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Surrogate model for carbon dioxide equilibrium absorption using aqueous Monoethanolamine (MEA)

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ABSTRACT

In this study, a surrogate model that describes the vapour-liquid equilibrium of CO₂ in a flue gas or biogas and an aqueous alkanolamine solution precisely, e.g. monoethanolamine (MEA), is adjusted. A surrogate model is an engineering method used when an outcome cannot be easily determined, hence a model of the outcome is used instead. Most engineering design problems require experiments and/or simulations to evaluate design objective and constraint functions as function of design variables. The vapour-liquid equilibrium data is simulated using the software OLI® which is suitable to work with electrolyte solutions. The system is made of a large number of compounds and chemical reactions which are readily implemented in OLI®. The aim of the study is to determine the distribution of CO₂ between the liquid and the gas phases. Therefore, a surrogate model is adjusted to the simulation results. The main variables affecting the carbon dioxide absorption are the type of chemical absorbent, concentrations and the operating temperature. The resulting surrogate model is critically evaluated to check its ability to reproduce satisfactorily the vapour-liquid MEA-CO₂-H₂O system. The model obtained, together with the mass balances, is useful to design absorption columns simplifying its resolutions.

Keywords: Monoethanolamine, carbon dioxide capture, alkanolamine, surrogate.

1. INTRODUCTION

Climate change is the greatest environmental threat of the century, with economic, social and environmental consequences of great magnitude. Without exception; citizens, businesses, economies and nature around the world are being affected. The weather has always varied along the Earth history; it is dynamic and unstable. The problem of climate change is that in the last century the pace of these changes has been greatly accelerated by the anthropogenic emissions of greenhouse gases, e.g. CO₂. Increasing world populations and corresponding emissions of CO₂ from combustion of fossil fuels (coal, oil and natural gas) as the main energy source are greatly contributing to global warming and therefore climate change. Hence, carbon capture and storage (CCS) is one of the main goals proposed in the Conference of the Parties (COP).

The capture of CO₂ from the combustion gases is done efficiently through chemical absorption with solvent processes, physical adsorption, and separation by membranes, processes of calcination/carbonation, etc. Among all these alternatives, the chemical absorption with alkanolamines is the nowadays most used industrially and with greatest potential in the future.

Scrubbing effluent industrial fluid streams of acid gases such as CO₂ and H₂S is an important industrial process operation. The technique has historically been applied for various reasons such as improving the calorific value of biogas streams and avoiding corrosion on process lines and fittings. Recently, a more compelling reason for scrubbing of carbon dioxide from process streams is the urgent need to reduce greenhouse gas emissions. CO₂ capture by absorption technology remains the most promising and most mature technology for CO₂ removal from exhaust gas streams, and a deep understanding of this technology is of global interest to reduce costs. Amine-based CO₂ solvents are the most studied absorbents for CO₂ capture by absorption (Aronu et al. 2011).

Several studies have been carried out on the solubility of CO₂ in aqueous monoethanolamine (MEA) solution. Tables presenting summaries of previous studies were presented by Jou et al. (1995), Kohl and Nielsen (1997) and Ma'mun et al. (2005). The experimental data of Jou

et al. (1995) covers a wide range of temperatures, pressures and loadings, however it is available only for 30 mass % MEA.

Although a large number of ‘end-of-pipe’ CO₂ separation technologies exist, there is agreement that the absorption–desorption process based on chemical solvents is the most mature and is most likely to be deployed in the near-to medium-term (Kather et al., 2008; Mac Dowell et al., 2010).

However, despite the technical feasibility, the economic penalty poses a huge barrier to the implementation of this technology at large scale. Solvent optimization and advanced process integration are two efficient ways to reduce the cost (Rochelle, 2009). A great deal of research effort has been devoted to exploring better alternatives to the traditional aqueous monoethanolamine (MEA) solvent, either through solvent blends or improved single solvents (Rochelle et al., 2001).

The behaviour of vapour-liquid equilibrium of CO₂-H₂O-MEA mainly depends on the concentration of MEA and the conditions of temperature and pressure at which the system is operated. The objective of this work is to adjust a model that describes in a simple way the complex vapour-liquid equilibrium that occurs in the chemical absorption of CO₂ in alkanolamine solutions, more precisely of the MEA-CO₂-H₂O system.

2. OBJECTIVES

The main objectives of this Master Final Project are:

- Simulation of vapour-liquid equilibrium data using OLI ® software
- Proposal of a novel surrogate model of the Vapour-Liquid Equilibrium for the chemical absorption of carbon dioxide in monoethanolamine (MEA).
- Model validation compared with simulated and experimental data.
- Determination of Monoethanolamine lost in the vapours.

3. MATERIALS AND METHODS

The simulation of the absorption of CO₂ using aqueous Monoethanolamine (MEA) is performed using OLI[®] software. The surrogate model is performed using a multilinear regression using Microsoft Excel[®]. The determination of the partial pressure of CO₂ at different concentrations of Monoethanolamine, temperatures and loading of CO₂/ MEA in the liquid is conducted. On the other hand, an assessment of the influence on the equilibrium in the presence of an inert gas (CH₄) instead of CO₂ is performed to check that the model is valid for biogas enrichment. The presence of Monoethanolamine (MEA) in the vapour phase is a parameter of great importance from the environmental point of view not addressed in the experimental studies from the literature.

3.1. OLI[®] ANALYSER

OLI Analyzer is a computing software for simulating aqueous-based chemical systems. It is a graphical program developed by OLI Systems, Inc. (Morris Plains, NJ, USA) that utilizes a predictive thermodynamic framework for calculating the physical and chemical properties of multiphase, aqueous-based systems.

The thermodynamic framework is applicable to multi component mixtures of chemicals in water, and is predictive over a wide range of temperature, pressure and concentration of interest. Supported by an in-place databank, the software allows users to predict the chemical and phase behaviour of mixtures of inorganic or organic chemicals in water. The program uses two different models to calculate thermodynamic parameters:

- **Aqueous (standard chemistry) model:** empirical extensions of the initial Debye–Hückel model.
- **Mixed Solvent Electrolyte (MSE) model:** based on the local composition concept which accounts for the Debye–Hückel model and its modifications.

In this study the Mixed Solvent Electrolyte model is used, because The MSE framework is OLI's newly developed model capable of reproducing speciation, chemical, and phase equilibria applicable to water-organic-salt systems in the full range of concentrations as well as aqueous electrolytes from dilute solutions to the fused salt limit.

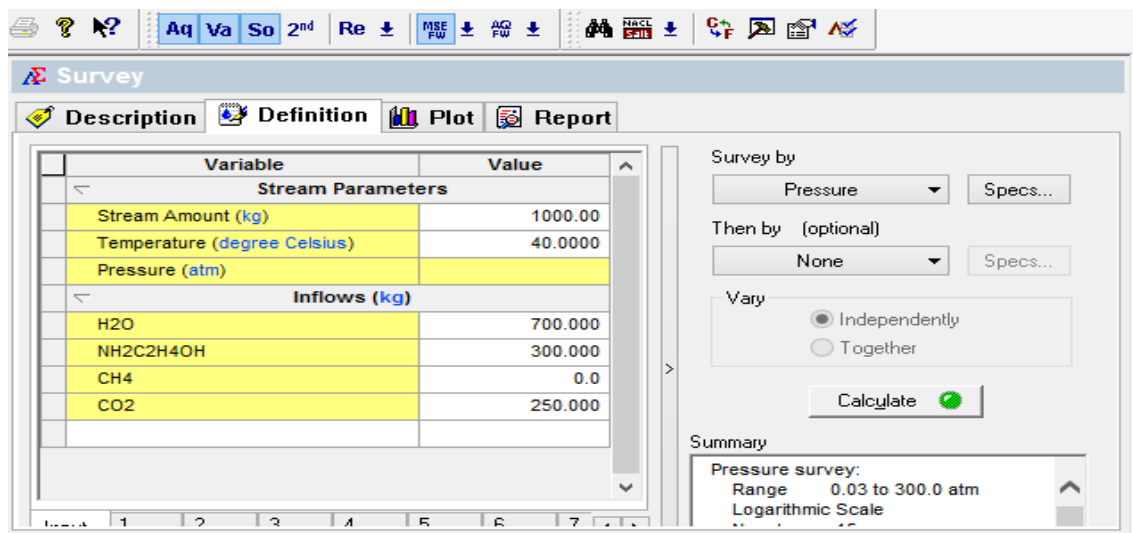


Figure 1. OLI Analyzer (Mixed Solvent Electrolyte model)

3.1.1. Low and high operating pressures

The following system is calculated at high and low operating pressures, to work at low pressures, the pressure with which it operates is 1 atm or lower. The pressure ranges for high pressure range from 0.03 to 300 atm. Several temperatures, amount of monoethanolamine (MEA), and dilution are used as input data, together with the amount of pure CO₂ fed. Simulations at lower pressures uses methane to help decreasing the partial pressure of CO₂, keeping the operating pressure fixed at 1 atm, and then the same procedure previously indicated is followed. The income amount of CH₄ is 50 kg.

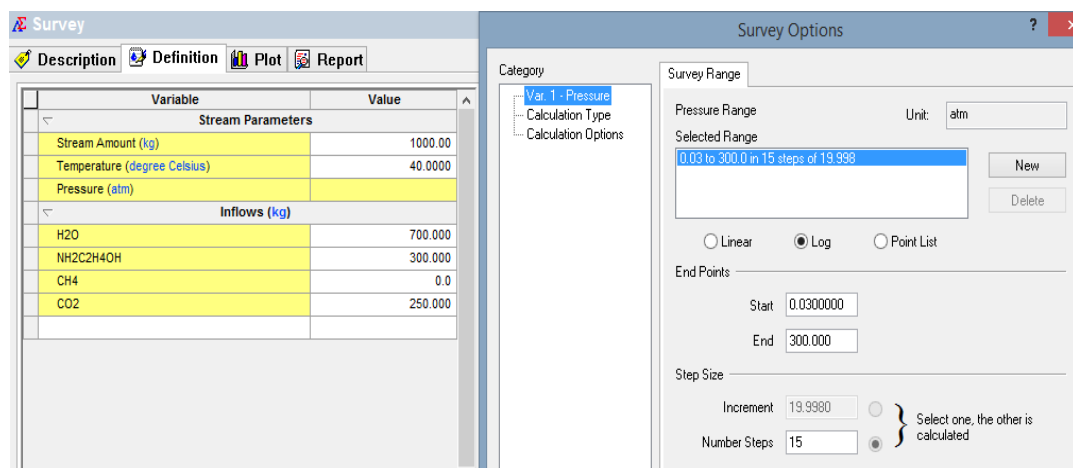


Figure 2. Simulation to high operating pressures (OLI ®)

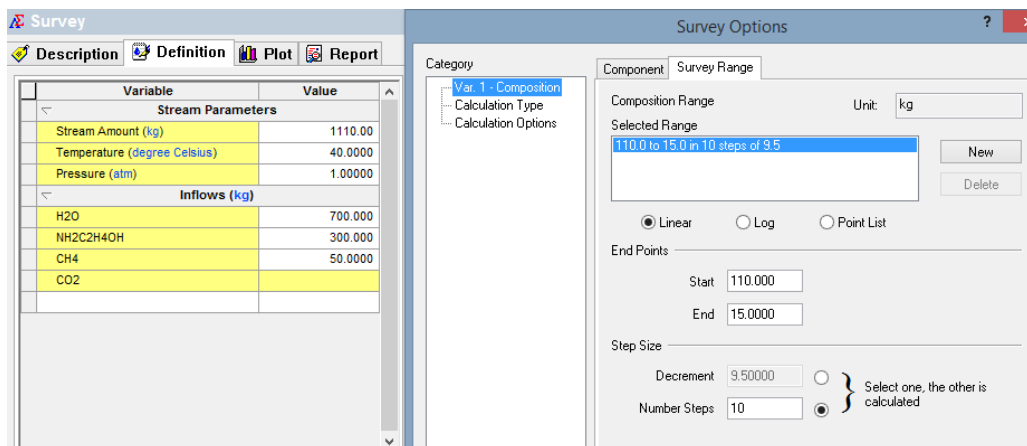


Figure 3. Simulation to low operating pressures (OLI ®)

3.1.2. Monoethanolamine (MEA) concentration and temperature simulation

Different amounts of monoethanolamine (MEA) are evaluated: 15, 30, 45 and 60 % wt. Operating temperatures varies from 40 to 120 °C.

3.1.3. Speciation Summary

Table 1. Classification of species produced

| User Inflows | Related Inflows | Liquid Species | Vapour Species |
|--|--------------------------------|--|--|
| H ₂ O | H ₂ CO ₃ | H ₂ O | H ₂ O |
| NH ₂ C ₂ H ₄ OH | | OH ⁻¹ | NH ₂ C ₂ H ₄ OH |
| CH ₄ | | NH ₃ C ₂ H ₄ OH ⁽⁺¹⁾ | CH ₄ |
| CO ₂ | | NH ₂ C ₂ H ₄ OH | CO ₂ |
| | | CH ₄ | |
| | | CO ₂ | |
| | | CO ₃ ⁻² | |
| | | HCO ₃ ⁻¹ | |
| | | C ₃ H ₆ NO ₃ ⁻¹ | |
| | | H ₃ O ⁺¹ | |

OLI® has implemented a large number of chemical reactions and compounds to simulate the absorption of CO₂. The liquid phase chemical composition is described using 10 compounds and the vapours phase is described using 4 compounds. Each scenario is obtained mixing the water/MEA liquid phase with the CH₄/CO₂ vapour phase (Table 1).

3.2. HENRY'S LAW

Henry's law defines that the amount of dissolved gas in a liquid at constant temperature is proportional to the partial pressure of the gas in the liquid (Eq. 1).

$$P = C \cdot kH \quad (1)$$

- P: partial pressure of gas.
- C: concentration of the gas (solubility).
- kH: Henry's constant.

The Henry law is widely used to model physical absorption but not complex systems with chemical absorption such as the CO₂/MEA system presented in the last section.

3.3. PARAMETERS OF THE NOVEL SURROGATE MODEL

In this section is presented a simple surrogated model for the carbon dioxide capture using MEA, as the Henry model is not useful for this kind of systems.

3.3.1. Loading CO₂/MEA (α)

Loading CO₂ that is present in the solution of MEA is calculated with Equation 2. Equation 2 is the ratio of moles of aqueous CO₂ and moles of aqueous MEA, both in their different ionic forms (Table 1).

$$\alpha = \frac{CO_2(aq) + CO_3^{-2} + HCO_3^{-1} + C_3H_6NO_3^{-1}}{C_3H_6NO_3^{-1} + NH_2C_2H_4OH(aq) + NH_3C_2H_4OH^{+1}} \quad (2)$$

3.3.2. Partial Pressure of CO₂ (OLI)

The partial pressure of CO₂ is calculated using Equation 3, the data obtained from the OLI® simulation. The partial pressure of CO₂ is calculated by the product of the molar fraction of

CO₂ in the vapours and the overall pressure (in Pa). The molar fraction of CO₂ is the ratio of the moles of CO₂ in the vapour and the totals moles of vapour.

$$Partial\ Pressure\ [Pa] = \frac{CO_2\ vapor\ (mol)}{Vapor\ total\ (mol)} \times 101,325\ [Pa] \quad (3)$$

3.3.3. Partial Pressure of MEA

The partial pressure of MEA is calculated using Equation 4, the data obtained from the OLI® simulation. The partial pressure of MEA is calculated by the product of the molar fraction of MEA in the vapours and the overall pressure (in Pa). The molar fraction of MEA is the ratio of the moles of MEA in the vapours and the totals moles of vapours.

$$Partial\ Pressure\ [Pa] = \frac{MEA\ vapour\ (mol)}{Vapor\ total\ (mol)} \times 101,325\ [Pa] \quad (4)$$

3.3.4. Experimental data fitting to a surrogate model

The independent variables chosen are the CO₂ load (α) and the operating temperature ($1/RT$), while the dependent variable is CO₂ partial pressure. The temperature is represented in K; R is the ideal gas constant (8.314 m³. Pa/K mol). Microsoft Excel® software is used to propose a surrogated model adjusting the experimental data.

3.3.5. Constraints of CO₂/MEA load modelling

In the industrial processes of CO₂ absorption with MEA (Fig. 4), the column of absorption and desorption (distillation) operates usually where the amount of α entering the absorption column is 0.2 (Jamal et al.,2006b; Luo et al.,2015), in the absorption column where α is charged to a value of 0.4, then this enters the desorption column, where it is discharged to 0.2 and is send back to the absorption column. The industrial interest to design absorption columns is on the above mentioned range of CO₂ load.

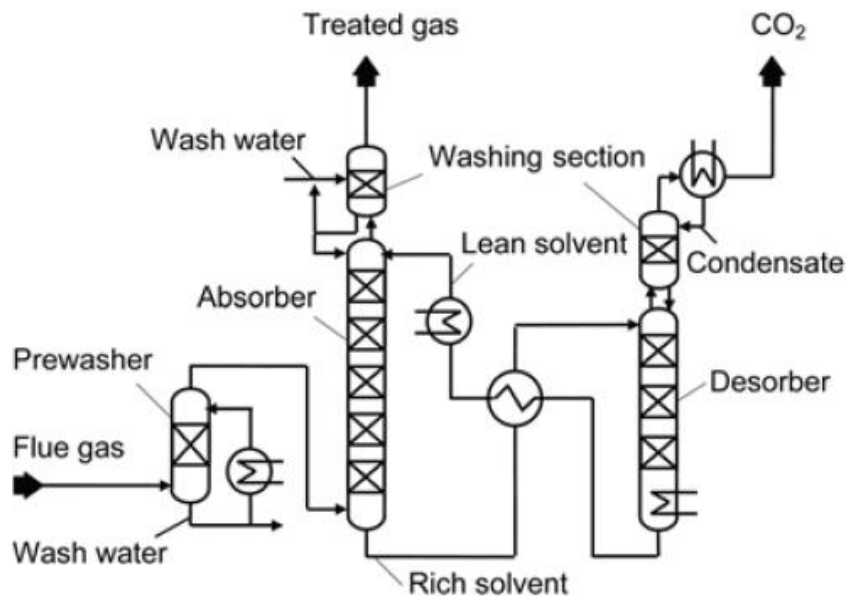


Figure 4. Flow scheme of the absorption/desorption process, Zhang et al. (2013)

Figure 4 shows the flue gas produced by a gas burner is fed into the pre-washer column by a blower. The pre-washer is built as a direct contact cooler to set the temperature of the flue gas at the absorber inlet and at the same time to make sure that the flue gas is saturated with water. The flue gas enters the absorber at the bottom with a temperature of approximately 40-50 °C. The regenerated solvent (lean solvent) is fed to the absorber top, typically at temperature of 40°C. Upon the CO₂ absorption into the liquid phase, absorption enthalpy is released, which leads to a temperature increase. To reduce solvent loss by flue gas, there is a washing section at the absorber top above the solvent inlet. A low amount of fresh deionized water is added into the washing water recycle stream to avoid a prohibitive accumulation of amine in the washing water.

The rich amine is pumped into the desorber through the rich lean heat exchanger, where the CO₂ rich solvent is heated to higher temperatures through the lean solvent from the desorber bottom. The bottom of the desorber contains electrical heating elements for partial evaporation of the solvent. For aqueous amine solutions, mainly water is evaporated. The vapour at the top of the desorber consists of water, CO₂ and some traces of amine. To retain the amine, also at the desorber top a washing section is installed. The vapour at the desorber top is led into the condenser where most of the water is removed so that almost pure CO₂ is obtained.

4. RESULTS AND DISCUSSION

The results of the simulation program OLI® of the vapour-liquid equilibrium for several concentrations of Monoethanolamine (MEA) 15, 30, 45 and 60% wt and several operating temperatures of 40, 60, 80, 100 and 120 °C, are shown in Figure 5. When methane is present, the results are not affected and matches with the results without methane. Therefore, the model is useful for biogas. At higher operating temperature, lower is the loading of CO₂ in the liquid; hence, the temperature is not favourable for the absorption as expected. To absorb or retain the same amount of CO₂ at a higher operating temperature, then the partial pressure of CO₂ should increase. When concentration of Monoethanolamine (MEA) is higher, is required a higher partial pressure of CO₂ for the same load of CO₂.

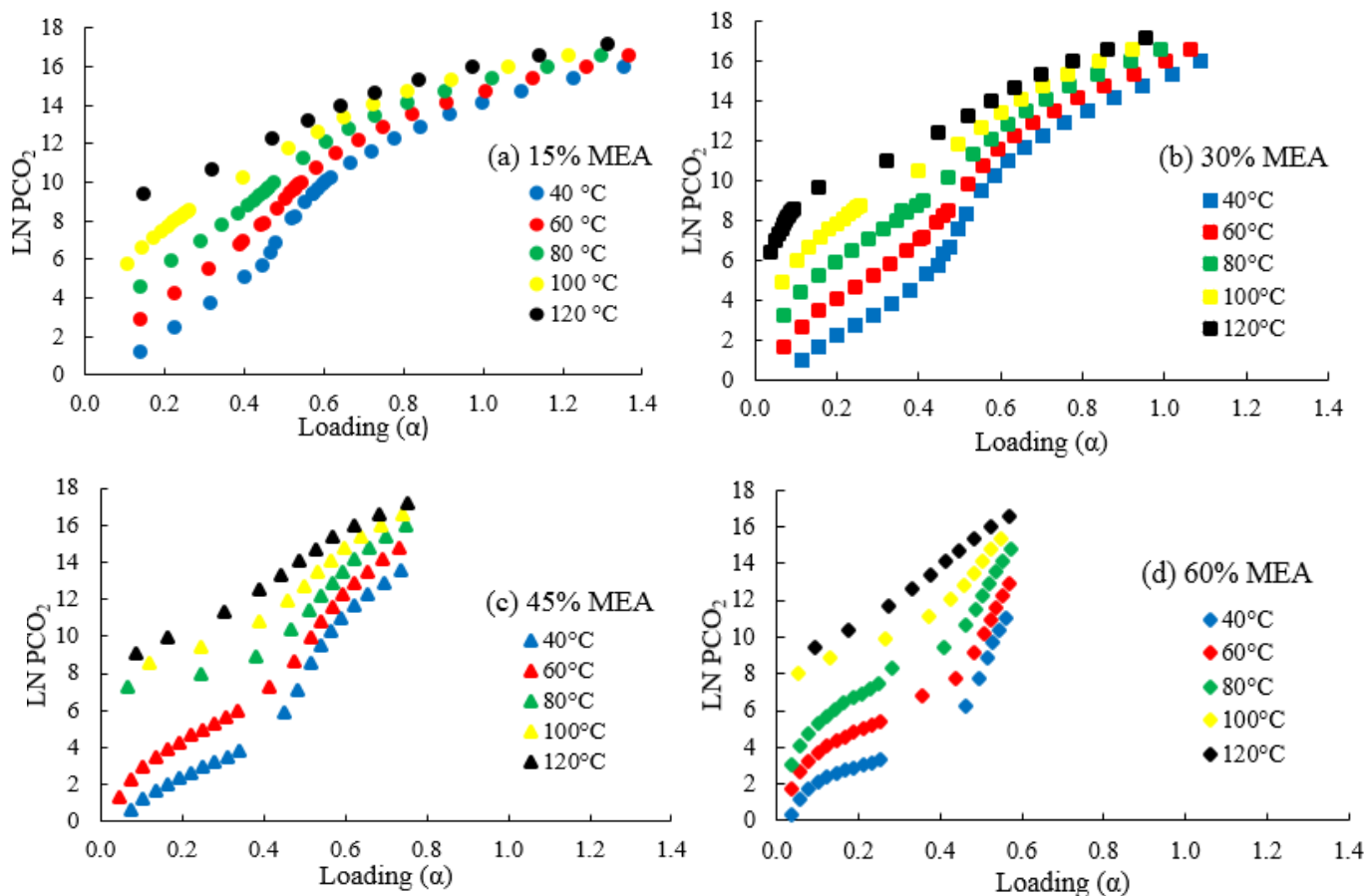


Figure 5. Logarithm of CO₂ partial pressure as a function of the loading of CO₂ in the liquid, for H₂O-CO₂-MEA system

4.1. Proposal for the surrogate model equation

The adjustment is obtained by a novel equation (Eq. 5) that at our knowledge has not been previously proposed in the literature. α is the load of CO₂ in the liquid, while temperature is represented in K, using the constant of ideal gas R (8.314 m³.Pa/K.mol). This equation is fitted to literature experimental data performing a multilinear regression. With this equation, the natural logarithm of the partial pressure of CO₂ is calculated.

$$LN PCO_2 = Intersection + X_1(\alpha) + X_2\left(\frac{1}{RT}\right) \quad (5)$$

Once multilinear regression of experimental data obtained considering the CO₂ load boundaries between 0.2 and 0.4 the three variables for the proposed equation are shown in table 2.

Table 2. Multilinear regression data

| Coefficients | |
|---------------------|------------|
| Intersections | 32.95 |
| Variable X 1 | 14.96 |
| Variable X 2 | -88,081.02 |

The regression is taking values of α from 0.2 to 0.4, and for all MEA (15, 30, 45 and 60% wt) concentrations.

4.2. Experimental-OLI data and proposed Model

Figure 6 shows the partial pressure of CO₂ for 15% wt solutions of monoethanolamine (MEA). The values obtained by OLI[®] (Table 3 in Appendix) are in very good agreement with experimental data. The values obtained by the surrogated model are in a range of load operation CO₂ from 0.2 to 0.4, and fit the experimental data (Table 7, 8.1 in Appendix) for 15% wt Monoethanolamine (MEA). The values obtained by the novel model fits better the experimental data than OLI[®] model when the temperature is 120 °C and low loads, e.g. 0.2.

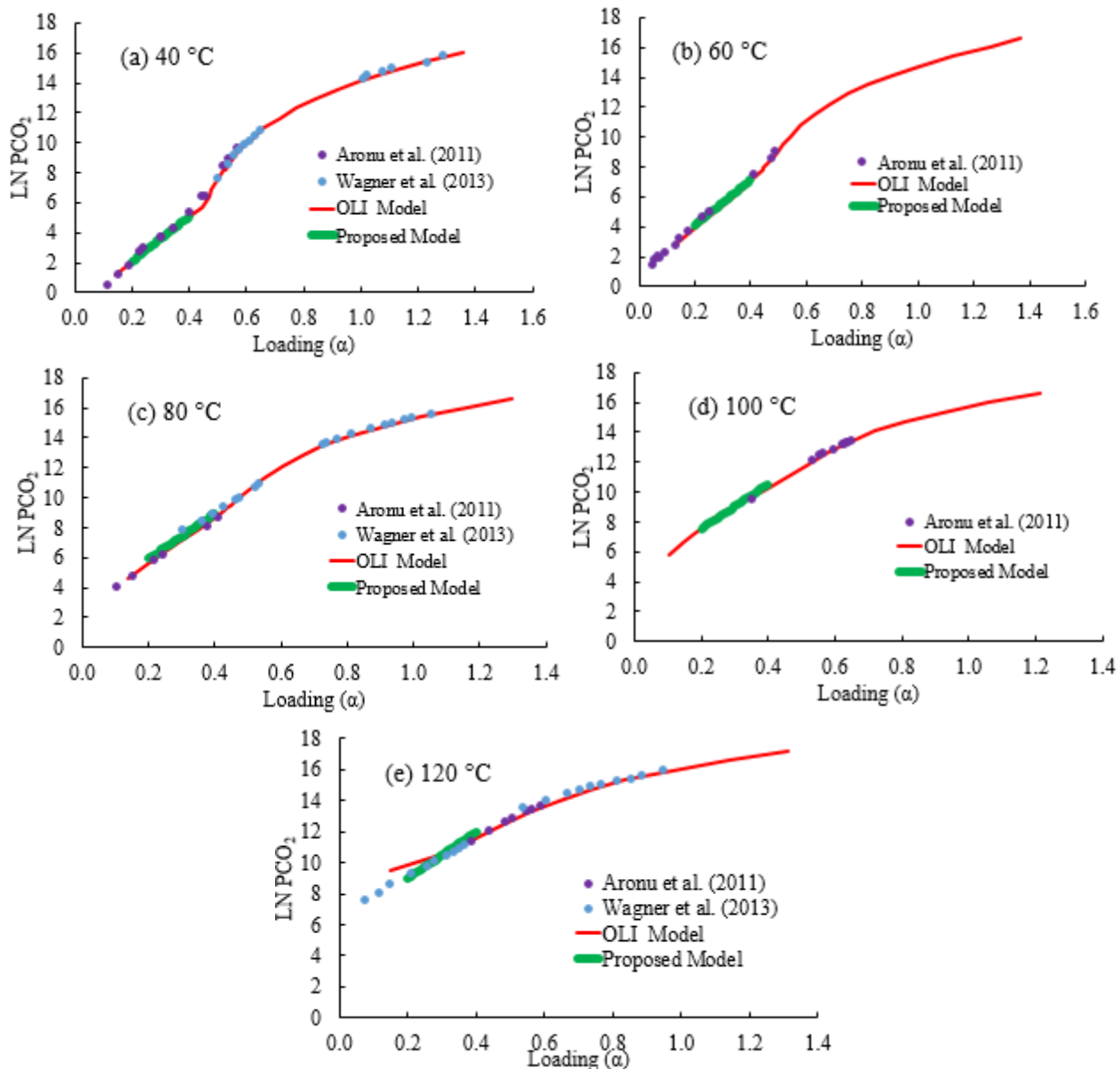


Figure 6. Logarithm of the partial pressure of CO₂ a function of the load of CO₂ in the liquid. Experimental data in literature of Wagner et al. (2013), Aronu et al. (2011), OLI[®] and Proposed model. MEA 15% by mass

Figure 7 shows the partial pressure of CO₂ results for 30% wt Monoethanolamine (MEA) solutions. Notice that the values of the proposed model are in accordance with the experimental data (table 7, 8.2, 9 and 10 in Appendix) and the values obtained by OLI[®] (Table 4 in Appendix) for 30% wt of Monoethanolamine (MEA). At a temperature of 120°C, OLI[®] values fit better to Jou et al. (1995) data than to the results of other authors. For this temperature of 120 °C, in the operating range of CO₂ absorption with Monoethanolamine (MEA), which is 0.2-0.4, the values obtained from OLI[®] and those of the proposed model

slightly overestimate the required partial pressure of CO₂ for the same load. However, the values of the model proposed fit the experimental data at the defined boundaries.

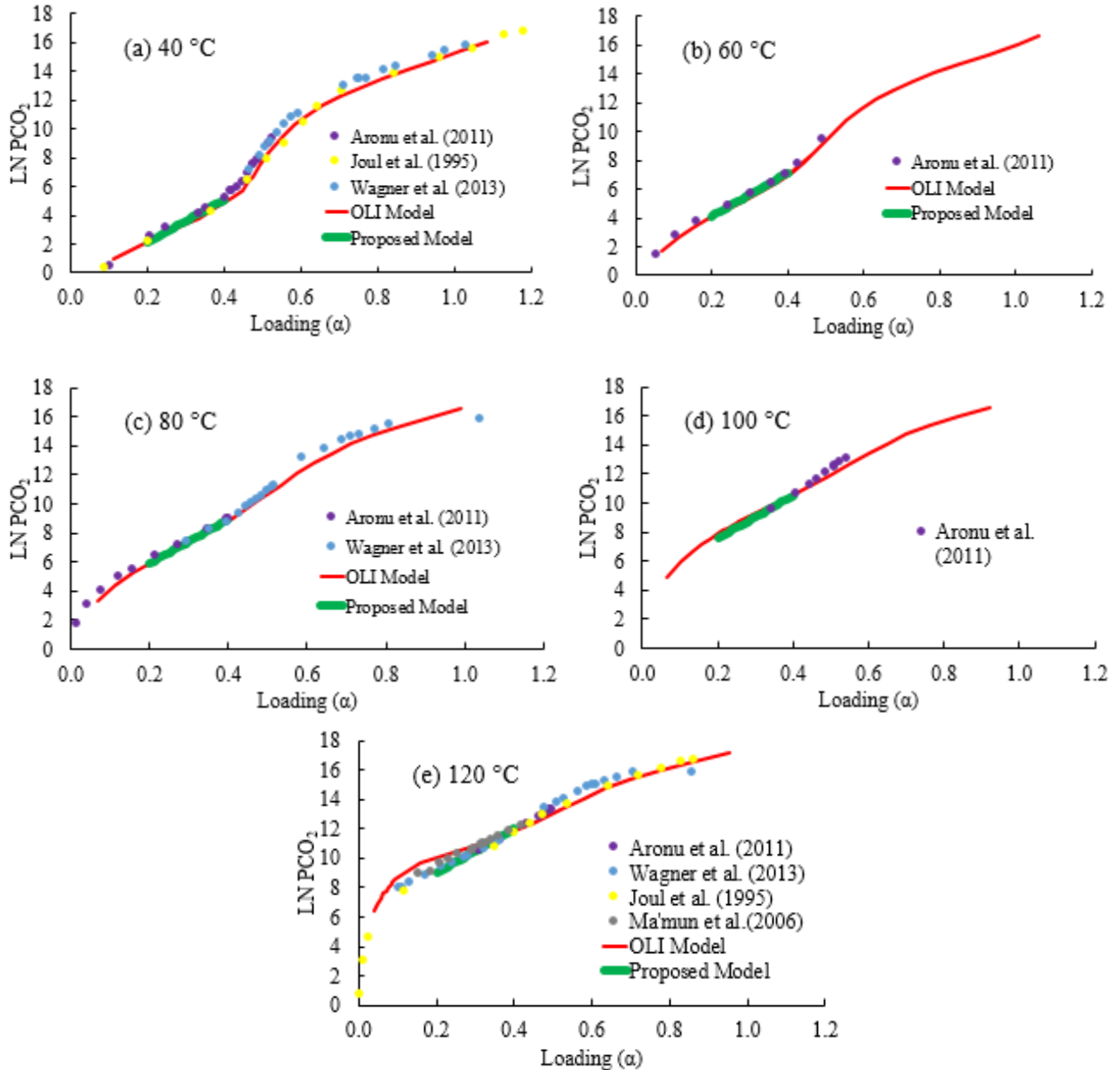


Figure 7. Logarithm of the partial pressure of CO₂ a function of the load of CO₂ in the liquid. Experimental data in literature of Jou et al (1995), Ma'mun et al (2005), Wagner et al (2013), Aronu et al. (2011), OLI® and Proposed model. MEA 30% by mass

Figure 8 shows the partial pressure of CO₂ for 45% wt of Monoethanolamine (MEA) solutions. The values of the proposed model fit the experimental data (Table 8.3 in Appendix) in all evaluated temperatures. OLI® (Table 5 in Appendix), experimental data in literature

and proposed model agree at temperatures of 40-60 °C. The values obtained by OLI® present a deviation at temperatures of 80 °C and higher.

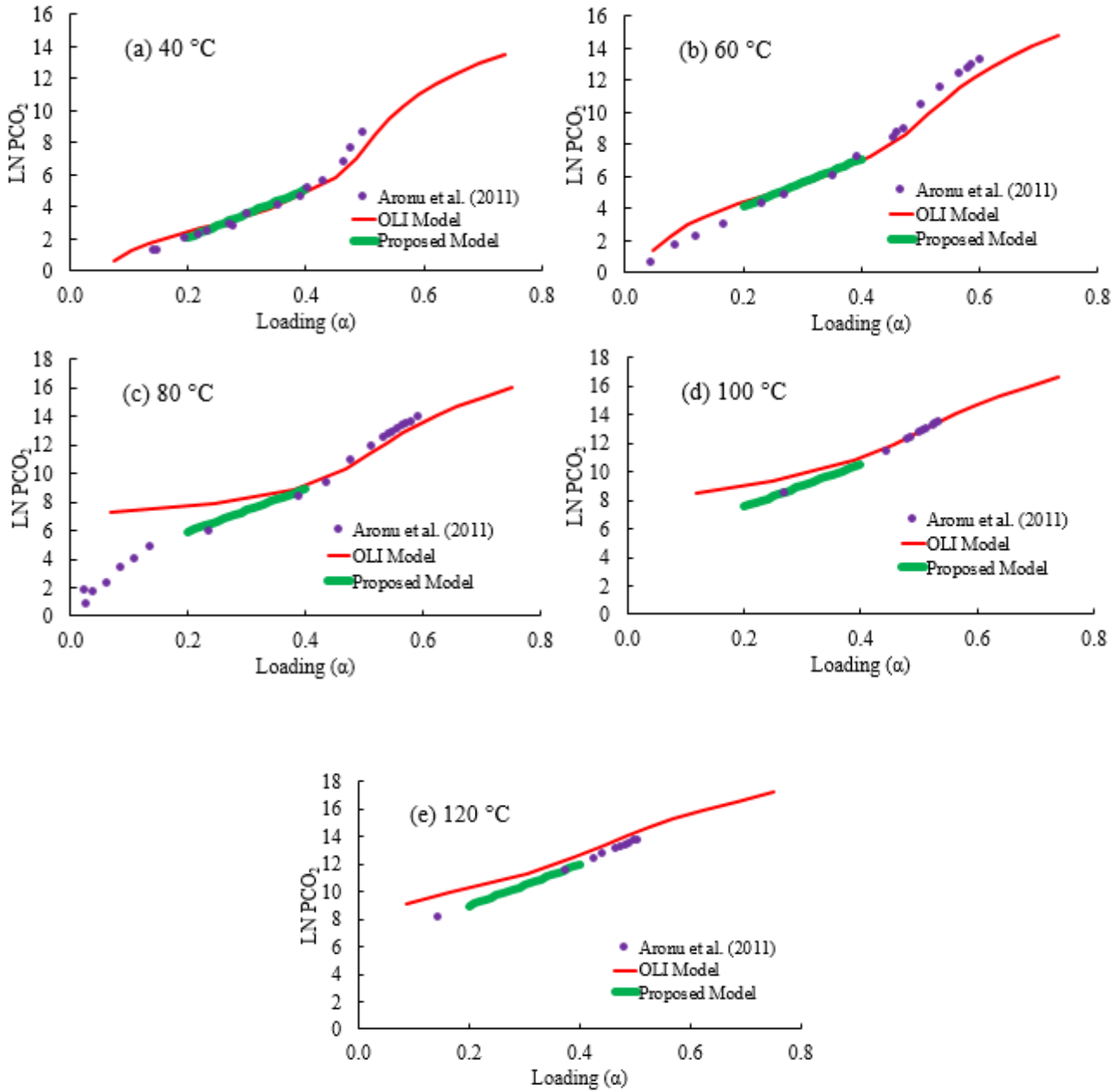


Figure 8. Logarithm of the partial pressure of CO₂ a function of the load of CO₂ in the liquid. Experimental data in literature of Aronu et al. (2011), OLI® and Proposal model. Monoethanolamine 45% by mass

Figure 9 shows the partial pressure of CO₂ for solutions of 60% wt of monoethanolamine (MEA). Similar to the data obtained for 45% wt of monoethanolamine (MEA), the values obtained by the proposed model and the experimental data in literature (Table 8.4 in Appendix) fit for all evaluated temperatures in the operating range of α (0.2 to 0.4). OLI ®

presents slight deviations from the experimental data in literature. At temperatures between 40 and 60 °C, OLI® underestimates the experimental data in literature at low loads and overestimates it at high loads. At temperatures higher than 80 °C, the values obtained by OLI® (Table 6 in Appendix) overestimated always the experimental data in literature.

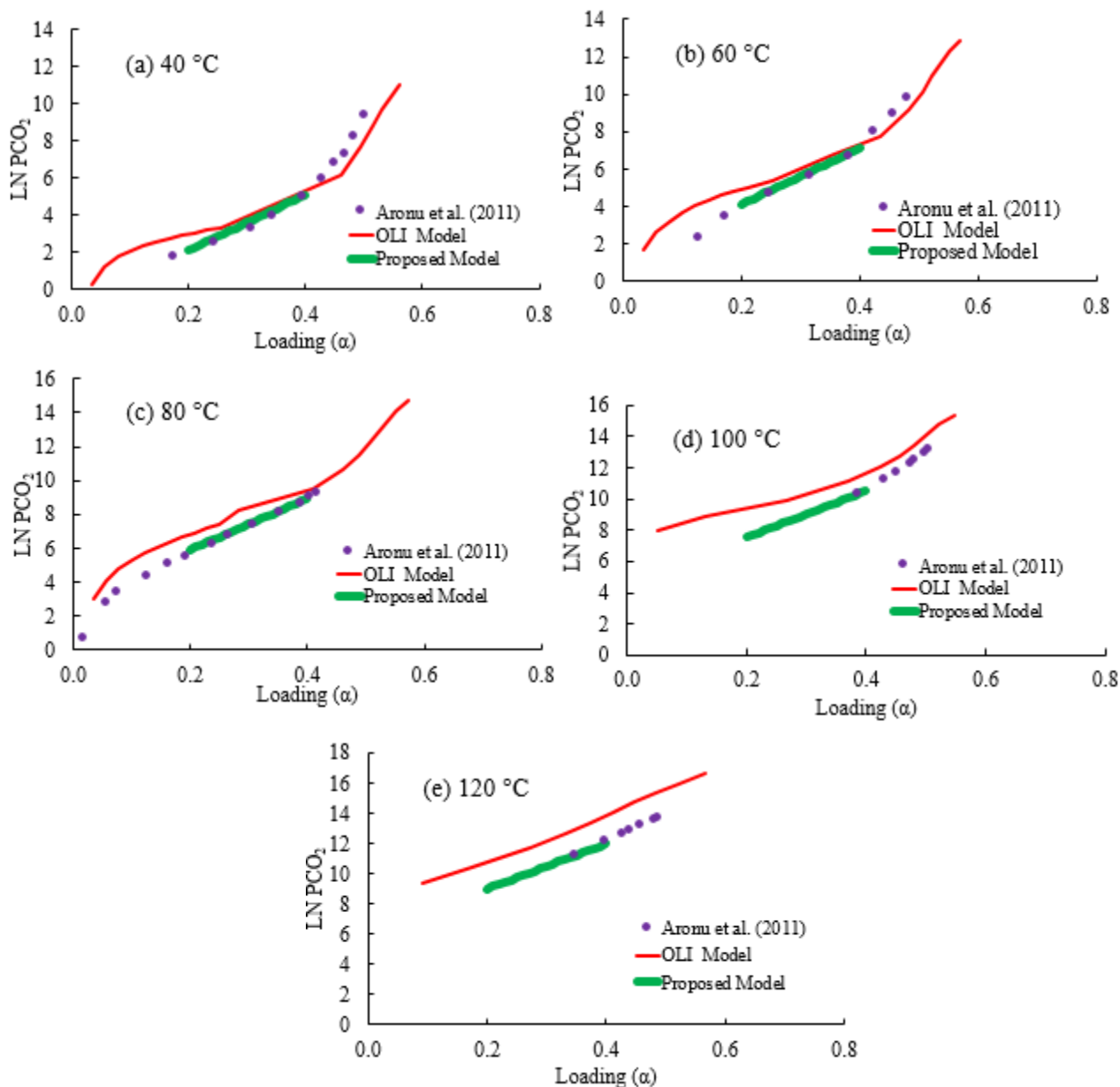


Figure 9. Logarithm of the partial pressure of CO₂ a function of the load of CO₂ in the liquid. Experimental data in literature of Aronu et al. (2011), OLI® and Proposal model. Monoethanolamine 60% by mass

4.3. Theoretical determination of the quantity of Monoethanolamine in vapour phase

The amount of MEA lost in the vapours is an important parameter from costs and environmental point of view, e.g. biogas combustion could produce NO_x . Figure 10 shows the vapour pressure of MEA obtained by 30% wt. solutions of MEA which is the MEA concentration most industrially used. The filled circles show the partial pressure of MEA in the absence of inert gases and each temperature is represented by a different colour. In the absence of inert when the load of CO_2 tends to zero, the curves converge to the same partial pressure of MEA regardless of the temperature. There is a specific load that depends on the temperature that minimizes the partial pressure of MEA. At lower operating temperatures, less is the partial pressure of MEA and the minimum is reached at a higher load. At temperature of $100\text{ }^\circ\text{C}$, the partial pressure of MEA in the vapours is above 6 ppm (threshold limit value), although it is pressurized to 10 bar column. For low loads in the presence of an inert gas, then the vapour partial pressure of MEA decreases and fails to converge to the common value indicated above.

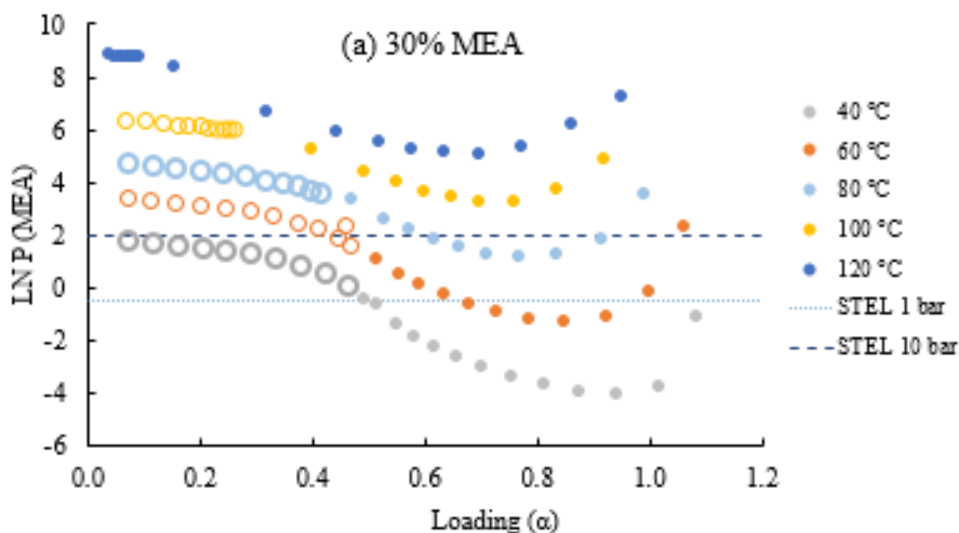


Figure 10. Vapours Pressure 30% MEA

Figure 11 shows the influence of the % MEA in aqueous solution. Partial pressure when the load tends to zero either depends on the % MEA. Lower is % MEA, lower is the minimum partial pressure of MEA that can be achieved.

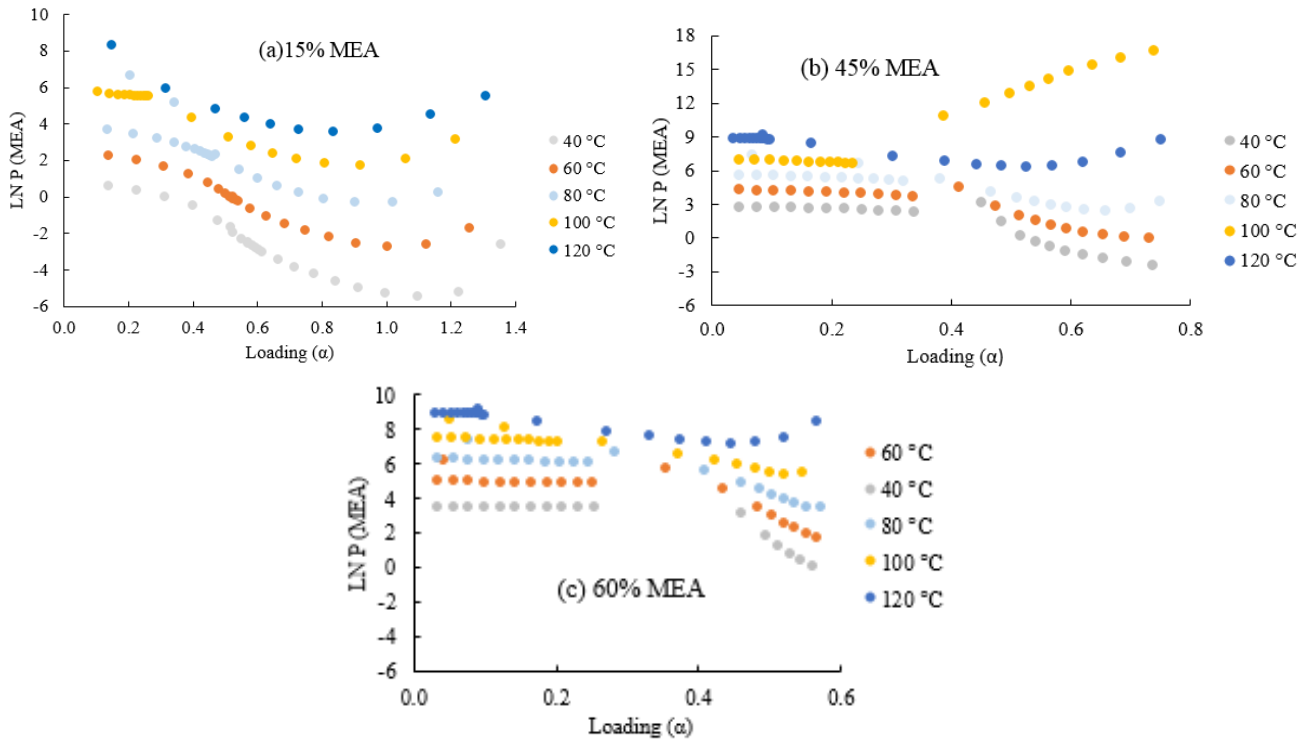


Figure 11. Vapours Pressure MEA. (a) 15% MEA. (b) 45% MEA. (c) 60% MEA

According to the proposed model, the CO₂ partial pressure depends on the load and temperature; therefore, different % MEA concentrations curves should match at a constant temperature. Figure 12 shows the concentration dependency of CO₂ partial pressure for the H₂O–MEA–CO₂ system as determined by experimental data in literature of Aronu et al. (2011) and novel model. The load versus the natural logarithm of partial pressure presents a sigmoidal shape. A good agreement is obtained with the novel model and the middle zone of the sigmoidal curve.

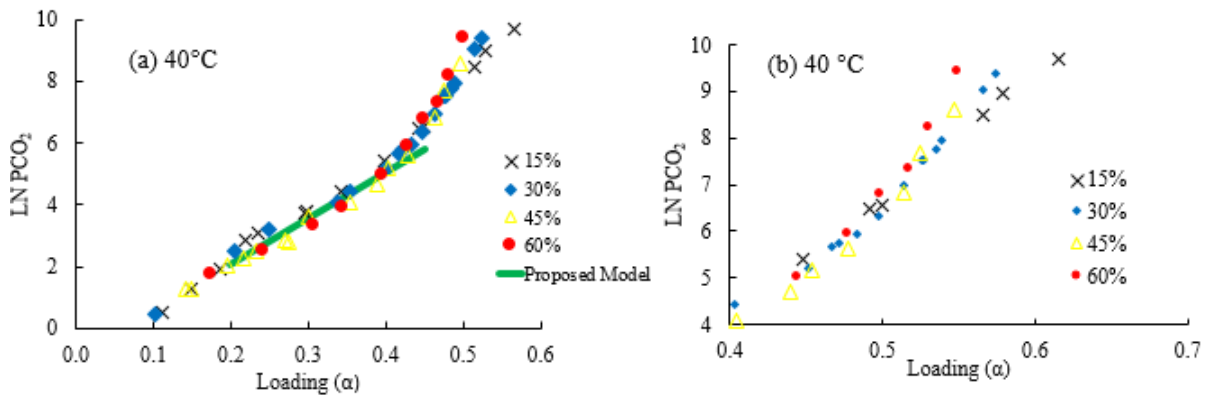


Figure 12. Concentration dependency of equilibrium CO₂ partial pressure of H₂O-MEA-CO₂ system at 40°C

The parity plot between results from experimental data in literature and OLI® model is shown in Figures 13 and 14; for 15, 30, 45 and 60% wt MEA. The figures show that the model predicts the CO₂ partial pressure very well even at different MEA concentrations. Figure 13 thus shows that the model precisely calculates CO₂ equilibrium in MEA at all concentration ranges up to 60 % wt.

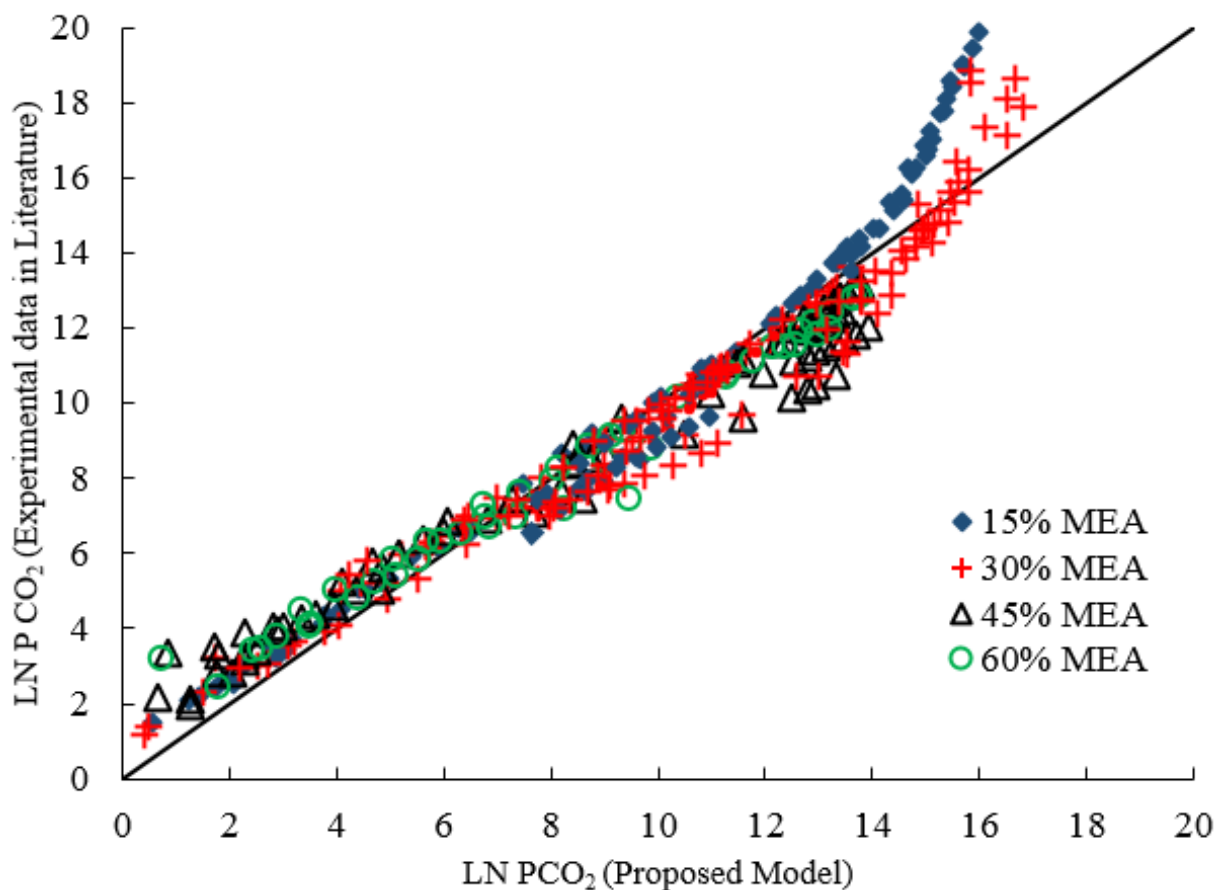


Figure 13. Parity plot between experimental literature and proposed model partial pressures

Figure 14 shows a parity plot of the results from the proposed model and the experimental data in literature and simulated data for 30 %. The figure indicates that the novel model is able to correlate existing equilibrium data in literature for H₂O–MEA–CO₂ system. The CO₂ partial pressure data of Aronu et al. (2011) is in general underestimated by the model, while the data of Jou et al. (1995) and Wagner et al. (2013) are generally overestimated.

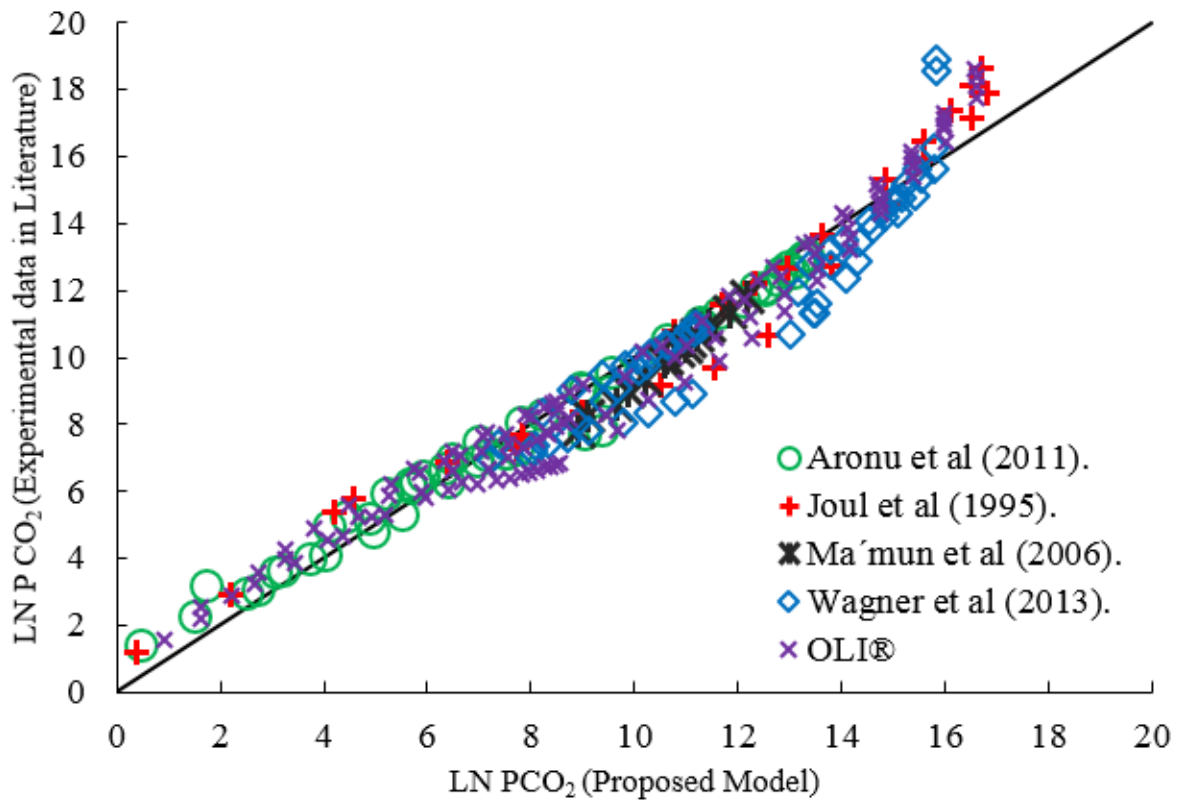


Figure 14. Parity plot between experimental literature and from OLI® and model

5. CONCLUSIONS

- The aim of the study is not the design and optimization of absorption column but to generate a surrogate model and compare the experimental and simulated data at different operation conditions.
- The novel surrogated model provides a good regression of all the experimental data.
- The OLI® model provides a good regression of the experimental data when MEA is between 15 to 30% wt. For high MEA concentrations of 45 and 60% wt, the OLI® model fits also the experimental data at 60 ° C but for temperatures above 80°C the model fits the experimental data only when the loading of CO₂ in the liquid phase exceeds 0.25 to 0.30.
- The loading CO₂ is operated in the range of 0.2 to 0.4, since in this range the lowest slope is presented, if one wants to work at higher load than 0.4, a large increase in pressure is required to obtain a small increase CO₂ load.
- Despite the amount of MEA in the vapours has very low values, they are above the recommended from the point of view of safety when the temperature is 100 °C. By security one could retain the MEA present using an acidic ion exchange resin and regenerate it with CO₂ vapours before entering column absorption (two columns would be required while one is on duty, the other is regenerated).
- The precise correlation between the behaviour of CO₂ equilibrium in aqueous solutions MEA provides a tool for better simulations of processes to reduce costs, better absorption column design as well as a better performance of the plant.

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APPENDIX

Table 3. Equilibrium solubility of CO₂ in aqueous 15 mass % MEA calculated by OLI

| 40 °C | | 60 °C | | 80 °C | | 100 °C | | 120 °C | |
|------------------------------|--------------------------|------------------------------|--------------------------|------------------------------|--------------------------|------------------------------|--------------------------|------------------------------|--------------------------|
| LN P CO ₂ (Pa) | α CO ₂ | LN P CO ₂ (Pa) | α CO ₂ | LN P CO ₂ (Pa) | α CO ₂ | LN P CO ₂ (Pa) | α CO ₂ | LN P CO ₂ (Pa) | α CO ₂ |
| 2.52 | 0.23 | 4.30 | 0.23 | 5.94 | 0.22 | 7.47 | 0.19 | 10.67 | 0.32 |
| 3.72 | 0.31 | 5.51 | 0.31 | 6.99 | 0.29 | 7.74 | 0.21 | | |
| 5.11 | 0.40 | 6.76 | 0.39 | 7.81 | 0.35 | 7.95 | 0.22 | | |
| | | 6.95 | 0.40 | 8.39 | 0.38 | 8.12 | 0.23 | | |
| | | | | 8.81 | 0.41 | 8.27 | 0.24 | | |
| | | | | | | 8.40 | 0.25 | | |
| | | | | | | 8.51 | 0.26 | | |
| | | | | | | 8.60 | 0.26 | | |
| | | | | | | 10.23 | 0.40 | | |

Table 4. Equilibrium solubility of CO₂ in aqueous 30 mass % MEA calculated by OLI

| 40 °C | | 60 °C | | 80 °C | | 100 °C | | 120 °C | |
|------------------------------|--------------------------|------------------------------|--------------------------|------------------------------|--------------------------|------------------------------|--------------------------|------------------------------|--------------------------|
| LN P CO ₂ (Pa) | α CO ₂ | LN P CO ₂ (Pa) | α CO ₂ | LN P CO ₂ (Pa) | α CO ₂ | LN P CO ₂ (Pa) | α CO ₂ | LN P CO ₂ (Pa) | α CO ₂ |
| 2.20 | 0.20 | 4.09 | 0.20 | 5.88 | 0.20 | 7.86 | 0.20 | 9.66 | 0.16 |
| 2.73 | 0.25 | 4.67 | 0.24 | 6.49 | 0.24 | 8.11 | 0.21 | 11.01 | 0.32 |
| 3.26 | 0.29 | 5.25 | 0.29 | 7.04 | 0.28 | 8.31 | 0.23 | 12.40 | 0.45 |
| 3.82 | 0.33 | 5.84 | 0.33 | 7.54 | 0.31 | 8.48 | 0.24 | | |
| 4.47 | 0.38 | 6.48 | 0.37 | 8.00 | 0.34 | 8.63 | 0.25 | | |
| 5.28 | 0.42 | 7.07 | 0.40 | 8.52 | 0.36 | 8.75 | 0.26 | | |
| | | | | 8.40 | 0.37 | 10.53 | 0.40 | | |
| | | | | 8.74 | 0.39 | | | | |

Table 5. Equilibrium solubility of CO₂ in aqueous 45 mass % MEA calculated by OLI

| 40 °C | | 60 °C | | 80 °C | | 100 °C | | 120 °C | |
|-----------------------------|--------------------------|-----------------------------|--------------------------|-----------------------------|--------------------------|-----------------------------|--------------------------|-----------------------------|--------------------------|
| LNP CO ₂ (Pa) | α CO ₂ | LNP CO ₂ (Pa) | α CO ₂ | LNP CO ₂ (Pa) | α CO ₂ | LNP CO ₂ (Pa) | α CO ₂ | LNP CO ₂ (Pa) | α CO ₂ |
| 2.36 | 0.19 | 4.30 | 0.19 | 7.95 | 0.25 | 9.41 | 0.25 | 9.96 | 0.17 |
| 2.65 | 0.22 | 4.65 | 0.22 | 8.92 | 0.38 | 10.84 | 0.39 | 11.34 | 0.30 |
| 2.93 | 0.25 | 4.99 | 0.25 | | | | | 12.50 | 0.39 |
| 3.21 | 0.28 | 5.33 | 0.28 | | | | | 13.34 | 0.44 |
| 3.51 | 0.31 | 5.67 | 0.31 | | | | | | |
| 3.84 | 0.34 | 6.03 | 0.34 | | | | | | |
| 5.88 | 0.45 | 7.28 | 0.41 | | | | | | |

Table 6. Equilibrium solubility of CO₂ in aqueous 60 mass % MEA calculated by OLI

| 40 °C | | 60 °C | | 80 °C | | 100 °C | | 120 °C | |
|-----------------------------|--------------------------|-----------------------------|--------------------------|-----------------------------|--------------------------|-----------------------------|--------------------------|-----------------------------|--------------------------|
| LNP CO ₂ (Pa) | α CO ₂ | LNP CO ₂ (Pa) | α CO ₂ | LNP CO ₂ (Pa) | α CO ₂ | LNP CO ₂ (Pa) | α CO ₂ | LNP CO ₂ (Pa) | α CO ₂ |
| 3.04 | 0.21 | 4.82 | 0.19 | 6.94 | 0.21 | 8.63 | 0.19 | 11.66 | 0.27 |
| 3.18 | 0.23 | 5.04 | 0.21 | 7.18 | 0.23 | 8.82 | 0.20 | 12.63 | 0.33 |
| 3.33 | 0.25 | 5.24 | 0.23 | 7.41 | 0.25 | 9.90 | 0.27 | 13.39 | 0.37 |
| 6.20 | 0.46 | 5.43 | 0.25 | 8.28 | 0.28 | 11.13 | 0.37 | 14.08 | 0.41 |
| | | 6.76 | 0.36 | 9.46 | 0.41 | 12.04 | 0.42 | | |
| | | 7.73 | 0.44 | | | | | | |

Table 7. Experimental literature (Wagner et al., 2010). Equilibrium solubility of CO₂ in aqueous MEA

| 15% MEA | | | | | | 30% MEA | | | | | |
|------------------------|-----------------------------|------------------------|-----------------------------|------------------------|-----------------------------|------------------------|-----------------------------|------------------------|-----------------------------|------------------------|-----------------------------|
| 40 °C | | 80 °C | | 120 °C | | 40 °C | | 80 °C | | 120 °C | |
| LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ |
| 7.74 | 0.49 | 7.93 | 0.30 | 7.63 | 0.07 | 7.23 | 0.47 | 7.37 | 0.29 | 7.98 | 0.10 |
| 8.69 | 0.53 | 8.55 | 0.36 | 8.16 | 0.11 | 8.09 | 0.49 | 8.23 | 0.35 | 8.04 | 0.12 |
| 9.20 | 0.55 | 8.99 | 0.39 | 8.64 | 0.15 | 8.71 | 0.51 | 8.79 | 0.40 | 8.35 | 0.13 |
| 9.60 | 0.57 | 9.46 | 0.42 | 9.33 | 0.20 | 9.11 | 0.52 | 9.38 | 0.43 | 8.88 | 0.17 |
| 9.99 | 0.59 | 9.92 | 0.46 | 9.90 | 0.25 | 9.77 | 0.54 | 9.82 | 0.45 | 9.41 | 0.21 |
| 10.24 | 0.60 | 10.08 | 0.47 | 10.17 | 0.28 | 10.28 | 0.56 | 10.04 | 0.46 | 9.68 | 0.24 |
| 10.59 | 0.62 | 10.81 | 0.52 | 10.80 | 0.33 | 10.80 | 0.58 | 10.30 | 0.47 | 10.09 | 0.27 |
| 10.94 | 0.64 | 11.00 | 0.53 | 10.57 | 0.31 | 11.10 | 0.59 | 10.59 | 0.49 | 10.23 | 0.28 |
| 14.41 | 1.00 | 13.60 | 0.72 | 11.21 | 0.36 | 13.01 | 0.71 | 10.92 | 0.50 | 10.64 | 0.32 |
| 14.57 | 1.02 | 13.79 | 0.74 | 10.97 | 0.35 | 13.45 | 0.75 | 11.16 | 0.51 | 11.04 | 0.35 |
| 14.83 | 1.07 | 14.00 | 0.77 | 13.57 | 0.53 | 13.51 | 0.75 | 11.27 | 0.52 | 11.15 | 0.36 |
| 15.05 | 1.10 | 14.30 | 0.81 | 14.12 | 0.60 | 13.52 | 0.77 | 13.15 | 0.59 | 11.20 | 0.36 |
| 15.47 | 1.23 | 14.69 | 0.87 | 14.56 | 0.66 | 14.09 | 0.82 | 13.80 | 0.64 | 13.38 | 0.48 |
| 15.90 | 1.28 | 14.95 | 0.91 | 14.73 | 0.70 | 14.33 | 0.85 | 14.35 | 0.69 | 13.79 | 0.51 |
| | | 15.06 | 0.93 | 15.01 | 0.73 | 15.10 | 0.95 | 14.62 | 0.71 | 14.04 | 0.53 |
| | | 15.28 | 0.97 | 15.11 | 0.76 | 15.41 | 0.98 | 14.81 | 0.73 | 14.55 | 0.57 |
| | | 15.37 | 0.99 | 15.36 | 0.81 | 15.81 | 1.03 | 15.15 | 0.77 | 14.83 | 0.59 |
| | | 15.66 | 1.05 | 15.51 | 0.85 | | | 15.52 | 0.81 | 14.99 | 0.60 |
| | | | | 15.70 | 0.88 | | | 15.83 | 1.04 | 15.04 | 0.61 |
| | | | | 15.98 | 0.95 | | | | | 15.25 | 0.63 |
| | | | | | | | | | | 15.47 | 0.67 |
| | | | | | | | | | | 15.79 | 0.71 |
| | | | | | | | | | | 15.82 | 0.86 |

Table 8.1. Experimental literature (Aronu et al., 2011). Equilibrium solubility of CO₂ in aqueous MEA (15%)

| 40 °C | | 60 °C | | 80 °C | | 100 °C | | 120 °C | |
|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|
| LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ |
| 0.53 | 0.11 | 1.44 | 0.05 | 4.10 | 0.10 | 9.59 | 0.35 | 11.45 | 0.39 |
| 1.25 | 0.15 | 1.72 | 0.06 | 4.88 | 0.15 | 12.23 | 0.53 | 12.11 | 0.44 |
| 1.92 | 0.19 | 1.92 | 0.08 | 5.87 | 0.21 | 12.54 | 0.55 | 12.68 | 0.48 |
| 2.83 | 0.22 | 2.05 | 0.07 | 6.26 | 0.24 | 12.67 | 0.56 | 12.90 | 0.50 |
| 3.07 | 0.24 | 2.24 | 0.10 | 8.20 | 0.37 | 12.99 | 0.59 | 13.35 | 0.54 |
| 3.75 | 0.30 | 2.71 | 0.14 | 8.75 | 0.41 | 13.26 | 0.62 | 13.51 | 0.56 |
| 3.81 | 0.30 | 3.15 | 0.14 | | | 13.34 | 0.63 | 13.74 | 0.59 |
| 4.44 | 0.34 | 3.73 | 0.18 | | | 13.38 | 0.63 | | |
| 5.40 | 0.40 | 4.57 | 0.23 | | | 13.46 | 0.64 | | |
| 6.50 | 0.44 | 4.98 | 0.25 | | | 13.54 | 0.65 | | |
| 6.55 | 0.45 | 7.50 | 0.42 | | | | | | |
| 8.48 | 0.52 | 8.60 | 0.48 | | | | | | |
| 8.97 | 0.53 | 9.02 | 0.49 | | | | | | |
| 9.68 | 0.57 | | | | | | | | |

Table 8.2. Experimental literature (Aronu et al., 2011). Equilibrium solubility of CO₂ in aqueous MEA (30%).

| 40 °C | | 60 °C | | 80 °C | | 100 °C | | 120 °C | |
|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|
| LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ |
| 0.47 | 0.10 | 1.50 | 0.05 | 1.72 | 0.02 | 9.58 | 0.34 | 10.56 | 0.31 |
| 2.51 | 0.21 | 2.73 | 0.11 | 3.09 | 0.04 | 10.65 | 0.41 | 11.31 | 0.36 |
| 3.20 | 0.25 | 3.75 | 0.16 | 4.02 | 0.08 | 11.28 | 0.44 | 12.34 | 0.43 |
| 4.10 | 0.34 | 4.90 | 0.24 | 4.95 | 0.12 | 11.65 | 0.46 | 12.83 | 0.46 |
| 4.44 | 0.35 | 5.71 | 0.30 | 5.52 | 0.16 | 12.11 | 0.49 | 12.97 | 0.47 |
| 5.21 | 0.40 | 6.47 | 0.36 | 6.42 | 0.22 | 12.52 | 0.51 | 13.18 | 0.49 |
| 5.68 | 0.42 | 7.00 | 0.39 | 7.13 | 0.27 | 12.53 | 0.51 | 13.27 | 0.49 |
| 5.76 | 0.42 | 7.82 | 0.43 | 8.23 | 0.35 | 12.80 | 0.52 | 13.35 | 0.50 |
| 5.94 | 0.43 | 9.51 | 0.49 | 8.98 | 0.40 | 13.08 | 0.54 | | |
| 6.35 | 0.45 | | | 9.02 | 0.40 | | | | |
| 6.97 | 0.46 | | | | | | | | |
| 7.51 | 0.48 | | | | | | | | |
| 7.51 | 0.48 | | | | | | | | |
| 7.75 | 0.49 | | | | | | | | |
| 7.96 | 0.49 | | | | | | | | |
| 9.05 | 0.52 | | | | | | | | |
| 9.38 | 0.52 | | | | | | | | |

Table 8.3. Experimental literature (Aronu et al., 2011). Equilibrium solubility of CO₂ in aqueous MEA (45%)

| 40 °C | | 60°C | | 80°C | | 100°C | | 120 °C | |
|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|
| LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ |
| 1.25 | 0.14 | 0.64 | 0.05 | 0.83 | 0.03 | 8.46 | 0.27 | 8.18 | 0.15 |
| 1.25 | 0.15 | 1.77 | 0.09 | 1.72 | 0.04 | 11.48 | 0.45 | 11.57 | 0.37 |
| 2.04 | 0.20 | 2.29 | 0.12 | 1.79 | 0.03 | 12.25 | 0.48 | 12.43 | 0.43 |
| 2.29 | 0.22 | 3.02 | 0.17 | 2.29 | 0.06 | 12.38 | 0.49 | 12.72 | 0.44 |
| 2.51 | 0.23 | 4.37 | 0.23 | 3.36 | 0.09 | 12.74 | 0.50 | 13.10 | 0.47 |
| 2.80 | 0.28 | 4.86 | 0.27 | 3.97 | 0.11 | 12.87 | 0.51 | 13.29 | 0.48 |
| 2.88 | 0.27 | 6.06 | 0.35 | 4.82 | 0.14 | 12.98 | 0.51 | 13.41 | 0.48 |
| 3.59 | 0.30 | 7.26 | 0.39 | 5.99 | 0.24 | 13.26 | 0.53 | 13.53 | 0.49 |
| 4.09 | 0.35 | 8.44 | 0.45 | 8.41 | 0.39 | 13.32 | 0.53 | 13.70 | 0.50 |
| 4.69 | 0.39 | 8.75 | 0.46 | 9.33 | 0.44 | 13.45 | 0.53 | 13.79 | 0.51 |
| 5.18 | 0.40 | 9.02 | 0.47 | 10.99 | 0.48 | | | | |
| 5.63 | 0.43 | 10.49 | 0.50 | 11.97 | 0.51 | | | | |
| 6.82 | 0.46 | 11.57 | 0.53 | 12.54 | 0.53 | | | | |
| 7.68 | 0.48 | 12.49 | 0.57 | 12.77 | 0.54 | | | | |
| 8.61 | 0.50 | 12.81 | 0.58 | 12.95 | 0.55 | | | | |
| | | 12.95 | 0.59 | 13.14 | 0.56 | | | | |
| | | 13.33 | 0.60 | 13.33 | 0.57 | | | | |
| | | | | 13.49 | 0.57 | | | | |
| | | | | 13.68 | 0.58 | | | | |
| | | | | 13.93 | 0.59 | | | | |

Table 8.4. Experimental literature (Aronu et al., 2011). Equilibrium solubility of CO₂ in aqueous MEA (60%)

| 40 °C | | 60°C | | 80°C | | 100°C | | 120 °C | |
|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|---------------------|--------------------------|
| LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ |
| 1.79 | 0.17 | 2.40 | 0.13 | 0.69 | 0.02 | 10.34 | 0.39 | 11.25 | 0.35 |
| 2.54 | 0.24 | 3.53 | 0.17 | 2.83 | 0.06 | 11.27 | 0.43 | 12.13 | 0.40 |
| 3.34 | 0.31 | 4.70 | 0.25 | 3.48 | 0.07 | 11.75 | 0.45 | 12.63 | 0.43 |
| 3.96 | 0.34 | 5.68 | 0.32 | 4.35 | 0.12 | 12.33 | 0.47 | 12.89 | 0.44 |
| 5.02 | 0.39 | 6.74 | 0.38 | 5.08 | 0.16 | 12.54 | 0.48 | 13.22 | 0.46 |
| 5.95 | 0.43 | 8.02 | 0.42 | 5.53 | 0.19 | 12.99 | 0.50 | 13.65 | 0.48 |
| 6.81 | 0.45 | 9.02 | 0.46 | 6.30 | 0.24 | 13.18 | 0.51 | 13.76 | 0.49 |
| 7.32 | 0.47 | 9.85 | 0.48 | 6.77 | 0.26 | | | | |
| 8.23 | 0.48 | | | 7.41 | 0.31 | | | | |
| 9.43 | 0.50 | | | 8.14 | 0.35 | | | | |
| | | | | 8.72 | 0.39 | | | | |
| | | | | 9.11 | 0.40 | | | | |
| | | | | 9.33 | 0.42 | | | | |

Table 9. Experimental literature (Jou et al., 1995). Equilibrium solubility of CO₂ in aqueous MEA (30%)

| 40 °C | | 120°C | |
|---------------------|--------------------------|---------------------|--------------------------|
| LN PCO ₂ | α CO ₂ | LN PCO ₂ | α CO ₂ |
| 0.39 | 0.09 | 0.70 | 0.003 |
| 2.19 | 0.20 | 3.10 | 0.01 |
| 4.22 | 0.37 | 4.59 | 0.02 |
| 6.40 | 0.46 | 7.74 | 0.12 |
| 7.85 | 0.51 | 10.75 | 0.35 |
| 9.00 | 0.56 | 11.71 | 0.40 |
| 10.49 | 0.61 | 12.31 | 0.44 |
| 11.54 | 0.65 | 12.95 | 0.47 |
| 12.59 | 0.71 | 13.62 | 0.54 |
| 13.81 | 0.84 | 14.85 | 0.64 |
| 14.91 | 0.97 | 15.57 | 0.72 |
| 15.60 | 1.05 | 16.09 | 0.78 |
| 16.52 | 1.13 | 16.51 | 0.83 |
| 16.81 | 1.18 | 16.69 | 0.86 |

Table 10. Experimental literature (Ma'mun et al., 2006). Equilibrium solubility of CO₂ in aqueous MEA (30%)

| 120°C | |
|---------------------|--------------------------|
| LN PCO ₂ | α CO ₂ |
| 8.90 | 0.16 |
| 9.11 | 0.18 |
| 9.65 | 0.21 |
| 9.88 | 0.23 |
| 10.23 | 0.26 |
| 10.58 | 0.29 |
| 10.61 | 0.30 |
| 10.86 | 0.31 |
| 10.98 | 0.32 |
| 11.05 | 0.33 |
| 11.22 | 0.34 |
| 11.44 | 0.36 |
| 11.83 | 0.39 |
| 12.16 | 0.42 |