# Process Modeling And Simulation

Course Code : CH620003

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# Assignment 2

## *Question 4*

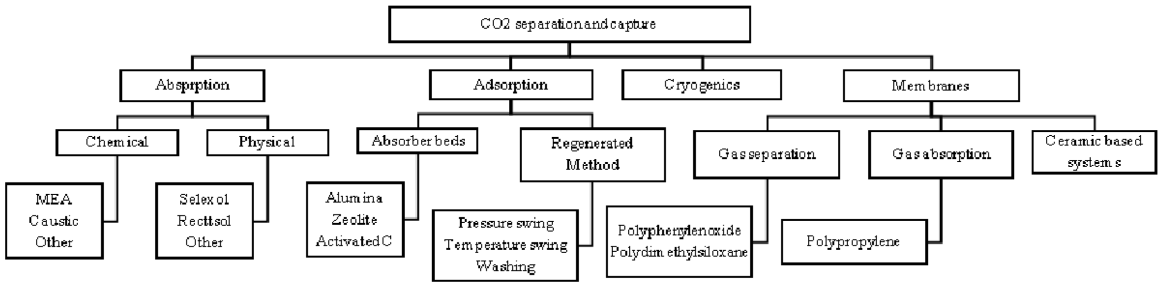
**Capture methods and technologies involve:** The best choice of capturing technology totally relies upon the properties of the enriched CO2 gas stream, which varies by the type of the power plant. Various kinds of gases can be extracted from the various CO2 capturing methods as shown in Table 1. Furthermore, pressure and contents of CO2 in the outlet stream gases, which are the most dominant parameters in selecting the best choice of the capturing technology of CO2, should be different for different methods.

| Gases to separate | Post-Combustion (fluegas) $CO_2/N_2$ | Pre-Combustion (shifted syngas) $CO_2/H_2$ | Oxy-fuel combustion (exhaust) $CO_2/N_2$ |
|---|---|---|---|
| P (kPa) | ~100 | 1000-8000 | ~100 |
| $CO_2$ (%) | 3-15 | 20-40 | 75-95 |

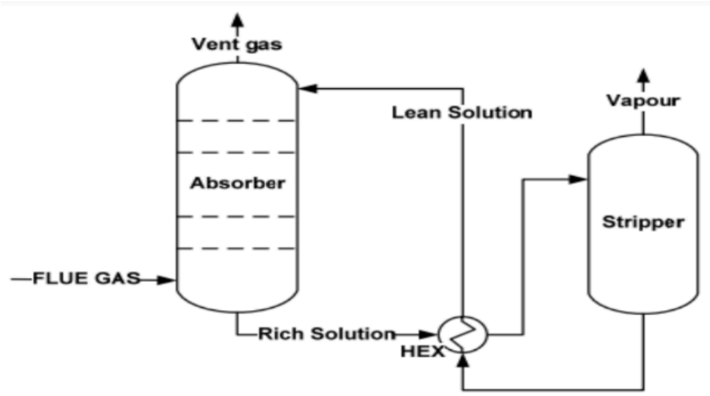
*Table 1*

It's impossible to choose between the different capture technologies right now because they're all too similar. Each has its own set of advantages and applications. However, the main focus of this assignment is on CO2 post-combustion capture method.

There are several techniques for extracting and collecting CO2 from flue gas. They are concentrating towards absorption, adsorption, membranes, cryogenics, among other physical and chemical processes as shown in figure  The choice of an appropriate technology always depends upon the CO2 flue gas traps, which primarily depends upon the kind of the power plant.




## Process Short Description




This is the basic operational flow diagram for an amine absorption unit as shown in the figure This is the traditional MEA-CO2 capturing flow diagram, which has been described and used in a variety of industrial and research activities. The provided process is an exothermic, reversible reaction between a weak base (MEA) and a weak acid(CO2) that leads to the formation of dissolved salts. In the absorber, the inlet gas is treated with a lean solvent. The solvent preferentially absorbs the acid gases. The CO2-enriched solution is preheated before reaching the stripper, where the reaction is reversed by adding heat. The lean solvent escapes the stripper and is cooled by mixing heat with the rich solvent. The residual solvent is transferred to the absorber. A high purity CO2 is extracted from the stripper's tip. A huge amount of heat is mandatory for the regeneration of rich solvent.

## Problem Statement

Aspen Plus Simulation of CO2 capturing from flue gases

- Cut-off the emissions of CO2 up to 85% by optimizing different parameters like MEA solvent, Lean in temperature, pressure, absorber packing height and reboiler duty by using ENTRL-RK method in Aspen Plus

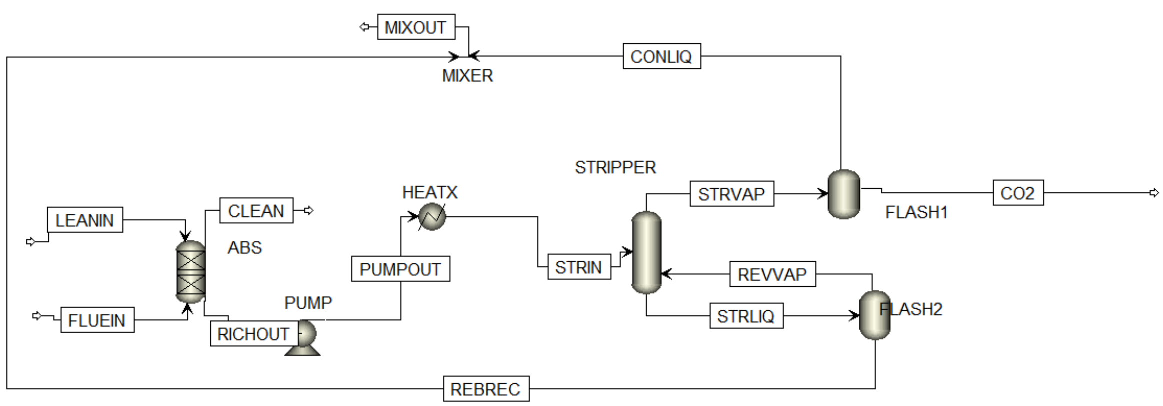
- To develop a better understanding of $CO_2$ post combustion process and the implementation for large scale $CO_2$ emitter application
- To get the optimum reboiler duty by using heat of low pressure steam (waste steam) to reduce the operational cost

## Simulation Approach

This simulation is supposed to address as a baseline for modeling the $CO_2$ capture mechanism with MEA. It can be used as a foundation for more complex models for production system optimization, and plant and equipment construction, among other aspects. Liquid and vapor properties can be determined by using unsymmetric electrolyte NRTL property method (ENRTL-RK) and PC-SAFT equation of state respectively, in rate-based method. $CO_2$, $H_2S$, $N_2$, $O_2$, $CH_4$, $C_2H_6$, and $C_3H_8$ are called Henry-components because Henry's law is applied to them.
The following main features are included in the model:

- Rate-based model of columns
- Unsymmetric electrolyte ENRTL-RK method for water and MEA vapors
- Proper blocks with icons
- Method based reactions kinetics

## Simulation Flow Sheet




Flue gases are injected in the absorber section, where $CO_2$ is absorbed by a Lean Solvent. As $CO_2$ is absorbed by Solvent, cleaned gases are released to the atmosphere from the top and solvent rich in $CO_2$ solution passes from the bottom of the absorber for further processing. The solvent used for absorption of CO2 is monoethanolamine (MEA). In the stripper section, the CO2 is separated (stripped) from the rich solvent and extracted from the top and can be stored after further processing and the lean solvent is recycled back to the absorber column.

## Process Description

Flue gases containing 19 mol % $CO_2$ having 1.03 bar pressure and 160-167C temperature is fed to the absorber. Before the flue gas is passed through the absorber column. It is necessary to remove NOx and SOx because they form heat stable salts with the amine solution. The absorber is a packed column which provides enough surface area for absorption of CO2. The absorption column uses sieve trays in order to
increase the surface area for CO2 absorption and proper mass transfer. The lean amine solution enters from the top (at stage 3) and flue gas enters from the bottom of the absorber (at stage 20). The flue gas and lean amine (solvent) counter current flow in the packed absorber and absorption of CO2 from flue gas to lean amine takes place. The flue gas after absorption of CO2 is released from the top (at stage 1) of the column as exhaust in the atmosphere and the rich amine leaves from the bottom of the absorber column. Lean amine means the amine which is stripped of CO2 and rich amine means the amine is loaded with CO2. The first stage of the absorber is kept for water. The water wash helps to remove any entrained amine present in the exhaust gases.

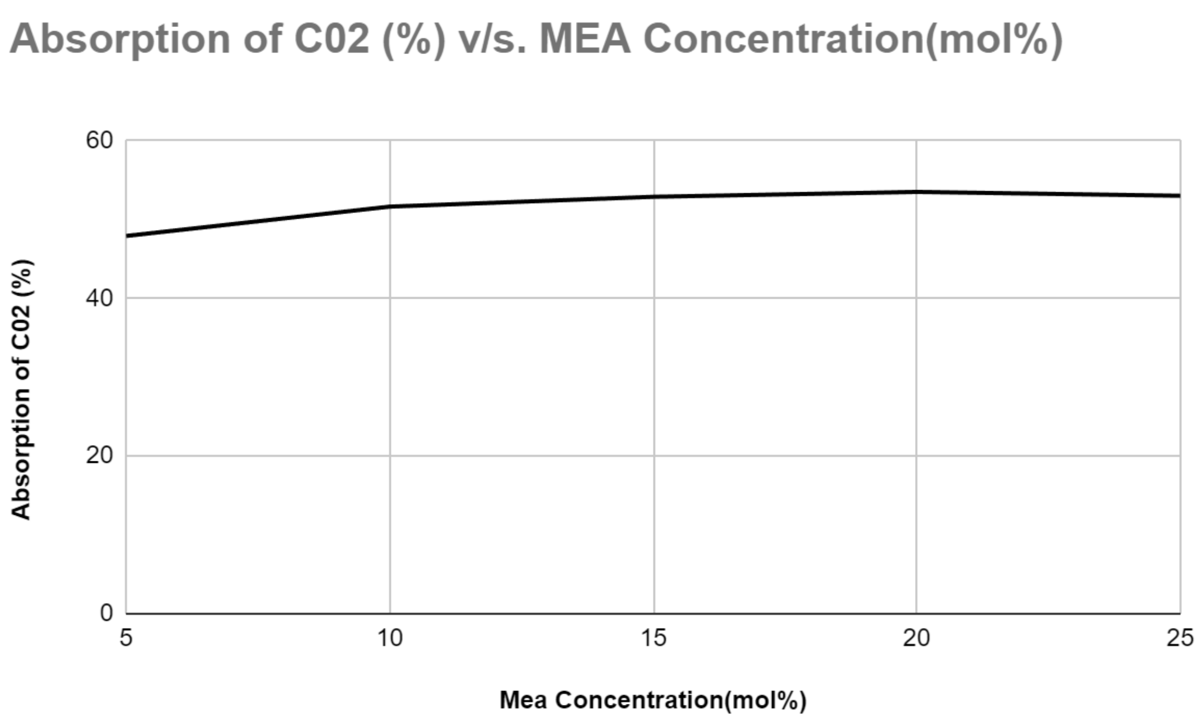
The rich amine passes through the pump which increases its pressure in order to go till the top of the absorber (stripper)column. Rich amine has high temperature because absorption of CO2 is an exothermic process. Before entering the absorber (stripper) column it passes through the cross-heat exchanger. The rich amine then pass-through heater, in heater it heats up to the required temperature. The rich amine then goes to the absorber (stripper) column. Absorber (Stripper) is a packed column with a kettle reboiler. The rich amine enters into the first stage of the column and flows downwards and the vapors from the re-boiler flows upwards. The vapors strip the CO2 from the rich amine and flow upwards and go through the condenser which condenses the water present in the vapors. Then CO2 gas is removed from the top in the vapor phase and the water comes out from the bottom. Then a part of this water flows through the top stage of the stripper column and the top stage acts as a water wash in order to remove any amine present in the Vapors. The reboiler in the stripper column requires heat duty in order to produce the vapors. The heat duty is provided by the power plant. The CO2 gas that is released from top of the stripper is dried and then sent for storage or to a particular industry for usage. The amine solvent (lean out) that is recovered from the bottom of the stripper having high temperature, exchange its heat in heat exchanger to rich amine. After it a makeup of amine is done and a part of the recovered amine solvent is purged and passed through the heater or cooler to achieve desired temperature and goes back to the absorber column.

## Results and Discussion

Our main aim is to develop a model which gives maximum CO2 removal efficiency while optimizing different parameters that affect the model performance. The most important parameters that affect the CO2 removal efficiency of a model are solvent parameters and reboiler duty. The performance of model in the form of CO2 removal efficiency is collected at various operational conditions by changing the different solvent parameters like concentration, pressure, temperature and reboiler duty in the reboiler of the stripper while the flue gas parameters remain constant.

### MEA concentration variation effect on CO2 removal (Absorption)

| **Mea Concentration(mol%)** | **Absorption of $C0_2$ (%)** |
|---|---|
| 5 | 47.93 |
| 10 | 51.65 |
| 15 | 52.9 |
| 20 | 53.52 |
| 25 | 53.03 |

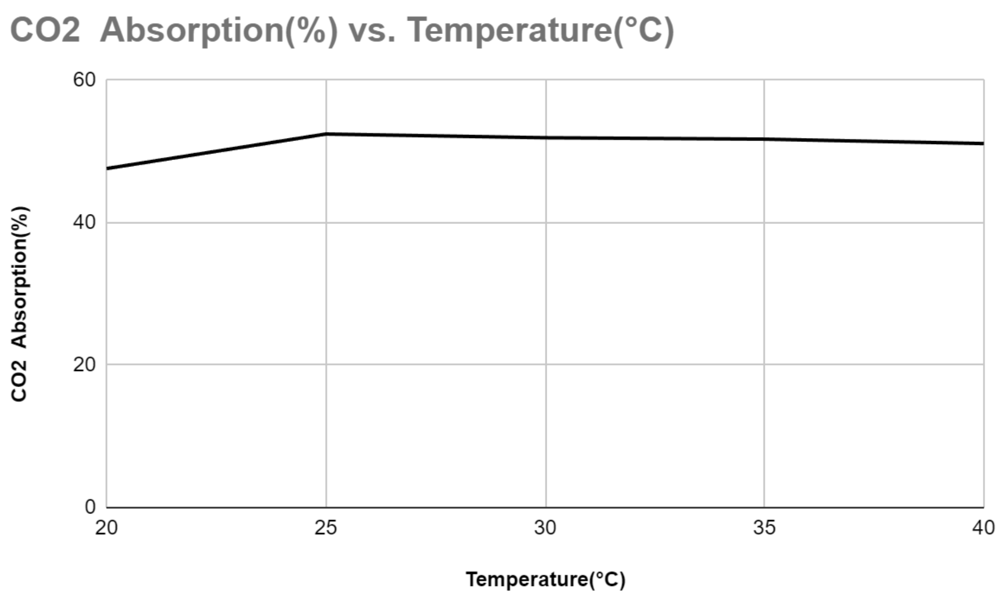


The removal efficiency of CO2 performance is collected in the absorber column of the model as given in figure 10. By varying MEA concentration for a closed loop system. It is analyzed that CO2 removal efficiency increased from 51.65 to 59.75% by changing concentration 10 to 20%. When the concentration is further increased from 20 to 30 % the removal efficiency decreased.CO2 removal efficiency gives maximum value at 20% of MEA concentration. Below 20 % of MEA, the absorption rate of CO2 decreases due to unavailability of sufficient MEA to react with CO2 in the absorption column. Above 20% concentration of MEA the trend of decrement of Absorption percentage is due to excess of MEA.

## Lean in (solvent) temperature variation effect on CO2 Absorption:

To check how much the lean in temperature will affect the absorption of CO2, the analysis is performed by simulating multiple runs by varying the solvent (lean in) temperature from 20C to 40C.

| **Temperature(°C)** | **$CO_2$ Absorption(%)** |
|---|---|
| 20 | 47.6 |
| 25 | 52.45 |
| 30 | 51.93 |
| 35 | 51.73 |
| 40 | 51.1133 |

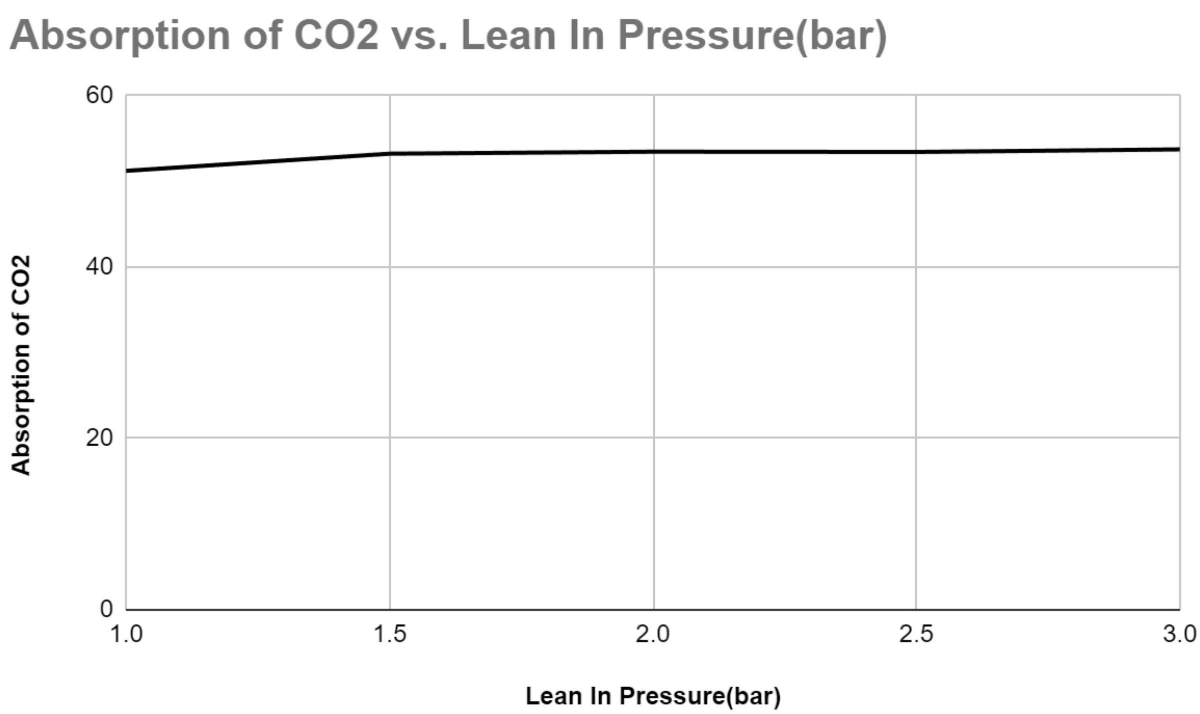


It can be seen that from above figure 11 the absorption of CO2 increases .2% as a result of increase in temperature from 20C to 25C. When temperature varies from 25 to 40 C the absorption of CO2 decreases 2%. Absorption of CO2 maximum at 25C. Absorption first increases at optimum temperature and then decreases by increasing temperature, it may be due to the evaporation of solvent and evaporation of solvent causes solvent loss.

### Lean in (Solvent) Pressure variation effect on CO2 Absorption:

To check lean in pressure behavior on CO2 absorption in the absorber column, the analysis is performed by simulating multiple runs by varying the solvent (lean in) pressure from1 to 3 bar.

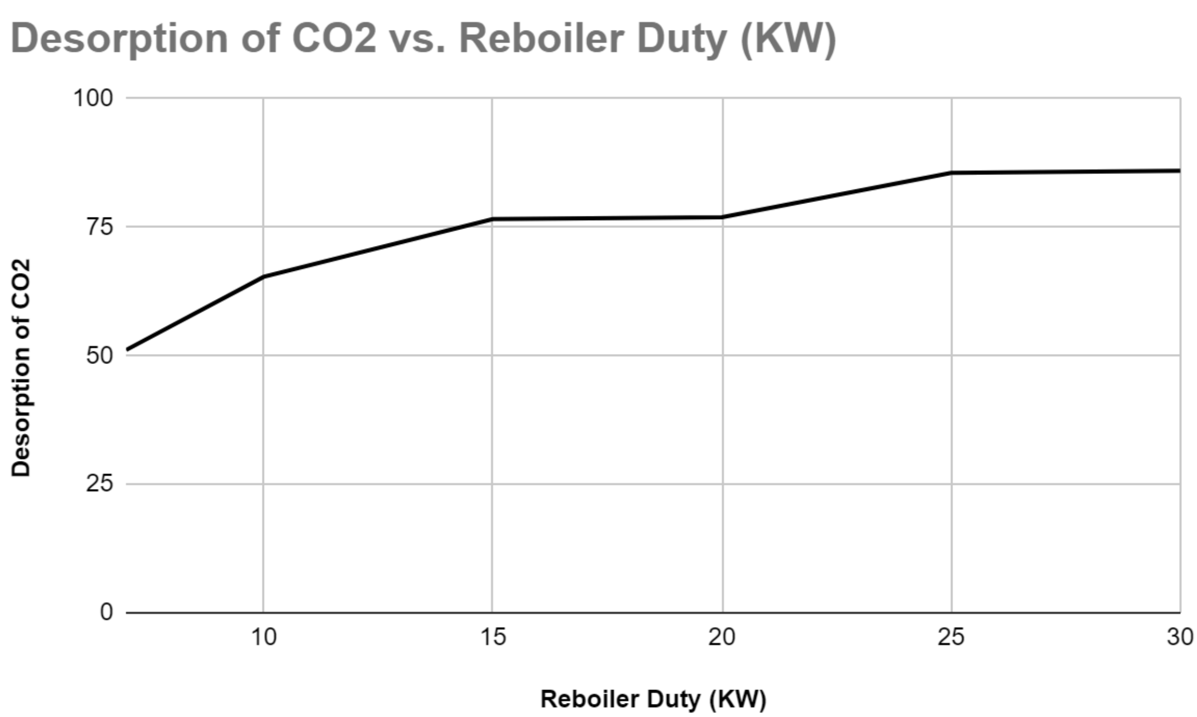
| **Lean In Pressure(bar)** | **Absorption of $CO_2$** |
|---|---|
| 1 | 51.23 |
| 1.5 | 53.23 |
| 2 | 53.464 |
| 2.5 | 53.432 |
| 3 | 53.734 |



By increasing pressure the absorption percentage also increases. Percentage of absorption increases from 51.23% to 53.734 % by varying pressure from 1 to 3 bar. It will give a maximum at 3 bars. Absorption of CO2 increases gradually by increasing pressure because higher pressure increases dilution of gas in solvent and it also prevents the vaporization of solvent in this way it reduces solvent losses.

## Reboiler duty variation effect on CO2 capture:

| **Reboiler Duty (KW)** | **Desorption of $CO_2$** |
|---|---|
| 7 | 51.12 |
| 10 | 65.345 |
| 15 | 76.595 |
| 20 | 76.935 |
| 25 | 85.565 |
| 30 | 85.955 |




The percentage of CO2 stripping is directly related to reboiler duty. As reboiler duty increases the percentage of CO2 desorption also increases. We get approximately 85% of CO2 stripping at 25 KW reboiler duty.

## Conclusion

**85.6%** of $CO_2$ is captured from flue gas using **25% by wt.** concentration of MEA and providing **25KW** reboiler duty at **40 $^{o}$C** Lean in Temperature and **2 bars** Lean in Pressure.