple heater was used as a starting point for the multistream heat exchanger. Outlet temperature was set to 104.5°C and  $\Delta P$  across the heater was assumed to be zero. Number of stages in the desorber was set to 8, including condenser and reboiler. The distillate rate was set to 4500 kmole/hr but was adjusted by using a design-spec to obtain a reboiler temperature of 120°C. The procedure is the same as in Figure 3–6 to Figure 3–8. A reflux ratio of 0.3 was chosen. Operating pressure was set to 2 bar with a Murphree efficiency of 1.0 on all stages.

The bottom product is split into two streams; semilean- and lean stream. The split fraction of the lean stream is 0.61. The lean stream goes through a valve where the pressure is reduced to 1.2 bar. Two transfer blocks are used to transfer outlet valve temperature and pressure to the separator. This is done to make it easier to run sensitivity analysis. The transfer block setup procedure can be seen in Figure 3–17 to Figure 3–19. The separator is given temperature and pressure estimates to get the iterations going. The top product of the separator is compressed up to 2 bar using the isentropic ASME model as a compressor type. Isentropic efficiency was set to 0.75. The compressor outlet enters the desorber On-Stage 8, which is the reboiler. At this point, the heater was replaced by a MHeatX model and the outlet streams selected together with their respective inlets. Outlet temperatures of the lean and semilean stream are used as specifications.



The bottom product of the separator is pumped at 4 bar, with a pump efficiency of 0.75, through the heat exchanger.  $\Delta P$  across the heat exchanger was assumed to be zero. The lean outlet temperature was set to 49.75°C. The lean stream is further cooled by a cooler down to 40°C with a pressure drop of 2.9 bar. In order to maintain the material balances through the system, the water loss and MEA loss was accounted for by mixing the regenerated amine solution with makeup streams of water and MEA. Two calculator blocks were used for this purpose. The calculator is based on Fortran coding and can be seen in Figure 3–9 to Figure 3–11. Initial values have to be used for the makeup streams in order for the simulation to start iterating. At this point, mass fraction in the lean stream entering the absorber was adjusted to match outlet stream of the mixer in order to get similar values. The semilean stream is pumped at 3.5 bar with a pump efficiency of 0.75 through the heat exchanger.  $\Delta P$  across the heat exchanger was assumed to be zero. The semilean outlet was set to 49.75°C. The semilean stream is further cooled by a semilean cooler down to 40°C with a pressure drop of 2.4 bar. The semilean stream is connected to the absorber, entering On-Stage 6. The lean flow rate was set to 75000 kmole/hr and further adjusted in order to obtain 85% removal of CO<sub>2</sub>.

*Table 3–10 Results of vapor recompression + split stream using Aspen Plus Equilibrium*

---

<b>Lean/Lean-In:</b>	
Molar flow [kmole/hr]	69500/69973 kmole/hr
Mass fractions:	
H <sub>2</sub> O	0.659/0.66
CO <sub>2</sub>	0.05/0.051
MEA	0.291/0.29
<b>Semilean:</b>	
Stage entry	6
Molar flow [kmole/hr]	42804 kmole/hr
Mass fractions:	
H <sub>2</sub> O	0.646
CO <sub>2</sub>	0.056
MEA	0.298
Rich to desorber temperature [°C]	100°C
Compressor outlet temperature [°C]	172.5°C

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<b>Equivalent energy consumption:</b>	3.19 MJ/kg CO <sub>2</sub>
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### 3.3.3 Aspen Plus/Rate-based

The rate-based example file found in the AspenTech folder was used for this simulation.

The sour-, lean-, sweet- and rich stream was added with values from table 3-1. Number of stages in the absorber was set to 10. The lean stream enters the absorber On-Stage 1 and the sour stream enters On-Stage 10. Top stage pressure was set to 1.1 bar.

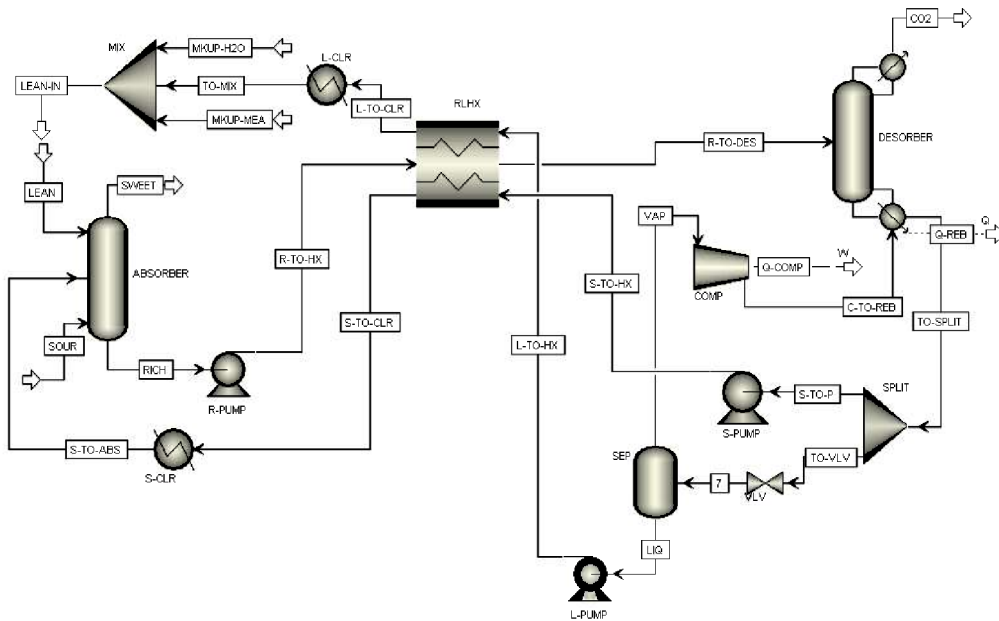


Figure 3–25 PFD of vapor recompression + split stream using Aspen Plus Rate-based

Table 3–11 Parameters used for rate-based calculations in the absorber and desorber

	Absorber	Desorber
Reaction condition factor	0.9	0.9
Liquid holdup	0.0015 m <sup>3</sup>	0.0015 m <sup>3</sup>
Packing material	Sulzer Mellapak 250Y	Sulzer Mellapak 250Y
Packing stages	1 – 10	2 – 7
Section diameter	17 meter	7.5 meter
Section height	12 meter	12 meter
Flow model	Mixed	Mixed
Interfacial area factor	1.2	1.0
Liquid film resistance phase	Discrxn	Discrxn
Vapor film resistance phase	Film	Film
Liquid film discretization points	5	5

A pump was added with a discharge pressure of 2 bar and a pump efficiency of 0.75. A regular heater was added with a specified outlet temperature of 104.5°C.

$\Delta P$  across the heater was assumed to be zero. Number of stages in the desorber was set to 8, which includes condenser and reboiler. Partial-vapor condenser was selected. Condenser pressure was set to 2 bar and kept constant. Distillate rate was initially set to 5500 kmole/hr with a reflux of 0.3. The heated rich stream enters the desorber On-Stage 3. A design-spec

block was used to maintain 85% removal of CO<sub>2</sub> in the desorber. As mentioned previously, the user may experience divergence and flooding at this point, regarding the desorber. This problem can be avoided by increasing the section diameter. This was done in this simulation but was at a later point decreased to its original value. Since the reboiler temperature does not depend on the distillate rate in rate-based calculations, the reboiler temperature was kept as calculated by Aspen Plus.

The bottom product is split into two streams; semilean- and lean stream. The split fraction for the lean stream is 0.61. The lean stream goes through a valve where pressure is reduced to 1.2 bar. Vapor is flashed and the stream goes into a separator. 1.2 bar was used as separator pressure and 105°C was used as an initial value. A transfer block was used to transfer the valve outlet temperature to the separator. Transfer block procedure can be seen in figure 3-15 to figure 3-17. The top product of the separator was compressed up to 2 bar using the isentropic ASME model as compressor type. Isentropic efficiency of 0.75 was used. The compressor enters the desorber On-Stage 8, which is the reboiler. The bottom product of the separator was pumped at 4 bar with a pump efficiency of 0.75.

The semilean stream enters a pump with a discharge pressure of 3 bar and a pump efficiency of 0.75. At this point, the heater was replaced with a MHeatX unit and inlets and outlets were connected. Two streams need to be specified in order for the heat exchanger to run. Semilean outlet- and lean outlet temperature was specified to be 5°C higher than the rich inlet temperature.  $\Delta P$  on all sides was assumed to be zero. This was done manually as there is no specification regarding cold inlet/hot outlet temperature difference when using a MHeatX unit. The semilean outlet was further cooled to 40°C using a cooler.  $\Delta P$  across the semilean cooler was set to 1.9 bar. The semilean cooler was not connected to the absorber at this point. The lean outlet was further cooled to 40°C using a cooler.  $\Delta P$  across the lean cooler was set to 2.9 bar.

In order to maintain the material balances through the system, the water loss and MEA loss was accounted for by mixing the regenerated amine solution with makeup streams of water and MEA. Two calculator blocks were used for this purpose. The calculator blocks can be seen in figure 3-9 to figure 3-11. Initial values have to be used for the makeup streams in order for the simulation to start. Mass fraction in the lean feed was adjusted to match outlet stream of the mixer in order to get similar values. At this point, the outlet of the semilean cooler was connected to the absorber. The semilean stream enters the absorber On-Stage 6. The molar flow rate of the lean feed was adjusted down to 65000 kmole/hr. A design-spec block was used to maintain 85% removal of CO<sub>2</sub> in the absorber.

Table 3–12 Results of vapor recompression + split stream using Aspen Plus rate-based

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<b>Lean/Low-In:</b>	
Molar flow [kmole/hr]	62098.4/62098.4 kmole/hr
Mass fractions:	
H <sub>2</sub> O	0.657/0.657
CO <sub>2</sub>	3.69E <sup>-8</sup> /3.71E <sup>-8</sup>
MEA	0.146/0.146
H <sub>3</sub> O <sup>+</sup>	2.46E <sup>-12</sup> /2.47E <sup>-12</sup>
OH <sup>-</sup>	7.1E <sup>-6</sup> /7.09E <sup>-6</sup>
HCO <sub>3</sub> <sup>-</sup>	5.1E <sup>-4</sup> /5.1E <sup>-4</sup>
CO <sub>3</sub> <sup>2-</sup>	1.9E <sup>-3</sup> /1.9E <sup>-3</sup>
MEA <sup>+</sup>	0.08/0.08
MEACOO <sup>-</sup>	0.12/0.12
<b>Semilean stage entry:</b>	
Stage entry	6
Molar flow [kmole/hr]	36401.7 kmole/hr
Mass fractions:	
H <sub>2</sub> O	0.634
CO <sub>2</sub>	3.47E <sup>-8</sup>
MEA	0.153
H <sub>3</sub> O <sup>+</sup>	2.4E <sup>-12</sup>
OH <sup>-</sup>	7.2E <sup>-6</sup>
HCO <sub>3</sub> <sup>-</sup>	4.5E <sup>-4</sup>
CO <sub>3</sub> <sup>2-</sup>	2.0E <sup>-3</sup>
MEA <sup>+</sup>	0.08
MEACOO <sup>-</sup>	0.13
Rich MEA to desorber temperature [°C]	106.7°C
Outlet compressor temperature [°C]	173.8°C
<b>Equivalent energy consumption:</b>	4.105 MJ/kg CO <sub>2</sub>

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### 3.3.4 Temperature profiles

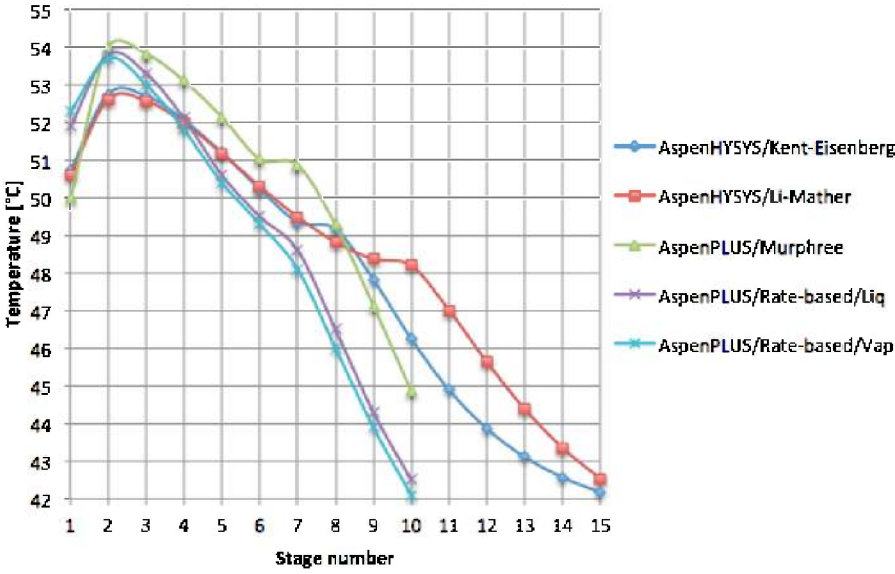


Figure 3-26 Temperature profiles in the absorber

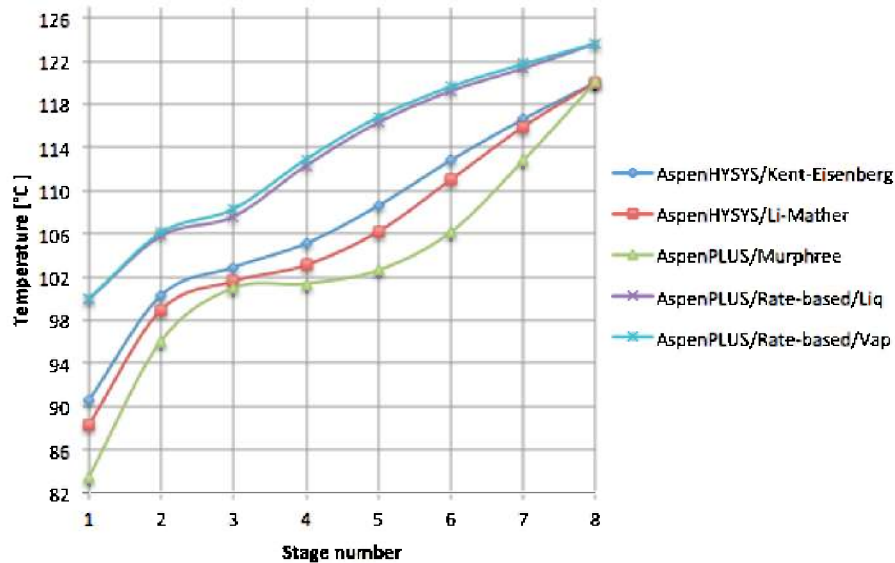


Figure 3-27 Temperature profiles in the desorber

## 3.4 Calculation strategies in Aspen HYSYS

The user will most likely experience convergence problems in the absorber and desorber. One solution is to manipulate any input specifications in the design/specs tab up and down to see if this might have an effect. The second solution is to change the solver for the column in which the problem is occurring. Change the solver from “*Inside-Out algorithm*” to “*Modified HYSIM Inside-Out algorithm*” with damping factor set to “*Adaptive*”.

Number of stages also has an impact on convergence. If the user has specified too many stages in a column, the column will diverge.

A problem with the Kent-Eisenberg and Li-Mather model is the wt-% of MEA and the temperature in a stream, which is limited to 30 wt-% MEA and 125°C. Even though these problems occur, the simulation will still be calculated with warnings and yellow streams (Øi 2007).

Convergence problems will occur more often the more complex a simulation becomes.

The adjust-operator is used instead of adjusting parameters manually, e.g. absorber efficiency.

For a complex simulation, the efficiency of the adjust-operator decreases and the simulation will tend to diverge. A mix of adjusting parameters manually and using an adjust-operator was used to achieve convergence for most of the Aspen HYSYS simulations.

## 3.5 Calculation strategies in Aspen Plus

Aspen Plus is more complicated simulation software compared to Aspen HYSYS.

When using Aspen Plus, the simulation should be run after a unit is added to the PFD. This is done to avoid problems and unnecessary waste of time. If a simulation displays many errors and warnings, the errors and warnings must be located and fixed. By running the simulation after a unit is added, this can be avoided.

Aspen HYSYS uses features like adjust, recycle and spreadsheet and are not available in Aspen Plus. Aspen Plus uses design-spec- and calculator blocks.

A design-spec block is used when a certain result is wanted, e.g. removal efficiency in the absorber. The user selects which parameter to vary and the lower and upper limit of the parameter that is to be varied. A calculator block is based on FORTRAN coding. The user chooses which parameters that are to be included in the code and where it is to be exported to. If the design- and calculator blocks are not specified correctly, the simulation will not start or it will not converge. See chapter 3.1.2 on how to set up such blocks correctly.

If a simulation is completed without using any of these features, it can be difficult to implement such blocks on a unit or stream. The user should implement them from the start of a simulation.

When using a design block, divergence may still occur. If the range between the lower and upper limit is too big or too low, the simulation might diverge.

Sometimes a unit will not converge simply because Aspen Plus wasn't able to perform enough iterations. Number of iterations can be increased; maximum is 200 iterations.

Another problem that may occur is that stages in columns dry up. By adjusting flow rate or number of stages in the column, the simulation will usually converge. Another solution is to reset the simulation to start from the beginning.

Rate-based simulations are more complex due to extra parameters that are needed in order to run the simulation. Same problems as mentioned above will occur but might occur more frequent. In rate-based simulations, the user specifies the height and width of a column and what type of packing material that is being used. Flooding may occur, especially in a distillation column, if the diameter is too low. By increasing the diameter, the flooding will be reduced.

If a design-block is used on a distillation column when running rate-based calculations and flooding occurs, the lower and upper limit of the design-spec block should be monitored when increasing the section diameter.



## 4 Variation of parameters

Some parameters have been changed in order to see the impact it would have on the energy consumption.

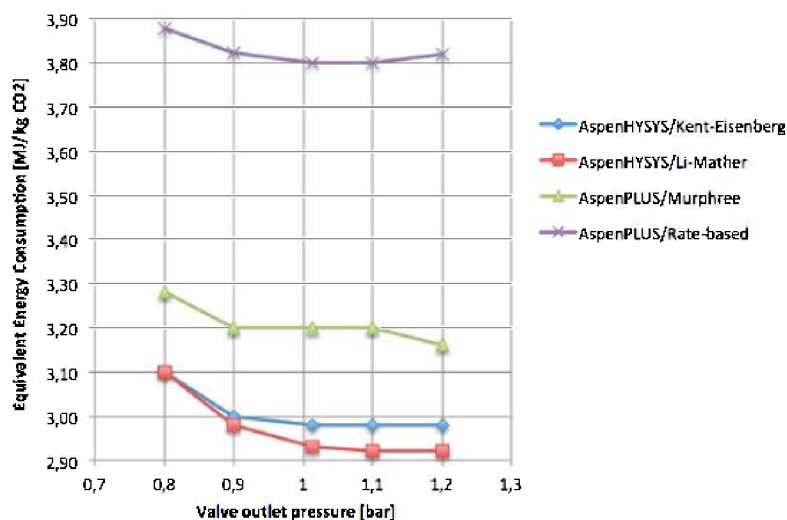
### 4.1 Valve outlet pressure

By increasing the pressure drop across the valve, the reboiler duty decreases. However, the compressor duty increases. In order to compare compressor- and reboiler duty, the compressor duty was multiplied with 4 in order to get equivalent duty. The valve outlet pressure was varied from 0.8 – 1.2 bar.

#### 4.1.1 Vapor recompression

*Table 4–1 Variation of valve outlet pressure for vapor recompression*

		Equivalent energy consumption [MJ/kg CO <sub>2</sub> ]				
Pressure [bar]		0.8	0.9	1.01	1.1	1.2
AspenHYSYS	K-E	3.10	3.00	2.98	2.98	2.98
AspenHYSYS	L-M	3.10	2.98	2.93	2.92	2.92
AspenPLUS	Eq	3.28	3.20	3.20	3.20	3.16
AspenPLUS	RB	3.88	3.82	3.80	3.80	3.82



*Figure 4–1 Variation of valve outlet pressure for vapor recompression*

A variation of the valve outlet pressure results in a reduction in equivalent energy consumption varying from 0.06 – 0.18 MJ/kg CO<sub>2</sub> removed. A valve outlet pressure of 1.2 bar gives the lowest equivalent energy consumption for most of the models. A more detailed study will show that optimum outlet pressure lies between 1.1 – 1.2 bar. Due to small difference in equivalent energy consumption, 1.2 bar has been used as optimum valve outlet pressure.

#### 4.1.2 Vapor recompression + split stream

Table 4–2 Variation of valve outlet pressure for vapor recompression + split stream

		Equivalent energy consumption [MJ/kg CO <sub>2</sub> ]				
Pressure [bar]		0.8	0.9	1.01	1.1	1.2
AspenHYSYS	K-E	3.13	3.11	3.10	3.12	3.12
AspenHYSYS	L-M	3.08	3.05	3.03	3.03	3.03
AspenPLUS	Eq	3.30	3.24	3.20	3.18	3.19
AspenPLUS	RB	4.10	4.08	4.08	4.07	4.11

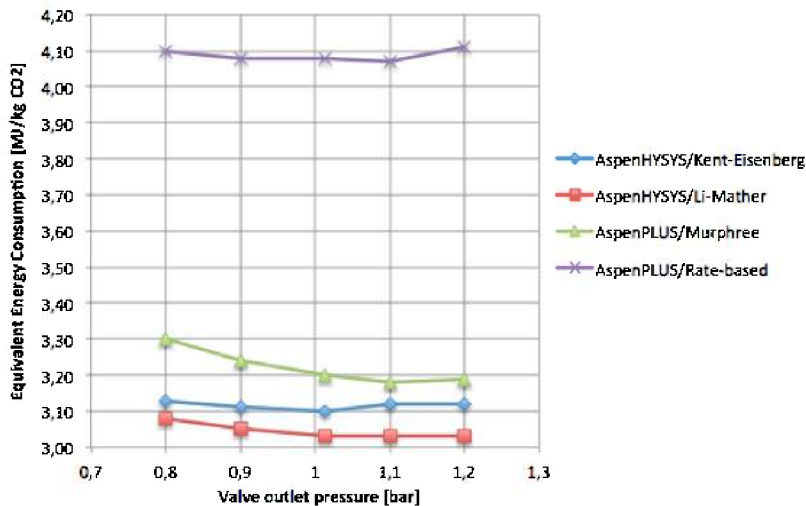


Figure 4–2 Variation of valve outlet pressure for vapor recompression + split stream

By varying the valve outlet pressure from 0.8 – 1.2 bar, the improvement is less for the vapor recompression combined with split stream configuration than it was for vapor recompression. In this configuration, 1.2 bar was used as optimum valve outlet pressure.

## 4.2 Flue gas temperature

The flue gas temperature was varied from 30°C to 40°C. While varying the flue gas temperature, the lean feed temperature was kept constant at 40°C. The removal efficiency in the absorber was kept constant at 85%. The temperature variation for vapor recompression and vapor recompression combined with split stream was performed at a valve outlet pressure of 1.2 bar.

### 4.2.1 Base case

Table 4–3 Variation of flue gas temperature for base case

		Energy consumption [MJ/kg CO <sub>2</sub> ]										
Temperature [°C]		30	31	32	33	34	35	36	37	38	39	40
HYSYS	K-E	3.31	3.32	3.34	3.35	3.36	3.38	3.40	3.42	3.44	3.46	3.48
HYSYS	L-M	3.17	3.19	3.21	3.23	3.25	3.27	3.30	3.32	3.35	3.38	3.42
AspenPLUS	Eq	3.17	3.18	3.20	3.21	3.24	3.25	3.27	3.30	3.32	3.34	3.37
AspenPLUS	RB	4.16	4.16	4.1	4.18	4.19	4.20	4.21	4.22	4.23	4.25	4.26

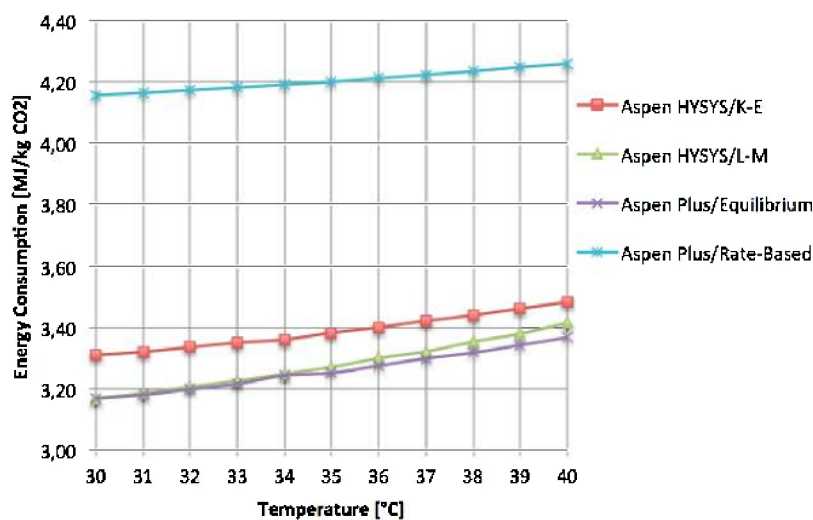


Figure 4–3 Variation of flue gas temperature for base case

All models have an increase in equivalent energy consumption when varying the flue gas temperature from 30 - 40°C. Aspen Plus rate-based gives the lowest increase of 0.1 MJ/kg CO<sub>2</sub> removed while Aspen HYSYS Li-Mather gives the highest increase of 0.25 MJ/kg CO<sub>2</sub> removed.

## 4.2.2 Vapor recompression

Table 4–4 Variation of flue gas temperature for vapor recompression

		Equivalent energy consumption [MJ/kg CO <sub>2</sub> ]										
Temperature [°C]		30	31	32	33	34	35	36	37	38	39	40
HYSYS	K-E	2.87	2.87	2.89	2.89	2.90	2.91	2.92	2.94	2.95	2.96	2.98
HYSYS	L-M	2.78	2.78	2.80	2.81	2.83	2.84	2.86	2.87	2.88	2.90	2.92
AspenPLUS	Eq	2.97	2.98	3.00	3.01	3.02	3.04	3.06	3.07	3.09	3.11	3.13
AspenPLUS	RB	3.72	3.73	3.74	3.75	3.75	3.76	3.77	3.78	3.79	3.81	3.82

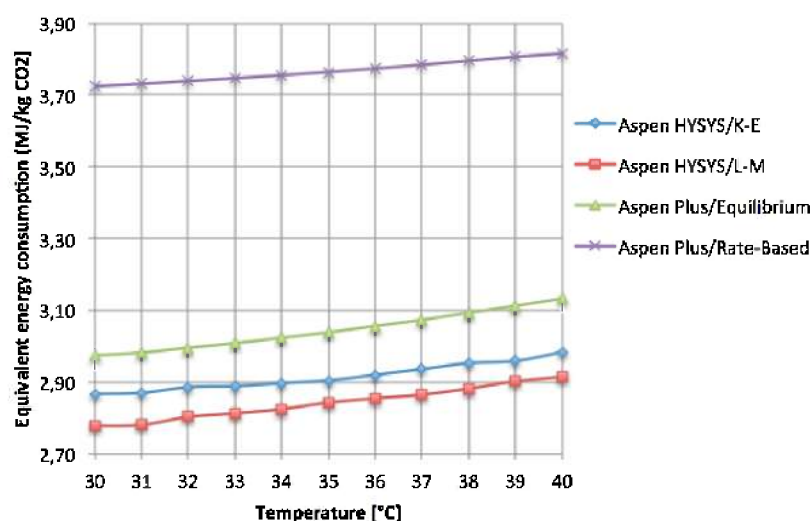


Figure 4–4 Variation of flue gas temperature for vapor recompression

All models have an increase in equivalent energy consumption when varying the flue gas temperature from 30 - 40°C. However, the increase is closer to each other in this configuration compared with the base case. Aspen Plus rate-based gives the lowest increase of 0.1 MJ/kg CO<sub>2</sub> removed while Aspen Plus equilibrium gives the highest increase of 0.16 MJ/kg CO<sub>2</sub> removed. Regarding the Kent-Eisenberg, Li-Mather and rate-based models, the temperature of the lean stream from the heat exchanger was below 40°C when the flue gas temperature varied from 30 - 32°C. The lean cooler was therefore not needed because it is not beneficial to heat the lean stream back up to 40°C. The temperature in the lean feed to the absorber was adjusted accordingly.

## 4.2.3 Vapor recompression + split stream

Table 4–5 Variation of flue gas temperature for vapor recompression + split stream

		Equivalent energy consumption [MJ/kg CO <sub>2</sub> ]										
Temperature [°C]		30	31	32	33	34	35	36	37	38	39	40
HYSYS	K-E	3.0	3.01	3.01	3.02	3.03	3.04	3.05	3.07	3.09	3.10	3.12
HYSYS	L-M	2.88	2.89	2.91	2.92	2.93	2.95	2.96	2.98	3.00	3.01	3.03
AspenPLUS	Eq	3.12	3.04	3.06	3.07	3.09	3.11	3.11	3.14	3.15	3.18	3.17

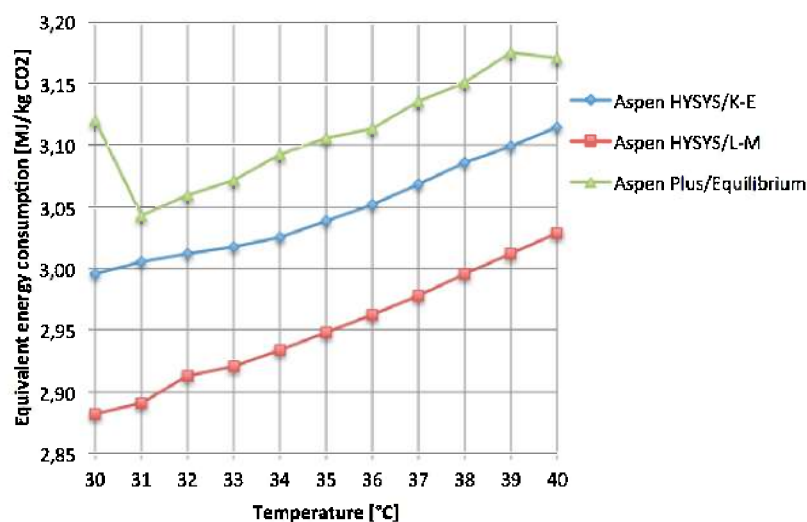


Figure 4–5 Variation of flue gas temperature for vapor recompression + split stream

Both of the Aspen HYSYS models have an increase in equivalent energy consumption while the Aspen Plus equilibrium model has a slight reduction from 30 - 31°C. Aspen Plus equilibrium model gives the lowest increase of 0.05 MJ/kg CO<sub>2</sub> removed while Aspen HYSYS Li-Mather gives the highest increase of 0.15 MJ/kg CO<sub>2</sub> removed. The Aspen Plus rate-based model has not been included due to convergence problems and difficulties with the simulation. Regarding both Aspen HYSYS models, the temperature of the lean stream from the heat exchanger was below 40°C when the flue gas temperature varied from 30 - 32°C. The lean cooler was therefore not needed because it is not beneficial to heat the lean stream back up to 40°C. The temperature in the lean feed to the absorber was adjusted accordingly.

## 4.3 Various parameters

Due to time consuming simulations, the valve outlet pressure and flue gas temperature were the only parameters that were varied in these simulations. A more complete study of parameter variation would include variation of Murphree efficiency, lean flow rate and number of stages. In Aspen HYSYS the number of stages in the absorber have been maximized for vapor recompression and vapor recompression combined with split stream.

In Aspen Plus, however, number of stages in the absorber has been kept constant at 10 stages. This is due to the complexity of the program and difficulties running simulations.

## 5 Discussion

There has been performed a lot of work on simulating CO<sub>2</sub> capture at TUC. However, most of this work is focusing on one simulation tool at the time and Aspen HYSYS has been the preferred tool.

For the base case, a  $\Delta T = 10^{\circ}\text{C}$  in the rich/lean heat exchanger has been used in earlier studies performed at TUC. The minimum temperature approach was then decreased to  $5^{\circ}\text{C}$  when simulating other configurations. In all the cases in this thesis, including base case, simulations was performed using a  $\Delta T = 5^{\circ}\text{C}$ . The reason for this is to get a better perspective on the improvement when simulating other configurations.

Kent-Eisenberg- and Li-Mather model gave approximately the same results, but the Li-Mather model was a little bit lower.

The Kent-Eisenberg model tends to diverge more often when a configuration gets more complex. This may affect adjust-operators used in the simulation and manual adjustments may be required. Convergence problems occurred in the simulations, especially for vapor recompression combined with split stream, and manual adjustments of the lean absorber feed and mass fractions was necessary to achieve 85% removal of CO<sub>2</sub>. As can be seen in the spreadsheets in the appendix, the removal efficiency varies from 85.0 – 85.27%. This is due to manual adjustments of the lean absorber feed. It is assumed that this difference is negligible and that the energy consumption would not be affected. However, there are uncertainties connected to this because small changes can have a big effect on different process parameters. The Li-Mather model is a more solid model than Kent-Eisenberg. The time for the iterations to complete is longer than for the Kent-Eisenberg model, but convergence will most likely be achieved.

In order to convert compressor duty to equivalent steam consumption, an efficiency of 0.25 was assumed. A further study on this efficiency and its accuracy should be performed.

The vapor recompression configuration has been simulated like described in chapter 2.7.

Outlet temperature of the compressor is calculated to  $170.7 - 173.8^{\circ}\text{C}$ . In literature, it is said that the compressed vapor returns to the reboiler at 2 bar and  $120^{\circ}\text{C}$ . It is uncertain what extent this temperature difference will have on the reboiler duty. There are several solutions for cooling down the compressed vapor. By using a cooler after the compressor, the temperature can be decreased to  $120^{\circ}\text{C}$ . When doing this, the vapor will condense and approximately 95% of the flow will be liquid. By injecting liquid instead of vapor back into the reboiler, the reboiler duty will increase.

Another solution is to compress the vapor in several steps and have water injection in between the compressor stages. A problem by doing this is that when compressing a vapor flow from 1 bar to 2 bar, the amount of compressor stages required are low. Uncertainties on how to handle the high temperature are high and a further study should be performed. A study on

degradation of MEA should also be performed regarding the conditions of the compressed vapor in these simulations.

Espen Hansen is one of few who have compared different simulation tools.

Uncertainties are connected to comparing the results in this thesis with results from Espen Hansen (Hansen 2011). He used a  $\Delta T = 10^\circ\text{C}$  in the rich/lean heat exchanger while a  $\Delta T = 5^\circ\text{C}$  was used in this thesis.

For the equilibrium model in Aspen Plus, Espen Hansen used the rate-based example file located in the AspenTech folder. This file contains old parameter sets. An electrolyte insert file was used for this thesis, which resulted in lower energy consumption. A description about this electrolyte insert file can be found in chapter 3.1.2.

For the rate-based model, Espen Hansen experienced problems with the rich/lean heat exchanger. Two heaters were used instead with approximately the same duty.

A HeatX unit was used in the simulations in this thesis and convergence problems occurred.

To get the HeatX model to converge, the section diameter of the desorber was increased to a point where convergence was achieved. The section diameter was then reduced to its original value later in the simulation. This resulted in lower energy consumption compared with Espen Hansen. The difference in energy consumption was calculated to approximately 0.2 MJ/kg  $\text{CO}_2$ . It was stated that the optimum pressure before compression was 1.2 bar for all the cases. From the profiles in chapter 4.1 it can be seen that this may not be the case.

For vapor recompression using the Aspen Plus rate-based model, the equivalent energy consumption increases when increasing the pressure from 1.1 – 1.2 bar. Rate-based calculations proved to be very difficult so this will most likely have an impact on the results.

For vapor recompression combined with split stream using Kent-Eisenberg, the equivalent energy consumption increases when the pressure is increased from 1.01 – 1.2 bar. In complex configurations, divergence occurred more often when using Kent-Eisenberg. This resulted in uncertainties regarding the accuracy of manual adjustments.

When the flue gas temperature was varied for vapor recompression combined with split stream using the Aspen Plus equilibrium model, the equivalent energy consumption decreased by 0.08 MJ/kg  $\text{CO}_2$  when the temperature was increased from 30 - 31 $^\circ\text{C}$ . This result is relatively small and may be a result of manual adjustments and the complexity of the configuration. Except for the Aspen Plus equilibrium model, all cases showed the same trend when varying the flue gas temperature. Temperature variation for vapor recompression combined with split stream using the rate-based calculations was not included. This was because of the difficulties of using the rate-based model.

The reason for including the combination of vapor recompression and split stream in this thesis was the reduction potential for the vapor recompression- and split stream configuration. Christian Berg et.al calculated an improvement of 0.65 MJ/kg  $\text{CO}_2$  for split stream compared to the base case. They calculated an improvement of 1.0 MJ/kg  $\text{CO}_2$  for vapor recompression compared to the base case.



The combination of the two configurations was therefore simulated to see if the reduction potential was greater or lower than the separate configurations.

This was not the case. The equivalent energy consumption for the combination was between 0.1- 0.3 MJ/kg CO<sub>2</sub> higher than that of vapor recompression.

The reason for this can be a combination of several things. The flow rate of the compressed vapor entering the reboiler is less, about 40%, than in that of vapor recompression. The stream entering the desorber has a larger flow rate, which is about 80000 kg/h, than in that of vapor recompression. A higher flow rate into the desorber will lead to a higher steam demand for the reboiler but will also result in greater heat loss in the rich/lean heat exchanger.

When comparing the cases, it can be seen that the energy consumption for the Kent-Eisenberg, Li-Mather and the Aspen Plus equilibrium model are approximately the same for all configurations. The rate-based calculations are approximately 0.8 – 1.0 MJ/kg CO<sub>2</sub> higher in all the configurations. This is because of the example file that was used for the rate-based calculations, which contains a different set of parameters compared to electrolyte insert file used in the equilibrium simulations.

## 6 Conclusion

Three different configurations were simulated using two different simulation tools, Aspen HYSYS and Aspen Plus. The configurations that were simulated were a base case, vapor recompression and vapor recompression combined with split stream. Kent-Eisenberg and Li-Mather were used in the Aspen HYSYS simulations while eNRTL (electrolyte Non-Random Two-Liquid) was used for the equilibrium and rate-based calculations in the Aspen Plus.

The CO<sub>2</sub> removal efficiency was kept constant at 85% in all cases. A Murphree efficiency of 0.25 was used in almost all cases. Murphree efficiency was not used in the rate-based simulations due to the presence of ionic species. In all Aspen HYSYS simulations besides for the base case, 15 stages were used in the absorption column. For the Aspen Plus simulations, 10 stages were used in absorption column. A  $\Delta T = 5^{\circ}\text{C}$  was used in the rich/lean heat exchanger for all simulations.

The energy consumption for the standard configuration was calculated to 3.37 – 4.26 MJ/kg CO<sub>2</sub>. The Aspen Plus equilibrium model calculated the lowest energy consumption while the Aspen Plus rate-based model calculated the highest.

The equivalent energy consumption for the vapor recompression configuration was calculated to 2.92 – 3.82 MJ/kg CO<sub>2</sub>. The equivalent energy consumption is equal to reboiler duty + 4 times compressor duty. The Aspen HYSYS Li-Mather model calculated the lowest equivalent energy consumption while the Aspen Plus rate-based model calculated the highest. The optimum pressure before compression was found to be 1.2 bar for except for the rate-based calculation of vapor recompression combined with split stream.

The equivalent energy consumption for vapor recompression combined with split stream was calculated to 3.0 – 4.1 MJ/kg CO<sub>2</sub>. The Aspen HYSYS Li-Mather model calculated the lowest energy consumption while the Aspen Plus rate-based model calculated the highest. The pressure before compression was kept at 1.2 bar.

The different models and tools calculated an improvement in equivalent energy consumption for vapor recompression varying from 0.2 – 0.5 MJ/kg CO<sub>2</sub>. The Aspen Plus equilibrium model calculated the lowest improvement while Kent-Eisenberg and Li-Mather calculated the highest. For vapor recompression combined with split stream, the improvement was calculated to 0.15 – 0.39 MJ/kg CO<sub>2</sub>. The Aspen Plus rate-based model calculated the lowest improvement while Aspen HYSYS Li-Mather model calculated the highest. This process configuration proved difficult to simulate using the rate-based model.

The results indicate that the vapor recompression configuration is considered to be the most reasonable configuration for reducing the energy consumption. This is in agreement with earlier studies. The most optimum process configuration and most optimum process parameters were calculated to be the same in almost all the simulation models.

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# Appendices

Appendix A: Thesis description

Appendix B: Aspen HYSYS base case spreadsheet

Appendix C: Aspen HYSYS vapor recompression spreadsheet

Appendix D: Aspen HYSYS vapor recompression combined with split stream spreadsheet

## Appendix A Thesis description



**Telemark University College**

**Faculty of Technology**

### **FMH606 Master's Thesis**

**Title:** Vapour recompression in absorption and desorption process for CO<sub>2</sub> capture

**TUC supervisor:** Associate Professor Lars Erik Øi

**Task Description:**

**Aim:**

Calculate the energy reduction potential using vapour recompression in CO<sub>2</sub> capture from atmospheric exhaust based on absorption in monoethanolamine.

**Tasks:**

1. Evaluation of earlier projects on process simulation of CO<sub>2</sub> capture using different process configurations like split-stream and vapour recompression.
2. Simulations of CO<sub>2</sub> capture especially using vapour recompression under different conditions and using different process simulation programs like Aspen HYSYS and Aspen Plus.
3. Calculations of the energy optimum conditions and search for a process with minimum energy consumption for CO<sub>2</sub> desorption.
4. Evaluation of uncertainties in the calculations.

**Background:**

The most studied method for removal of CO<sub>2</sub> from atmospheric exhaust is by the help of amine solutions. Aspen HYSYS has been much used in student projects at Telemark University College for process simulation of CO<sub>2</sub> removal. There are several possibilities to improve the existing models. Split-stream and vapour recompression are possible configurations.



References:

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**Student:** Stian Kvam

**Practical arrangements:**

The work will mainly be carried out at Telemark University College.

**Signatures:**

Supervisor (date and signature):

10/4-13 Lars Erik Øi

Student (date and signature):

10/4-13 Stian Kva

## Appendix B Aspen HYSYS base case spreadsheet

Spreadsheet: SPRDSHT-1

Current Cell: A1 Variable: Angles in: Exportable:

	A	B	C	D	E
1					
2	CO2 Sour Gas	139532.7563 kg/h		Q-Reboiler	4.125e+008 kJ/h
3	CO2 Sweet Gas	20926.4751 kg/h		Massflow CO2	118486.4369 kg/h
4	CO2 Removal Eff.	85.00	%		
5				Energy Consumptio	3.482
6	H2O Sour Gas	5703.5000 kgmole.			
7	H2O loss Abs	8463.8337 kgmole.			
8	H2O loss Des	2445.7523 kgmole.			
9	H2O loss Total	5206.09 kgmole/h			
10					
11	MEA loss Abs	30.3023 kgmole/h			
12	MEA loss Des	0.6502 kgmole/h			
13	MEA loss Total	30.9525 kgmole/h			
14					
15					
16					
17					
18					
19					
20					

Connections Parameters Formulas **Spreadsheet** Calculation Order User Variables Notes

Delete Function Help... Spreadsheet Only...  Ignored

Figure B-1 Spreadsheet for base case using Kent-Eisenberg

Spreadsheet: SPRDSHT-1

Current Cell: D19 Variable: Angles in: Exportable:

	A	B	C	D	E	F
1						
2	H2O Loss Sweet	8346.8362 kgmole.		Q-Reboiler	4.070e+008 kJ/h	
3	H2O Loss CO2	2265.6281 kgmole.		Massflow CO2	119162.9940 kg/h	
4	H2O Sour Gas	5703.5000 kgmole.				
5	H2O Total Loss	4908.96 kgmole/h		Energy Con.	3.416	MJ/kg
6						
7	MEA Loss Sweet	29.7837 kgmole/h				
8	MEA Loss CO2	0.5548 kgmole/h				
9	MEA Total Loss	30.3385 kgmole/h				
10						
11	CO2 Sour Gas	139532.7563 kg/h				
12	CO2 Sweet Gas	20929.8990 kg/h				
13	Removal Eff.	85.00	%			
14						
15						
16						
17						
18						
19						

Connections Parameters Formulas **Spreadsheet** Calculation Order User Variables Notes

Delete Function Help... Spreadsheet Only...  Ignored

Figure B-2 Spreadsheet for base case using Li-Mather



# Appendix C Aspen HYSYS vapor recompression spreadsheet

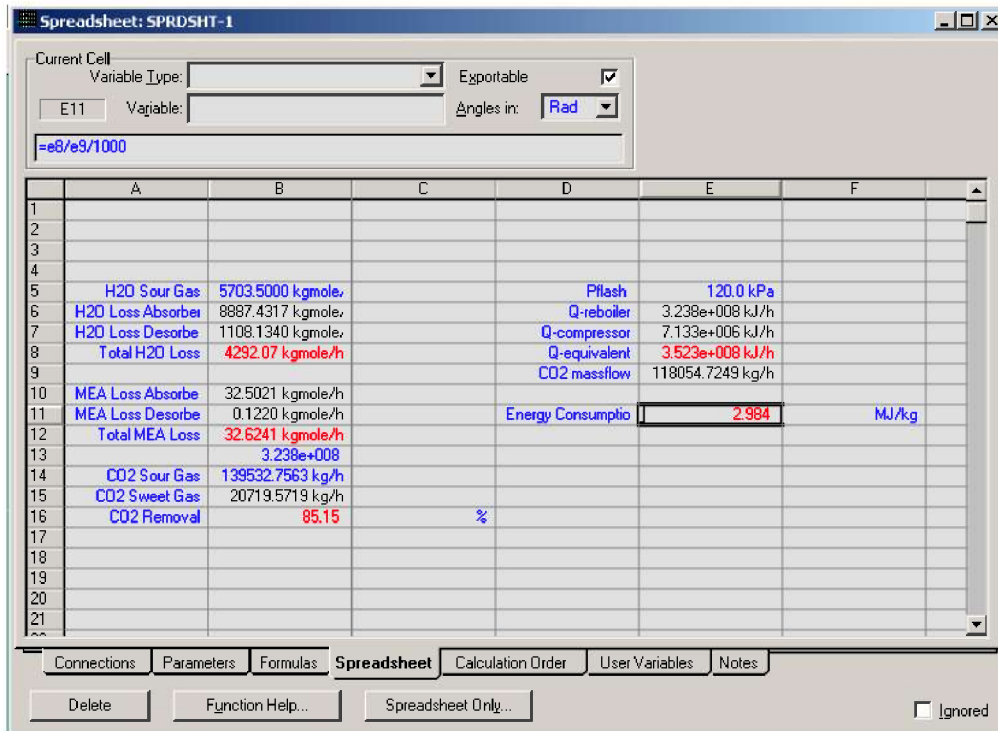


Figure C-1 Spreadsheet for vapor recompression using Kent-Eisenberg

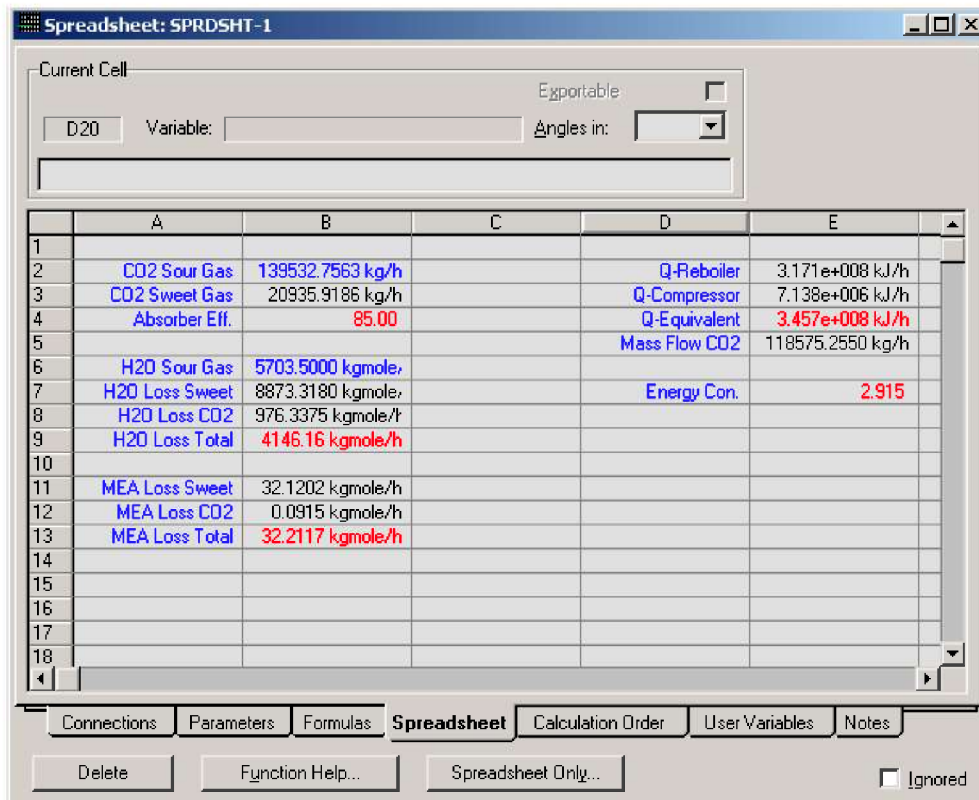


Figure C-2 Spreadsheet for vapor recompression using Li-Mather

# Appendix D Aspen HYSYS vapor recompression + split stream spreadsheet

Spreadsheet: SPRDSHT-1

Current Cell: Variable Type: [ ] Exportable:

B19 Variable: [ ] Angles in: [ ]

	A	B	C	D	E	F
1						
2	CO2 Sour Gas	139532.7563 kg/h		Q-Reboiler	3.530e+008 kJ/h	
3	CO2 Sweet Gas	20552.8863 kg/h		Q-Compressor	4.395e+006 kJ/h	
4	Absorber Eff.	85.27		Q-Equivalent	3.706e+008 kJ/h	
5				CO2 Mass Flow	118933.4980 kg/h	
6	H2O Sour Gas	5703.5000 kgmole/h				
7	H2O Loss Sweet	8844.0862 kgmole/h		Energy Con.	3.116	
8	H2O Loss CO2	1533.3557 kgmole/h				
9	H2O Loss Total	4673.94 kgmole/h				
10						
11	MEA Loss Sweet	32.0411 kgmole/h				
12	MEA Loss CO2	0.2492 kgmole/h				
13	MEA Loss Total	32.2903 kgmole/h				
14						
15	Rich to HX Temp	42.21 C				
16	Lean to Cooler Temp	47.21 C				
17	dT	5.000 C				
18						
19						
20						

Connections Parameters Formulas **Spreadsheet** Calculation Order User Variables Notes

Delete Function Help... Spreadsheet Only...  Ignored

Figure D-1 Spreadsheet for vapor recompression + split stream using Kent-Eisenberg

Spreadsheet: SPRDSHT-1

Current Cell: Variable Type: [ ] Exportable:

B18 Variable: [ ] Angles in: [ ]

	A	B	C	D	E	F
1						
2	CO2 Sour Gas	139532.7563 kg/h		Q-Reboiler	3.428e+008 kJ/h	
3	CO2 Sweet Gas	20627.9547 kg/h		Q-Compressor	4.403e+006 kJ/h	
4	Absorber Eff.	85.22		Q-Equivalent	3.605e+008 kJ/h	
5				CO2 Mass Flow	118993.5655 kg/h	
6	H2O Sour Gas	5703.5000 kgmole/h				
7	H2O Loss Sweet	8788.0315 kgmole/h		Energy Con.	3.029	
8	H2O Loss CO2	1347.2452 kgmole/h				
9	H2O Loss Total	4431.78 kgmole/h				
10						
11	MEA Loss Sweet	31.6535 kgmole/h				
12	MEA Loss CO2	0.1878 kgmole/h				
13	MEA Loss Total	31.8412 kgmole/h				
14						
15	Rich to HX Temp	42.56 C				
16	Lean to Cooler Temp	47.56 C				
17	dT	5.002 C				
18						
19						
20						

Connections Parameters Formulas **Spreadsheet** Calculation Order User Variables Notes

Delete Function Help... Spreadsheet Only...  Ignored

Figure D-2 Spreadsheet for vapor recompression + split stream using Li-Mather