Modelling of CO_2 Capture by Reactive Absorption and Stripping

The CO_2 post-combustion capture by chemical absorption-stripping is a process consisting in the reactive absorption by an aqueous chemical solution and subsequent regeneration of the solvent by means of a reactive stripping process. The process has been studied since the '50s and a very exhausting literature exists on different topics, such as the choice of a proper solvent, the study of the kinetics, the synthesis of different process configurations etc.

The objective of this study is to show a systematic procedure for the steady-state model-based design of a CO2 post-combustion capture plant by reactive absorption and stripping using Monoethanolamine (MAE) as solvent. The first part is dedicated to the process modelling in one of the most powerful process simulation software, Aspen Plus.

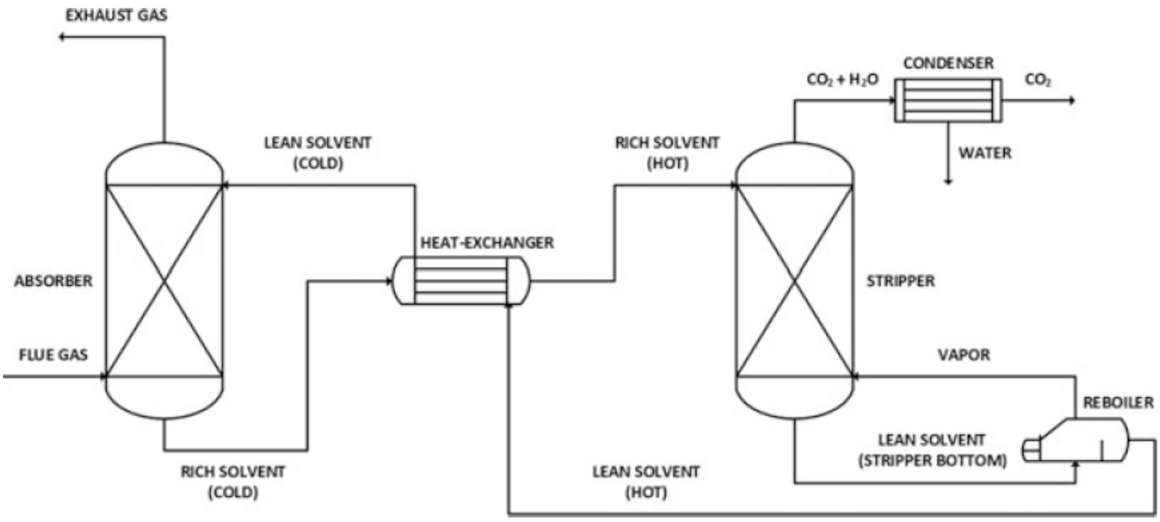
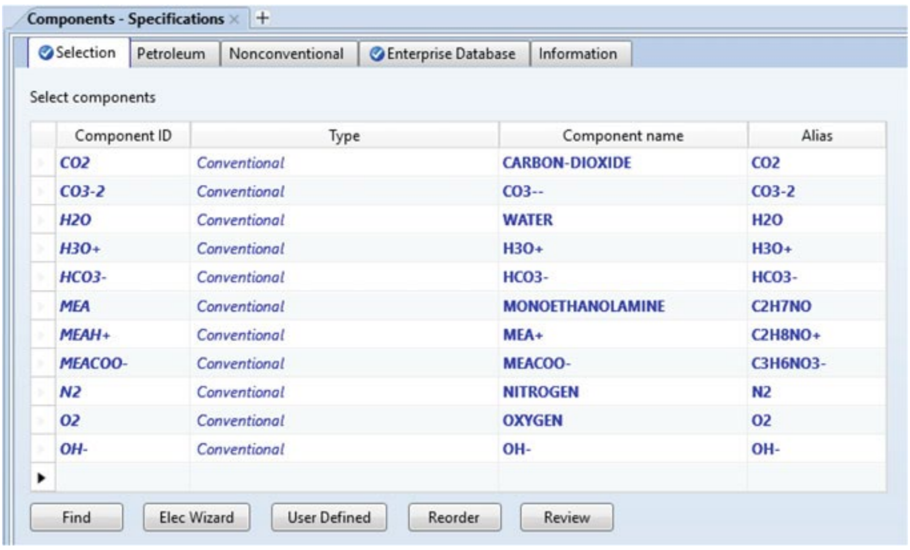


Fig. : Simplified flowsheet of a CO_2 capture by reactive absorption-stripping plant



Component ID	Type	Component name	Alias
CO2	Conventional	CARBON-DIOXIDE	CO2
CO3-2	Conventional	CO3--	CO3-2
H2O	Conventional	WATER	H2O
H3O+	Conventional	H3O+	H3O+
HCO3-	Conventional	HCO3-	HCO3-
MEA	Conventional	MONOETHANOLAMINE	C2H7NO
MEAH+	Conventional	MEA+	C2H8NO+
MEACOO-	Conventional	MEACOO-	C3H6NO3-
N2	Conventional	NITROGEN	N2
O2	Conventional	OXYGEN	O2
OH-	Conventional	OH-	OH-

Fig. : List of components in the Aspen Properties®—Components—Specifications panel

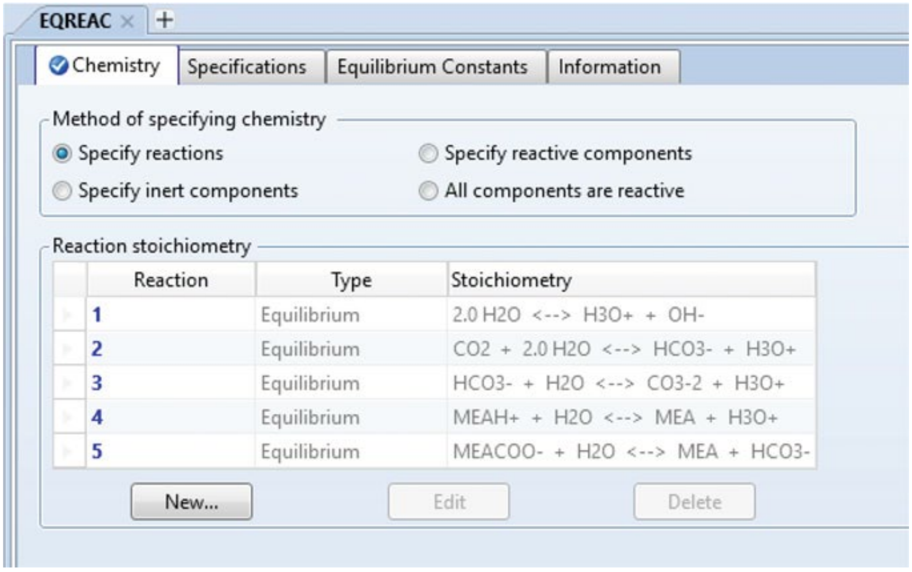


Fig. Equilibrium reactions for the CO_2-MEA-H_2O system

The Elec-NRTL model was coupled with the Redlich-Kwong Equation of State for the computation of the non-idealities of the vapor/gas phase, is used for this study.

Due to the reactive nature of the process, a proper set of reactions must be specified in the Reactions panel. As reported in numerous works on the CO_2 post-combustion capture with MEA, both kinetic and equilibrium reactions are involved written as following.

$$2H_2O \rightleftarrows H_3O^+ + OH^-$$

$$MEA^+ + H_2O \rightleftarrows H_3O^+ + MEA$$

$$HCO_3^- + H_2O \rightleftarrows H_3O^+ + CO_3^{2-}$$

$$CO_2 + MEA + H_2O \rightleftarrows MEACOO^- + H_3O^+$$

$$CO_2 + OH^- \rightleftarrows HCO_3^-$$

For what concerns the equilibrium reactions, for the determination of the equilibrium constants as a function of temperature, Aspen Plus offers two methods:

- **Standard Gibbs free-energy change.** In this case the equilibrium constant has the following rigorous expression

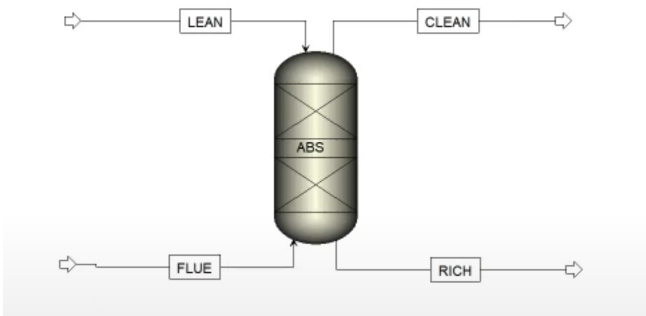
  $$K_{eq} = \exp\left(-\frac{\Delta G^0}{RT^L}\right)$$

  Where the values of the ΔG^0 are retrieved from the Aspen Properties® database.
- **Parameter-based correlation.** In this case the equilibrium constant has the following form

  $$\ln\left(K_{eq}\right) = A + \frac{B}{T^L} + C\ln\left(T^L\right) + DT^L$$

  where the coefficients A, B, C, D can be found in literature.

Model Validation for the Absorber



Aspen Flowsheet of Absorption Column

For this case study we have referred Tontiwachwuthikul P, Meisen A, Lim CJ (1992) CO2 absorption by NaOH, Monoethanolamine and 2-Amino-2-Methyl-1-Propanol solutions in a packed column. Chem Eng Sci 47(2):381–390

Source	Tontiwachwuthikul et al.	
Run	T22	
Stream	Flue gas	Lean amine
Temperature (K)	288.15	292.15
Molar flow (mol/s)	0.14	1.04
CO_2 (mol frac)	0.191	0
MEA (mol frac)	0	0.055
H_2O (mol frac)	0.1	0.945
N_2 (mol frac)	0.709	0
Pressure (kPa)	103.15	103.15

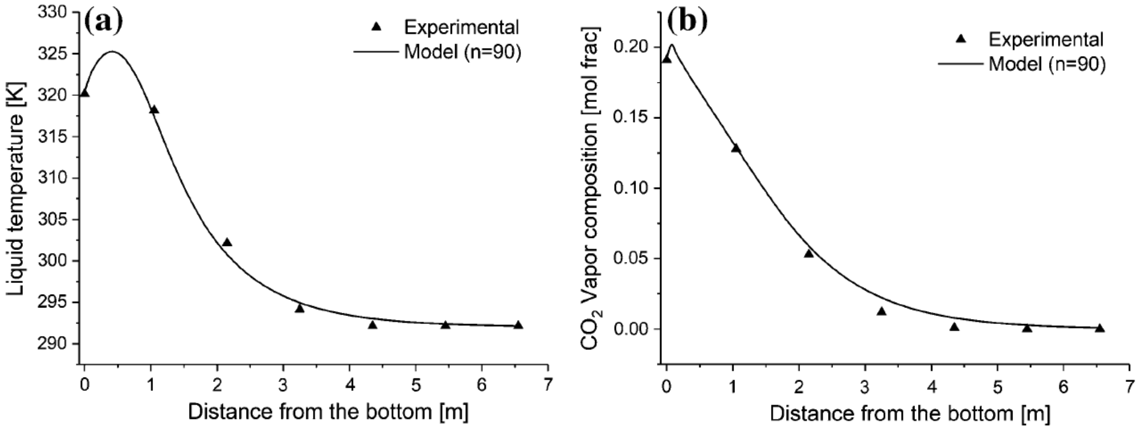
Feed characterization

Packing height (m)	6.55
Column diameter (m)	0.1
Packing type	12.7 mm Berl Saddles
Void fraction (m^3/m^3)	0.62
Dry specific area (m^2/m^3)	465

Column and packing features

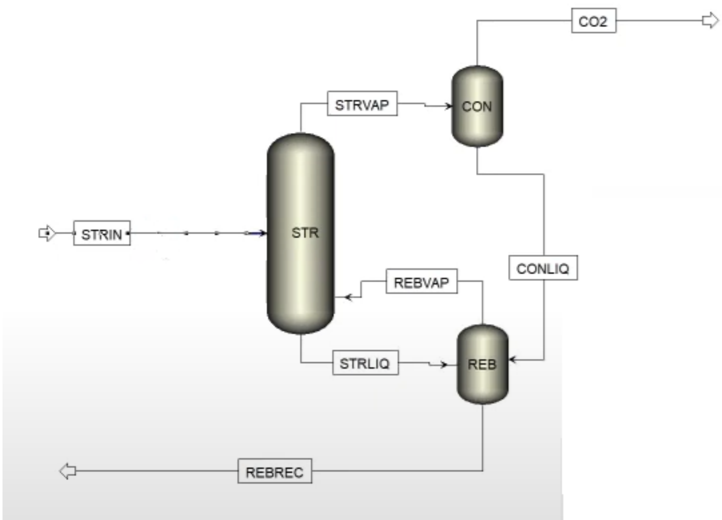
Run	T22
Packing type	Random
Wetted surface area	Onda
Material transfer coefficients	Onda
Heat transfer coefficients	Chilton and Colburn
Fractional liquid hold-up	Stichlmair

Rate-based correlations



Comparison between absorber (a) liquid temperature and (b) CO_2 vapor composition Profiles obtained in Aspen Plus with the experimental data

Model Validation for the Stripper



Aspen Flowsheet of Stripping Column

For this study we have referred Tobiesen FA, Juliussen O, Svendsen HF (2008) Experimental validation of a rigorous desorber model for CO_2 post-combustion capture. Chem Eng Sci 63(10):2641–2656

Source	Tobiesen et al.
Run	1
Stream	Rich amine
Temperature (K)	389.91
Molar flow (kmol/h)	10.71
CO_2 (mol frac)	0.0348
MEA (mol frac)	0.1102
H_2O (mol frac)	0.8549
N_2 (mol frac)	0
Pressure (kPa)	196.96

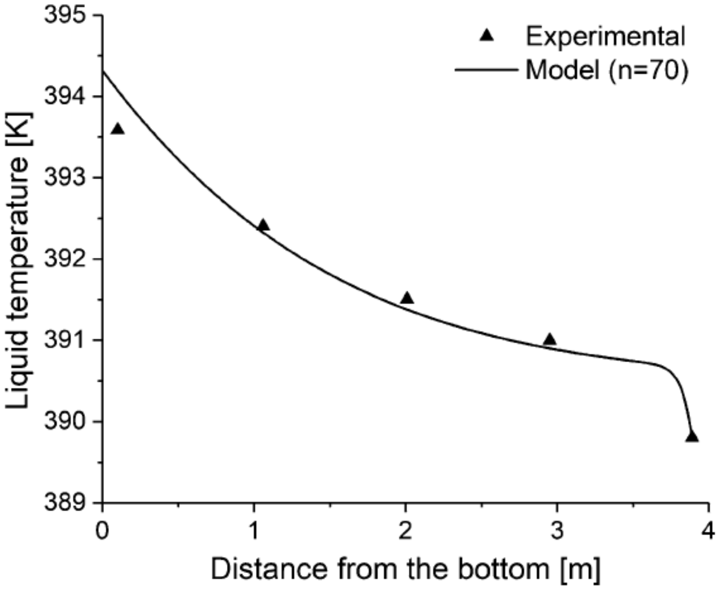
Feed characterization

Packing height (m)	3.89
Column diameter (m)	0.1
Packing type	Sulzer Mellapak 250Y
Void fraction (m^3/m^3)	0.987
Dry specific area (m^2/m^3)	256

Column and packing features

Run	1
Condenser/Top pressure (kPa)	196.96
Pressure drop (kPa)	1
Condenser temperature (K)	288.15
Reboiler duty (kW)	11.6

Operating conditions



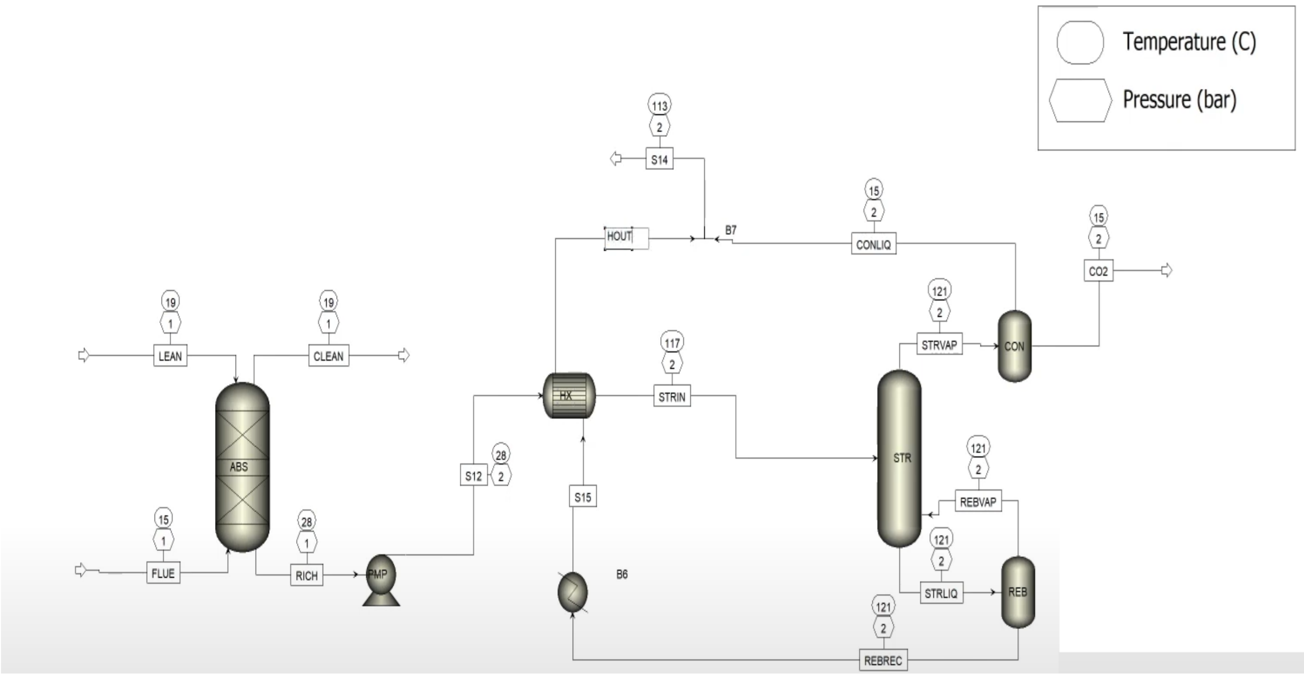
Comparison between the model liquid temperature profile and the experimental data

Cross Heat-Exchanger Design

The cross heat-exchanger represents the connection between the absorption and the stripping sections. In fact, here the rich solvent from the bottom of the absorber is heated using the sensible heat of the lean solvent coming from the reboiler. The heat-exchanger should be designed to maximize the exchange between the two streams.

In particular, the Aspen Exchanger Design and Rate (Aspen EDR) was used to evaluate the average heat transfer coefficient. Then, the Shortcut mode within Aspen Plus was used to evaluate the exchange area. Table below resumes the results for the design of the cross heat-exchanger.

Parameter	Value
Heat Duty (MW)	112.6
Average heat transfer coefficient [W/(m^2 K)]	338.34
Exchange area (m^2)	28,892



Complete Aspen Plus Flow Sheet with both absorber and stripper

Results

Following are the final results of the complete case study, which shows 99.12% CO_2 at 15 number of stages, which is similar to experimental values available in literature.

Performance	Number of segments				
	15	30	50	80	90
CO_2 removal %	99.12	99.45	99.56	99.62	99.63
Loading out	0.455	0.457	0.457	0.457	0.457