Influence of five model parameters on the performance of a CO₂ absorber column by a loaded aqueous MEA solution

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Abstract. Rigorous packed-bed absorber modeling and simulation are significant for post-combustion CO₂ capture processes design. Hence, a good knowledge and judicious selection of model parameters are essential to ensure reliable predictions. In this paper, the reactive absorption of CO₂ into loaded aqueous monoethanolamine solution was modeled, furthermore, the effects of five different parameters (kinetic model, enhancement factor, enthalpy of absorption, CO₂ diffusivity, and vapor pressure) were investigated. Finally, this study revealed that some model parameters have a large influence on the column performance, contrary to others. In addition, methods and correlations that generally provide more accurate predictions of the empirical data relative to the other cases involved in this research were determined for each model parameter. It was also found that the model deviation was reduced by 18% and 4% for the liquid temperature and liquids CO₂ loading profiles, respectively, while comparing between the worst and the best case.

Nomenclature

| Symbol | Definition |
|--------|------------|
| a      | Interfacial area [m²/m³] |
| CA,1   | Free CO₂ molar concentration [mol/m³] |
| CPG    | Heat capacity in the gas phase [J/(mol K)] |
| CPL    | Heat capacity in the liquid phase [J/(mol K)] |
| CS,i   | Heat capacity of species i in the gas phase [J/(mol K)] |
| DAG    | Gas phase CO₂ diffusivity [m²/s] |
| DL,j   | Species j diffusivity in the liquid phase [m²/s] |
| DS,j   | Species j diffusivity in water [m²/s] |
| dH     | Hydraulic diameter [m] |
| E      | Enhancement factor |
| GB     | Flow rate of carrier gas B [mol/(s m²)] |
| He     | Henry’s constant |
| hG     | Convective heat transfer coefficient [J/(s K m²)] |
| k2     | Kinetic constant [m³/(kmol s)] |
| kG,i   | Component i mass-transfer coefficient in the gas side [kmol/(kPa m² s)] |
| kLA    | Mass transfer coefficient in the liquid phase [m/s] |
| L      | Liquid flow rate [mol/(s m³)] |
| P      | Gas-phase total pressure [Pa] |
| Pw     | Water vapor pressure [Pa] |

| Symbol | Definition |
|--------|------------|
| T₀     | Standard temperature [298.15 K] |
| Tg     | Temperature in the gas side [K] |
| TL     | Temperature in the liquid bulk [K] |
| xₜ     | Mole fraction of water in the liquid phase |
| y₁     | The bulk gas side mole fraction of species i |
| y₁,1   | Species i mole fraction at the gas side interface |
| Z      | Column height [m] |

Greek letters

| Symbol | Definition |
|--------|------------|
| αCO₂   | CO₂ loading [mol CO₂/mol MEA] |
| ΔHrx   | Enthalpy of absorption [kJ/mol of CO₂] |
| ΔHvap,S | Heat of vaporization of water [J/mol] |
| ω      | Acentric factor |
| γₛ     | Activity coefficient of water in the liquid phase |

Subscripts

| Symbol | Definition |
|--------|------------|
| A      | Carbon dioxide |
| ARD%   | Average relative deviation percentage |
| B      | Carrier gas |
| MEA    | Monoethanolamine |
| R      | MEA |
| S      | Water vapor |

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1. Introduction

Significant efforts have been made to reduce greenhouse gas emissions and mitigate the global warming IPCC (2007). In this area, particular attention has been given to carbon dioxide removal using the post-combustion process on the basis of the absorption-desorption with chemical solvents. In recent years, remarkable progress has been made in this area of research. New solvents that increase the CO2 capture in post-combustion processes (Akinola et al., 2019; Ali Saleh Bairq et al., 2019; Gheni et al., 2018; Mohammadpour et al., 2019; Wang et al., 2019).

Reliable dimensioning, scaling, and monitoring post-combustion processes require the use of an accurate packed bed absorber modeling and simulation (Llano-Restrepo and Araujo-Lopez, 2015). Therefore, a good knowledge and judicious selection of model parameters are essential to ensure rigorous predictions. In this context, several studies on diverse process parameters have been published in literature (Abu-Zahra et al., 2007; Afkhamipour and Mofarahi, 2013, 2014; Khan et al., 2011; Kvamsdal and Rochelle, 2008; Kvamsdal and Hillestad, 2012; Mofarahi et al., 2008; Wu et al., 2010).

Abu-Zahra et al. (2007) investigated absorber inlet temperature, lean amine loading, concentration, and stripper pressure sensitivities. Furthermore, the process that recovers carbon dioxide from flue gas was studied by Mofarahi et al. (2008) where the effect of both operating conditions and design parameters on the absorber and stripper columns was presented. In addition, a statistical analysis and a combination between the sensitivity analysis and the neural networks modeling were carried out by Wu et al. (2010) to investigate the interactions between similar main process parameters. However, the studies on the selection of rate-based model parameter correlations in packed columns are scarce. Khan et al. (2011) applied the rate-based model to perform a sensitivity analysis using different mass transfer coefficients in a packed column. Furthermore, in the aim of determining the temperature bulge position and magnitude, Kvamsdal and Hillestad (2012) focused on the selection of the rate-based model parameter correlations for prediction of physical properties and kinetics, they investigated also their effects on mass and energy balances. Afkhamipour and Mofarahi (2013, 2014) performed a rate-based model sensitivity analysis, once by varying different mass transfer correlations, and another time by combining these correlations with different kinetic models.

In the current paper, the reactive absorption of CO2 with loaded aqueous monoethanolamine solution in a packed-bed absorber was modeled and simulated, in addition, the effects of five different parameters (kinetic model, enhancement factor, enthalpy of absorption, CO2 diffusivity in aqueous solution of MEA, and vapor pressure) on the column performance were investigated by performing a parametric study based on step-by-step approach.

2 Rate-based model

For modeling the CO2 absorption in a packed column, three forms of the rate-based model were developed: the Continuous Differential Contactor (CDC) model, the Continuous Film Reaction (CFR) model, and Non-Equilibrium Stage (NEqS) model. In this study, the last version of the CDC model was applied, indicating that this model was first proposed by Pandya (1983) based on the differential-change approach suggested by Treybal (1969) which was largely employed by many authors, and since it presents some inconsistent simplifications or assumptions, Llano-Restrepo and Araujo-Lopez (2015) revised the model using the finite difference approach and introduced a new improved version as shown below:

\[
\frac{dY_A}{dz} = -\frac{k_{GA} aP(y_A - y_{A,1})}{G_B},
\]

\[
\frac{dY_S}{dz} = -\frac{k_{GS} aP(y_S - y_{S,1})}{G_B}.
\]

The mole fractions of CO2 and water vapor \(y_{A,1}\) and \(y_{S,1}\), respectively, at the interface are given by:

\[
y_{A,1} = \frac{y_A P + \left( \frac{E_{y_A}}{k_{GA}} \right) C_A}{1 + \left( \frac{E_{y_A}}{k_{GA}} \right)},
\]

\[
y_{S,1} = x_S \gamma_S P_{sat} / P.
\]

Noting that, the model considers the liquid phase as an ideal solution. Thus \(\gamma_S = 1\) and Raoult’s law \(y_{S,1} = x_S P_{sat} / P\) is valid.

- A total mole balance for both liquid and gas phases:

\[
\frac{dL}{dz} = G_B \left( \frac{dY_A}{dz} + \frac{dY_S}{dz} \right).
\]

- Temperature gradients for the gas and liquid phases:

\[
\frac{dT_G}{dz} = \frac{-h_G(T_G - T_L) a}{G_B \left( C_{p,G} + Y_A C_{p,G} + Y_S C_{p,S} \right)}.
\]
\[
\frac{dT_L}{dz} = \frac{G_B}{LC_{p,L}} \left\{ \left( C_{p,B}^{(g)} + Y_A C_{p,A}^{(g)} + Y_S C_{p,S}^{(g)} \right) \frac{dT_G}{dz} + \int_{T_0}^{T_G} C_{p,A}^{(g)} \, dT - \Delta H_{p,x}^{(abs)}(T_0) - \int_{T_0}^{T_G} C_{p,L} \, dT \right\} \frac{dY_A}{dz} + \int_{T_0}^{T_G} C_{p,S}^{(g)} \, dT - \Delta H_{vap,S}(T_0) - \int_{T_0}^{T_G} C_{p,L} \, dT \right\} \frac{dY_S}{dz} \right\}.
\]

Indicating that the energy balance neglects heat losses through the wall of the absorber column (an adiabatic column is assumed).

For the resolution of these differential equations a computer program was coded in Matlab software.

The correlations used for estimating the different physicochemical and transport properties are listed in Table A1.

## 3 Kinetic model

A large number of experimental and theoretical studies have been reported in literature on the kinetics of the reaction between CO2 and an uncharged aqueous MEA since 1950s (Blauwhoff et al., 1983; Danckwerts and Sharma, 1966; Faramarzi, 2010; Fregua and Rochelle, 2003; Hikita et al., 1977, 1979; Horng and Li, 2002; Jamal et al., 2006; Kucka et al., 2002, 2003; Kvamsdal et al., 2009; Luo et al., 2012; Pinsent et al., 1956; Plaza, 2011; Versteeg et al., 1996; Ying and Eimer, 2013). However, only few researchers have studied kinetics of CO2 absorption into partially carbonated MEA solutions (Aboudheir et al., 2003; Dang and Rochelle, 2003; Dugas and Rochelle, 2011; Littel et al., 1992; Luo et al., 2015; Puxty et al., 2010). Among these research works, only two termolecular kinetic models of carbon dioxide reacting with loaded aqueous MEA solution have been found (Aboudheir et al., 2003; Luo et al., 2015), Table A2 includes both models, the mechanism that they are based on and their validity ranges.

## 4 Enhancement factor

Since the last century, many researchers have studied the enhancement factor used to compute the mass transfer rates from gases to liquids (Brian et al., 1961; Cussler, 2009; DeCoursey, 1982; DeCoursey and Thring, 1989; Gaspar and Fosbol, 2015; Gilliland et al., 1958; Hatta, 1928; Hikita et al., 1982; Hogendoorn et al., 1997; Last and Stichlmair, 2002; Van Krevelen and Hofijzer, 1948; Van Swaaij and Versteeg, 1992; Van Wijngaarden et al., 1986; Versteeg et al., 1989; Wellek et al., 1978; Yeramian et al., 1970). Consequently, a great variety of models have been developed (Brian et al., 1961; Cussler, 2009; Gaspar and Fosbol, 2015; Last and Stichlmair, 2002; Van Krevelen and Hofijzer, 1948; Wellek et al., 1978; Yeramian et al., 1970). A list of expressions allowing the calculation of enhancement factor is provided in Table A3.

## 5 Heat of absorption

Although MEA is believed to be the most commonly used solvent for the CO2 removal, only limited data on the direct measurements of the heat of absorption of the reaction between CO2 and aqueous solutions of MEA have been published (Arcis et al., 2011; Carson et al., 2000; Kim, 2009; Kim and Svendsen, 2007; Mathonat et al., 1998).

Few researchers, in their works, used fixed values for the enthalpy of absorption prediction (Kolil and Nielsen, 1997; Kvamsdal and Rochelle, 2008; Pandya, 1983), however, others have developed new correlations to calculate the enthalpy of absorption on the basis of existing empirical data available in literature (Kim, 2009, Llano-Restrepo and Araujo-Lopez, 2015). All these correlations and fixed values for the heat of absorption estimation are summarized in Table A4.

## 6 Vapor pressure

Over the years, various temperature dependent equations for water vapor pressure estimation have been developed. In this study, we will consider the ones that are most commonly used in literature (Ambrose and Walton, 1989, Antoine, 1888, Riedel, 1954). These correlations are written in Table A5.

## 7 CO2 diffusivity in aqueous solutions of MEA

Because of the reaction occurring between CO2 and the amine solutions, the CO2 diffusivity in the MEA solution cannot be determined directly. Therefore, Clarke (1964) proposed the N2O analogy method which has been then adopted by many researchers. This approach can be expressed as follows:

\[
D_{CO2,L} = D_{N2O,L} \left( \frac{D'_{CO2}}{D'_{N2O}} \right).
\]

Various measurements have been reported in literature on the N2O diffusivity in aqueous solutions of MEA on a broad range of MEA concentration and temperature (Clarke, 1964; Cullen and Davidson, 1957; Sada et al., 1978; Li and Lai, 1995; Ko et al., 2001; Ying and Eimer, 2012). Based on these experimental data, different correlations have been developed which are listed in Table A6.

## 8 Parametric study

The effects of changing the empirical correlations or fixed values on the column performance (liquid temperature and liquid CO2 loading profiles) were investigated for each model parameter following step-by-step approach, that
Table 1. Summary of the model parameter correlations used in each cases.

| 1. Kinetic model | Enhancement factor | Enthalpy of absorption | Vapor pressure | CO₂ diffusivity | Number of cases |
|------------------|--------------------|------------------------|----------------|----------------|-----------------|
| Variable         | Fixed              | Fixed                  | Fixed          | Fixed          | 2 cases         |
| (a) Luo et al. (2015) | Gaspar and Fosbøl (2015) | Llano-Restrepo and Araujo-Lopez (2015) based on Arcis et al. (2011) data | Antoine (1888) | Ying and Eimer (2012) |
| (b) Aboudheir et al. (2003) | | | | |

| 2. Enhancement factor | Fixed | Variable | Fixed | Fixed | Fixed | 8 cases |
|-----------------------|-------|----------|-------|-------|-------|---------|
| Luo et al. (2015)     | (a) Van Krevelen and Hoftijzer (1948) | Llano-Restrepo and Araujo-Lopez (2015) based on Arcis et al. (2011) data | Antoine (1888) | Ying and Eimer (2012) |
| (b) Brian et al. (1961) | | | | |
| (c) Yeramian et al. (1970) based on penetration theory | | | | |
| (d) Yeramian et al. (1970) based on surface renewal theory | | | | |
| (e) Welk et al. (1978) | | | | |
| (f) Last and Stichlmair (2002) | | | | |
| (g) Cussler (2009) | | | | |
| (h) Gaspar and Fosbøl (2015) | | | | |

| 3. Enthalpy of absorption | Fixed | Fixed | Variable | Fixed | Fixed | 5 cases |
|---------------------------|-------|-------|----------|-------|-------|---------|
| Luo et al. (2015)         | Van Krevelen and Hoftijzer (1948) | (a) Kohl and Nielsen (1997) | Antoine (1888) | Ying and Eimer (2012) |
| (b) Pandya (1983) | | | | |
| (c) Kim (2009) | | | | |
| (d) Llano-Restrepo and Araujo-Lopez (2015) based on Kim and Svendsen (2007) data | | | | |
| (e) Llano-Restrepo and Araujo-Lopez (2015) based on Arcis et al. (2011) data | | | | |

| 4. Vapor pressure | Fixed | Fixed | Fixed | Variable | Fixed | 3 cases |
|-------------------|-------|-------|-------|----------|-------|---------|
| Luo et al. (2015) | Van Krevelen and Hoftijzer (1948) | Llano-Restrepo and Araujo-Lopez (2015) based on Arcis et al. (2011) data | (a) Antoine (1888) | Ying and Eimer (2012) |
| (b) Riedel (1954) | | | | |
| (c) Ambrose and Walton (1989) | | | | |

| 5. CO₂ diffusivity | Fixed | Fixed | Fixed | Variable | 3 cases |
|-------------------|-------|-------|-------|----------|---------|
| Luo et al. (2015) | Van Krevelen and Hoftijzer (1948) | Llano-Restrepo and Araujo-Lopez (2015) based on Arcis et al. (2011) data | Antoine (1888) | (a) Ko et al. (2001) |
| (b) Jamal (2002) | | | | |
| (c) Ying and Eimer (2012) | | | | |
Table 2. Simulation results for runs (R 3, 8, 13–15, 18, 21–23) of Sonderby et al. (2013).

| 1. Kinetic model | Run 3 | Run 8 | Run 13 | Run 14 | Run 15 | Run 18 | Run 21 | Run 22 | Run 23 |
|------------------|-------|-------|--------|--------|--------|--------|--------|--------|--------|
| ARD% for the liquid CO2 loading profile | Case 1-a | 3.719 | 3.373 | 5.074 | 5.146 | 5.188 | 2.101 | 2.099 | 1.552 | 1.804 |
| ARD% for the liquid temperature profile | Case 1-a | 2.015 | 4.278 | 2.686 | 2.738 | 1.823 | 5.091 | 2.532 | 2.530 | 2.593 |
| 2. Enhancement factor | | | | | | | | | |
| ARD% for the liquid CO2 loading profile | Case 2-a | 3.709 | 3.359 | 5.055 | 5.144 | 5.174 | 2.055 | 2.095 | 1.550 | 1.762 |
| Case 2-b | 3.764 | 3.412 | 5.111 | 5.154 | 5.220 | 2.213 | 2.102 | 1.559 | 1.833 |
| Case 2-c | 3.736 | 3.459 | 5.135 | 5.170 | 5.256 | 2.334 | 2.101 | 1.565 | 1.867 |
| Case 2-d | 3.735 | 3.461 | 5.155 | 5.171 | 5.258 | 2.340 | 2.100 | 1.565 | 1.870 |
| Case 2-e | 3.728 | 3.467 | 5.152 | 5.166 | 5.260 | 2.350 | 2.100 | 1.563 | 1.867 |
| Case 2-f | 3.733 | 3.491 | 5.189 | 5.191 | 5.285 | 2.417 | 2.100 | 1.571 | 1.891 |
| Case 2-g | 3.800 | 3.595 | 5.284 | 5.361 | 2.688 | 2.103 | 1.600 | 1.961 |
| ARD% for the liquid temperature profile | Case 2-a | 2.008 | 4.260 | 2.664 | 1.814 | 5.078 | 2.522 | 2.521 | 2.583 |
| Case 2-b | 2.038 | 4.330 | 2.744 | 1.867 | 5.160 | 2.579 | 2.573 | 2.630 |
| Case 2-c | 2.061 | 4.385 | 2.727 | 1.867 | 5.160 | 2.579 | 2.573 | 2.630 |
| Case 2-cl | 2.063 | 4.387 | 2.726 | 1.867 | 5.160 | 2.579 | 2.573 | 2.630 |
| Case 2-e | 2.068 | 4.396 | 2.716 | 1.869 | 5.164 | 2.578 | 2.569 | 2.625 |
| Case 2-f | 2.073 | 4.418 | 2.720 | 1.885 | 5.183 | 2.603 | 2.594 | 2.650 |
| Case 2-g | 2.127 | 4.540 | 2.762 | 1.934 | 5.263 | 2.654 | 2.642 | 2.695 |
| Case 2-h | 2.015 | 4.278 | 2.686 | 1.823 | 5.091 | 2.532 | 2.530 | 2.593 |
| 3. Enthalpy of absorption | | | | | | | | | |
| ARD% for the liquid CO2 loading profile | Case 3-a | 3.858 | 3.456 | 5.153 | 5.188 | 2.286 | 2.099 | 1.587 | 1.767 |
| Case 3-b | 4.394 | 3.462 | 5.231 | 5.256 | 2.655 | 2.108 | 1.605 | 1.772 |
| Case 3-c | 4.406 | 3.464 | 5.235 | 5.259 | 2.648 | 2.159 | 1.606 | 1.773 |
| Case 3-cl | 4.439 | 3.469 | 5.244 | 5.262 | 2.666 | 2.160 | 1.608 | 1.782 |
| Case 3-e | 3.709 | 3.359 | 5.055 | 5.174 | 2.055 | 2.095 | 1.550 | 1.762 |
| ARD% for the liquid temperature profile | Case 3-a | 7.478 | 6.220 | 4.871 | 4.131 | 5.190 | 5.573 | 5.746 | 5.239 |
| Case 3-b | 8.961 | 6.425 | 9.382 | 8.889 | 5.703 | 7.793 | 5.881 | 5.416 |
| Case 3-c | 9.151 | 6.603 | 9.543 | 9.018 | 6.763 | 7.925 | 5.944 | 5.415 |
| Case 3-cl | 9.600 | 7.006 | 9.916 | 9.384 | 6.968 | 6.118 | 6.908 | 5.623 |
| Case 3-e | 2.008 | 4.260 | 2.664 | 1.814 | 5.078 | 2.522 | 2.521 | 2.583 |
| 4. Vapor pressure | | | | | | | | | |
| ARD% for the liquid CO2 loading profile | Case 4-a | 3.709 | 3.359 | 5.055 | 5.144 | 5.174 | 2.055 | 2.095 | 1.550 | 1.762 |
| Case 4-b | 9.361 | 6.438 | 7.141 | 5.794 | 5.201 | 3.237 | 3.839 | 2.813 | 3.567 |
| Case 4-c | 3.888 | 4.825 | 5.984 | 5.492 | 5.199 | 3.074 | 2.370 | 2.003 | 3.146 |
| ARD% for the liquid temperature profile | Case 4-a | 2.008 | 4.260 | 2.664 | 1.814 | 5.078 | 2.522 | 2.521 | 2.583 |
| Case 4-b | 15.078 | 11.868 | 17.137 | 17.035 | 9.689 | 12.278 | 18.383 | 17.308 | 18.346 |
| Case 4-c | 7.634 | 9.843 | 5.712 | 6.536 | 4.125 | 8.212 | 6.963 | 6.908 | 6.908 |
| 5. CO2 diffusivity | | | | | | | | | |
| ARD% for the liquid CO2 loading profile | Case 5-a | 3.732 | 3.516 | 5.229 | 5.221 | 5.252 | 2.421 | 2.098 | 1.591 | 1.964 |
| Case 5-b | 3.828 | 5.150 | 6.107 | 5.378 | 6.191 | 5.961 | 2.554 | 2.578 | 2.884 |
| Case 5-c | 3.709 | 3.359 | 5.055 | 5.144 | 5.174 | 2.055 | 2.095 | 1.550 | 1.762 |
| ARD% for the liquid temperature profile | Case 5-a | 2.085 | 4.438 | 2.739 | 2.765 | 1.861 | 5.178 | 2.628 | 2.621 | 2.673 |
| Case 5-b | 3.567 | 6.305 | 2.928 | 2.571 | 6.254 | 3.115 | 3.662 | 3.521 |
| Case 5-c | 2.008 | 4.260 | 2.664 | 2.734 | 1.814 | 5.078 | 2.522 | 2.521 | 2.583 |
means, each time the best correlation for the parameter $X$ calculation is determined then used (or fixed) to study the next parameter, and so on. For a better understanding, Table 1 shows the different methods used for model parameters calculation in each case.

In this paper, the average relative deviation percentage ARD% was the criterion used to compare model predictions with experiments, and it was computed by using the following equation:

$$\text{ARD} = 100 \times \frac{1}{n} \sum_{i=1}^{n} \left( \frac{x_i^\text{cal} - x_i^\text{Exp}}{x_i^\text{Exp}} \right). \quad (9)$$

9 Results and discussion

In this research work, the model simulation was based on the experimental data reported in the literature by Sonderby et al. (2013) using a pilot-scale CO$_2$ absorption column, where 23 experiments were performed, denoted (R1–R23). However, in this study, only 9 runs (R 3, 8, 13–15, 18, 21–23) were taken into account, as shown in Table 2. This selection was founded on two criteria: a low experimental error and a large number of points (measurements) in each run.

All the simulation results, displayed in terms of liquid temperature and liquid CO$_2$ loading average relative deviation percentages (ARD%) for all runs (R 3, 8, 13–15, 18, 21–23) and all cases (21 cases), are summarized in Table 2.

In this section, the results presented in Table 2 are discussed in general terms, that means, they will be discussed only in respect of the simulation deviation between the different runs, and then a detailed discussion is given for each parameter separately (in Sects. 9.1–9.5).

The Case 5-c is selected as a base case for this discussion because it represents a combination between the correlations that provide the lowest ARD%. Accordingly, it has been noticed that for the liquid CO$_2$ loadings, the ARDS% are in the range of 1–6%. A maximum ARD% of ±5% is obtained for runs (R13–15), while the minimum ARD% of ±2% is obtained for runs (R18, 21–23). Furthermore, for the liquid temperature, the ARDS% for the different runs are varying also between 1% and 6%. A maximum ARD% of ±5% is obtained for Run 18, an ARD% of 4.260% is also given by Run 8, while the other runs (R3, 13–15, 21–23) have an ARD% of ±2%. This difference in ARD% between the different runs might be cause by the experimental errors which are different from a run to another, and it is believed that the reasons of these deviations are: The use of manual instruments instead of digital readouts which...
require a calibration prior to each run. Moreover, the difficulty to reach the adiabatic conditions at the laboratory scale which is assumed in the model development. Finally, pressure and heat losses along the column.

9.1 Kinetic model

A sensible selection of kinetic models is important for obtaining accurate predictions. In regards to this area, the liquid-phase temperature and liquid CO₂ loading have been simulated using two different kinetic models (Aboudheir et al., 2003, Luo et al., 2015).

Figure 1 illustrates the simulation results in respect of the empirical values obtained from runs R21 and R22 of Sonderby et al. (2013). According to this figure, it has been noticed that the liquid temperature and the liquid CO₂ loading profiles simulated by using the kinetic model suggested by Luo et al. (2015) are more accurate than the ones obtained while using the kinetic model of Aboudheir et al. (2003). The use of the kinetic model of Aboudheir et al. (2003) is somewhat under predicts the liquid temperature and the liquid CO₂ loading. This low accuracy presented by this kinetic model might be affected by the instrumental methods employed to obtain kinetic data, and the empirical correlations of physical properties (CO₂ diffusivity and solubility in aqueous solutions) employed for kinetic model development. Furthermore, it has been also observed that the kinetic models have a large influence on both, liquid CO₂ loading and liquid temperature. And according to the results obtained from Cases 1.a to 1.b for all runs, presented in Table 2, the same conclusions are found.

9.2 Enhancement factor

On the basis of the results presented in Table 2 for the Cases 2.a–2.h, it can be deduced that the effect of the different enhancement factor models on the performance of the columns is not very significant. The ARD% between the simulation results and pilot-plant measured data are very close for all cases, the difference is in the order of ±0.1% for both liquid temperature and liquid CO₂ loading. The lowest ARD% is obtained by using the model developed by Van Krevelen and Hoftijzer (1948), while the highest ARD% is given from the model suggested by Cussler (2009).
9.3 Enthalpy of absorption

The simulated liquid temperature and liquid CO₂ loading profiles were compared with measurements taken from runs R21 and R22 of Sonderby et al. (2013), as shown in Figure 2, to study the effect of the enthalpy of absorption on the absorber performance.

Accordingly, it has been noticed that the influence of the enthalpy of absorption on the liquid CO₂ loading is very small, the different profiles obtained for R21 and R22 are almost overlapped, there is just a slight difference in the last 3 m of the absorber height, where the lowest ARD% is obtained from the correlation of Llano-Restrepo and Araujo-Lopez (2015) based on Arcis et al. (2011). On the other hand, the effect is very high for the liquid temperature profiles. It has been observed that the use of the fixed value of 118.2 kJ/mol, given by Kohl and Nielsen (1997), under-predicts the liquid temperature profile for both runs R21 and R22 with ARD% of 5.573% and 5.746%, respectively. Furthermore, the liquid temperature profiles obtained by using the fixed value of 84.4 kJ/mol reported by Pandya (1983) and the two correlations developed by Kim (2009) and Llano-Restrepo and Araujo-Lopez (2015) based on Kim and Svendsen (2007) data are closely superposed with ARDs% of 7.793, 7.925, and 8.114%, respectively, for R21, and ARDs% of 5.881, 5.944 and 6.118%, respectively, for R22, they exhibit a good accord with experimental data in the initial 3 m then they over-predict the liquid temperature for the rest of the column.

Finally, the correlation suggested by Llano-Restrepo and Araujo-Lopez (2015) based on Arcis et al. (2011) data provides the lowest ARD% of 2.522% and 2.521%, with respect to R21 and R22, the overall agreement in this case between simulated liquid temperature profile and measurements is generally good.

From the results of Table 2, regarding the Cases 3.a–3.e for all runs, it has been noticed that it leads to the same conclusions.

9.4 Vapor pressure

Different correlations for vapor pressure estimation (see Tab. A5) were employed to simulate the liquid temperature and the liquid CO₂ loading using the experimental data of Sonderby et al. (2013), the results for R21 and R22 are illustrated in Figure 3.

As shown in Figure 3, the influence of the vapor pressure on both, the liquid temperature and the liquid CO₂ loading is important. According to runs R21 and R22, the results obtained while using the correlation developed by Antoine (1888) show a good agreement with experimental data, contrary to the correlation suggested by Riedel (1954)
where the ARD% is very large (see Tab. 2), it overestimates the liquid temperature and the liquid CO2 loading, while the use of Ambrose and Walton (1989) correlation under-predicts them. All in all, and according to these results as well as the results shown in Table 2 for the Cases 4.a–4.d, it has been concluded that the correlation developed by Antoine (1888) leads to the most accurate simulation results.

9.5 CO2 diffusivity in aqueous solutions of MEA

The influence of CO2 diffusivity in aqueous solutions of MEA on the column performance is studied by using the measurements taken from Sonderby et al. (2013). The results, shown in Figure 4, are presented in terms of liquid temperature and liquid CO2 loading.

According to this figure, it has been noticed that the influence of the CO2 diffusivity in aqueous MEA solution on the column performance is not very large, all the three correlations show a good agreement with experimental data, the profiles obtained from the correlations of Ko et al. (2001) and Ying and Eimer (2012) are almost overlapped with very close ARD% (see Tab. 2). However, the use of the correlation of Jamal (2002) under-predicts both, liquid temperature and liquid CO2 loadings profiles. The lowest ARD% is obtained from the correlation suggested by Ying and Eimer (2012), while the highest ARD% is given from the correlation developed by Jamal (2002), and according to Table 2 for the cases 5.a–5.c, the same is observed for the other runs.

9.6 The added value of this study to the modeling and simulation

In general, the experimental techniques, the number of measurements, as well as the assumptions behind the different model parameter correlations are the main reason of the discrepancies between experimental data and simulated profiles, therefore, a good selection of such correlations is of high importance which is the key objective of this parametric study. And in order to prove its significance on obtaining reliable modeling and simulation results, a comparison between a combination of different model parameters that present the highest and the lowest ARDs% was performed (only this two cases were chosen since the number of possible combinations is very large), in other words, the difference in deviation between the worst case and the best one is investigated in this section, Table 3 summarized the model parameter correlations used in each case.

According to the comparison results illustrated in Figure 5, for different runs (R 3, 8, 13–15, 18, 21–23) of Sonderby et al. (2013), we can come up with the following conclusions:
Table 3. List of the different model parameter correlations used in each case.

| Model properties        | Case 1                                             | Case 2                                             |
|-------------------------|---------------------------------------------------|---------------------------------------------------|
| Kinetic model           | Aboudheir et al. (2003)                           | Luo et al. (2015)                                 |
| Enhancement factor      | Cussler (2009)                                    | Van Krevelen and Hoftijzer (1948)                  |
| Heat of absorption      | Llano-Restrepo and Araullo-Lopez (2015) based on Kim and Svendsen (2007) data | Llano-Restrepo and Araullo-Lopez (2015) based on Arcis et al. (2011) data |
| Vapor pressure          | Riedel (1954)                                    | Antoine (1888)                                   |
| CO₂ diffusivity         | Jamal (2002)                                      | Ying and Eimer (2012)                             |

10 Conclusion

One of the challenges faced while modeling and simulating the reactive absorption of CO₂ into loaded aqueous monoethanolamine solution in a packed-bed absorber is the proper calculation of the model parameters, hence, a parametric study was performed by using different cases of five different model parameters (kinetic model, enhancement factor, heat of absorption, CO₂ diffusivity in aqueous solutions of MEA, and vapor pressure). Consequently, the following points can be deduced:

- Among the model parameters studied in this paper, only kinetic model and vapor pressure have a large influence on the liquid CO₂ loading.
- Some parameters present a large influence on the liquid temperature (kinetic model, heat of absorption, and vapor pressure). Therefore, they should be chosen very carefully.
- The effect of the enhancement factor and CO₂ diffusivity is not very important, hence, a wrong choice of the model does not lead to severe deviation.
- The kinetic model introduced by Luo et al. (2015), the widely used model developed by Van Krevelen and Hoftijzer (1948) for the enhancement factor prediction, the developed correlation of Llano-Restrepo and Araullo-Lopez (2015) on the basis of Arcis et al. (2011) data for the heat of absorption estimation, vapor pressure expression of Antoine (1888), and the correlation of Ying and Eimer (2012) for the diffusivity of CO₂ in loaded aqueous MEA solution calculation generally provide more accurate predictions of the empirical values relative to the other cases employed in this analysis. This combination of correlations is obtained using the step-by-step approach where the coupling between different processes or phenomena is neglected. Therefore, another optimum model could be found while using another methods of performing the paramedic study.

In addition, the comparison between the two combinations of different model parameters that present the highest and the lowest ARDs% revealed that the model deviation

![Fig. 5. Comparison results for runs (R 3, 8, 13–15, 18, 21–23) of Sonderby et al. (2013).](image-url)
could be reduced by 18% and 4% for the liquid temperature and liquid CO₂ loading profiles, respectively.

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## Appendix

**Table A1.** List of correlations used for the calculation of physicochemical and transport properties.

| Property | Correlation | Property | Correlation |
|----------|-------------|----------|-------------|
| Density of pure MEA | Jayarathna et al. (2013) | Henry's constant of N$_2$O in aqueous MEA solution | Jiru et al. (2012) |
| Density of water | Kell (1975) | Diffusivity of MEA in water | Snijder et al. (1993) |
| Density of CO$_2$-loaded MEA solution | Weiland et al. (1998) | Surface Tension of CO$_2$-loaded aqueous MEA solution | Jayarathna et al. (2013) |
| Viscosity of water | Swindells taken from Weast (1984) | Heat capacity of liquid MEA | Agbonghae et al. (2014) |
| Viscosity of CO$_2$-loaded MEA solution | Weiland et al. (1998) | Heat capacity of liquid water | Agbonghae et al. (2014) |
| Henry's constant of CO$_2$ in water | Jamal (2002) | Heat capacity of CO$_2$-loaded aqueous MEA solution | Agbonghae et al. (2014) |
| Henry's constant of N$_2$O in water | Jamal (2002) | Heat of vaporization | Pitzer and Curl (1957) |

**Gas phase properties**

| Property | Correlation | Property | Correlation |
|----------|-------------|----------|-------------|
| Gas phase density | Soave (1972); Holderbaum and Gmehling (1991) | Gas phase CO$_2$ diffusivity | Wilke (1950) |
| Gas phase viscosity | Poling et al. (2001) | Thermal conductivity of pure gases | Ely and Hanley method taken from Reid et al. (1987) |
| Gas phase heat capacities | Smith et al. (2005) | Gas phase thermal conductivity | Wassiljewa-Mason-Saxen method taken from Poling et al. (2001) |
| Gas phase binary diffusivities | Fuller method taken from Poling et al. (2001) | Gas phase water vapor diffusivity | Blanc’s expression taken from Poling et al. (2001) |

**Mass and heat transfer properties**

| Property | Correlation | Property | Correlation |
|----------|-------------|----------|-------------|
| Mass transfer coefficients | Billet and Schultes (1999) | Gas phase heat transfer coefficient | Geankoplis (2003) |
| Effective interfacial area | Billet and Schultes (1999) | Mass-transfer-corrected gas-phase heat transfer coefficient | Pandya (1983) |
| Liquid holdup of packing | Billet and Schultes (1999) | | |
Table A2. Summary of kinetic models for CO$_2$ reacting with loaded aqueous MEA solution.

| References            | Mechanism type                     | Validity ranges | Kinetic constant expressions                                                                 |
|-----------------------|------------------------------------|-----------------|-----------------------------------------------------------------------------------------------|
| Aboudheir et al. (2003) | Termolecular mechanism             | 3–9 M           | $k_2 = \sum_i k_{2,i} \text{[base, }i\text{]}$                                                   |
|                       |                                    | 293–333 K       | $k_2 = k_{2,\text{MEA}}[\text{MEA}] + k_{2,\text{H}_2\text{O}}[\text{H}_2\text{O}]$       |
|                       |                                    | 0.1–0.5 mole CO$_2$/mole MEA | $k_{2,\text{MEA}} = 4.61 \times 10^9 \exp\left(\frac{-4412}{T}\right)$ |
|                       |                                    |                 | $k_{2,\text{H}_2\text{O}} = 4.55 \times 10^6 \exp\left(\frac{-3287}{T}\right)$     |
| Luo et al. (2015)     | Termolecular mechanism             | 1 and 5 M       | $k_2 = \sum_i k_{2,i} \text{[base, }i\text{]}$                                                   |
|                       |                                    | 298–343 K       | $k_2 = k_{2,\text{MEA}}[\text{MEA}] + k_{2,\text{H}_2\text{O}}[\text{H}_2\text{O}]$       |
|                       |                                    | 0–0.4 mole CO$_2$/mole MEA  | $k_{2,\text{MEA}} = 2.003 \times 10^{10} \exp\left(\frac{-4742}{T}\right)$         |
|                       |                                    |                 | $k_{2,\text{H}_2\text{O}} = 4.147 \times 10^{6} \exp\left(\frac{-3110}{T}\right)$     |

Table A3. Summary of the enhancement factor models.

| References             | Reaction condition/Theory     | Enhancement factor expressions                                                                 |
|------------------------|-------------------------------|-------------------------------------------------------------------------------------------------|
| Van Krevelen and       | 2nd order irreversible reaction | $E_{i_{\text{film}}} = 1 + \left(\frac{C_B D_B}{v D_{\text{AL}} C_{\text{AL}}}\right)$          |
| Hoftijzer (1948)       | Film theory                   |                                                                                                 |
|                       |                               | $E_{i_{\text{film}}} = \frac{\tan h}{\tan h} \left(\frac{\sqrt{g_{\text{film}} g_{\text{AL}}}}{g_{\text{film}} g_{\text{AL}}}\right)$ |
|                       | Irreversible 2nd order reaction | $E_{i_{\text{pen}}} = \sqrt{\frac{D_{\text{AL}}}{D_B}} + \sqrt{\frac{D_B}{D_{\text{AL}}} \left(\frac{C_B}{v D_{\text{AL}} C_{\text{AL}}}\right)}$ |
|                       | Penetration theory            |                                                                                                 |
|                       |                               | $E_{i_{\text{pen}}} = \frac{1 - \left(\frac{E_{i_{\text{pen}}}}{E_{1_{i}}-1}\right)}{\tan h} \left(\frac{1 - \left(\frac{E_{i_{\text{pen}}}}{E_{1_{i}}-1}\right)}{\tan h}\right)$ |
| Brian et al. (1961)    | 2nd order irreversible reaction | $E_{1_{i_{\text{pen}}}} = \text{Ha} \left\{1 + \frac{x}{\text{SR}_{\text{AL}}}\right\} \text{erf}\left(\sqrt{\frac{\text{SR}_{\text{AL}}}{\pi}}\right) + \frac{1}{2\text{H}_{\text{AL}}} \exp\left(\frac{-4\text{H}_{\text{AL}}}{\pi}\right)$ |
|                       | Penetration and surface-renewal theories | $E_{1_{i_{\text{pen}}}} = 1 + \left(\frac{C_B}{v C_{\text{AL}}}\right)$                      |
|                       |                               | $E_{i_{\text{pen}}} = \frac{\left(E_{i_{\text{pen}}}^\text{SR}\right)^2}{2\left(E_{i_{\text{pen}}}-1\right)} \left[\sqrt{1 + \frac{4\left(E_{i_{\text{pen}}}^\text{SR}\right)}{E_{i_{\text{pen}}}^\text{SR}-1}} - 1\right]$ |
|                       |                               | $E_{\text{surf}} = \frac{\text{Ha}^2}{2\left(E_{i_{\text{pen}}}-1\right)} \left[\sqrt{1 + \frac{4\left(E_{i_{\text{pen}}^\text{SR}}\right)^2 + E_{i_{\text{pen}}^\text{SR}}^\text{SR} \text{Ha}^2 \left(E_{i_{\text{pen}}}-1\right)}{\text{Ha}^2} - 1\right]$ |

(Continued on next page)
### Table A3. (Continued)

| References                  | Reaction condition/Theory                      | Enhancement factor expressions                                      |
|-----------------------------|------------------------------------------------|---------------------------------------------------------------------|
| Wellek et al. (1978)        | 2nd order irreversible reaction                | $E_i^{film} = \frac{(Ha)}{\tan(h(Ha))}$                           |
|                             | Film theory                                     | $E_i^{film} = 1 + \left( \frac{C_R D_R}{y A_1 \cdot C_1} \right)$   |
|                             |                                                 | $E_i^{film} = 1 + \frac{1}{\left( (1/E_i^{film}) - 1 \right)^{1.35} + (1/E_i^{film})^{1.35}}^{1/1.35}$ |
| Last and Stichlmair (2002) | 2nd order irreversible reaction                | $E_{surf} = 1 + \frac{1}{\left( 1 - E_i^{film} \right) + \frac{1}{\left( 1/E_i^{film} \right)^{1.35}}}$ |
|                             | Surface-renewal theory                          | $E_i^{film} = (Ha) \cot(h(Ha))$                                    |
| Cussler, 2009               | Fast reaction                                   | $E_i^{film} = (Ha) \cot(h(Ha))$                                    |
| Gaspar and Fosbøl (2015)   | 2nd order reversible reaction                  | $E_i^{film} = 1 + \left( \frac{C_R D_R}{y A_1 \cdot C_1} \right)$   |
|                             | Film theory                                     | $(1 - E_i^{film}) Y^2 + Ha(y_{A1} - 1) Y + E_i^{film} - y_A = 0$    |
|                             |                                                 | $Y = \sqrt{y_R^{'} - y_A}$                                         |
|                             |                                                 | $E_i^{film} = Ha \sqrt{y_R^{'} - y_A}$                             |

### Table A4. Summary of heat of absorption correlations and fixed values.

| References                          | Heat of absorption correlations and fixed values                                      |
|-------------------------------------|---------------------------------------------------------------------------------------|
| Kohl and Nielsen (1997)            | (118.2 kJ/mol)                                                                        |
| Pandya (1983)                      | (84.4 kJ/mol)                                                                          |
| Kim (2009)                         | $-\Delta H^{(ab)}_r = 84.68 - 0.1135t_L + 0.0027t_L^2$                               |
|                                    | $t_L = T_2 - 273.15$                                                                  |
| Llano-Restrepo and Araujo-Lopez     | $-\Delta H^{(ab)}_r = 85.2903 - 38.5592z_{CO_2} + 193.189(z_{CO_2})^2 - 317.759(z_{CO_2})^3 + 124.958(z_{CO_2})^4$ |
| based on Kim and Svendsen (2007)   |                                                                                       |
| data                               |                                                                                       |
| Llano-Restrepo and Araujo-Lopez     | $-\Delta H^{(ab)}_r = B_0 + B_1 z_{CO_2} + B_2 (z_{CO_2})^2 + B_3 (z_{CO_2})^3$ with: |
| based on Arcis et al. (2011) data  |                                                                                       |
|                                    | $B_0 = 111.171 - 4.62336 P + 0.0772299 P^2$                                           |
|                                    | $B_1 = -4.33417 + 12.6306 P - 0.222503 P^2$                                          |
|                                    | $B_2 = -72.9602 - 13.3031 P + 0.244333 P^2$                                          |
|                                    | $B_3 = 3.72612 + 7.62998 P - 0.135737 P^2$                                           |
Table A5. Summary of water vapor-pressure correlations.

| References                  | Correlations |
|-----------------------------|--------------|
| Antoine (1888)              | \( P_{\text{sat}} = 10^5 \times 10^{\left[5.11564 \cdot \frac{10^{0.507}}{288.15 + 230.15} \right]} \) |
| Riedel (1954)               | \( P_{\text{sat}} = 10^5 \times \exp \left[ \left( A^+ + B^+ \ln T_r + C^+ T_r^6 \right) + \ln P_c \right] \) with: |
|                             | \( A^+ = -35Q \) |
|                             | \( B^+ = -36Q \) |
|                             | \( C^+ = 42Q + \alpha_c \) |
|                             | \( D^+ = -Q \) |
|                             | \( K \) to be 0.0838 |
|                             | \( Q = K (3.758 - \alpha_c) \) |
|                             | \( \alpha_c = \frac{3.758K\psi_b + \ln(P_c/1.01325)}{K\psi_b - \ln T_{br}} \) |
|                             | \( \psi_b = -35 + \frac{2}{T_{br}} + 42\ln T_{br} - T_{br}^6 \) |
| Ambrose and Walton (1989)   | \( P_{\text{sat}} = 10^5 \times \exp \left[ \left( f^{(0)} + \omega f^{(1)} + \omega^2 f^{(2)} \right) + \ln P_c \right] \) |
|                             | \( f^{(0)} = -5.97616(1-T_r) + 1.29874(1-T_r)^{1.5} - 0.60394(1-T_r)^{2.5} - 1.06841(1-T_r)^3 \) |
|                             | \( f^{(1)} = -5.03365(1-T_r) + 1.11565(1-T_r)^{1.5} - 5.41217(1-T_r)^{2.5} - 7.46628(1-T_r)^3 \) |
|                             | \( f^{(2)} = -0.64771(1-T_r) + 2.41539(1-T_r)^{1.5} - 4.26979(1-T_r)^{2.5} + 3.25259(1-T_r)^3 \) |
Table A6. A list of CO₂ diffusivity correlations in aqueous MEA solution.

| References          | CO₂ diffusivity correlations                                                                                                                                 |
|---------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Ko et al. (2001)    | \[ D_{N_{20}}^\text{N}_{20} = 5.07 \times 10^{-6} \exp \left( \frac{-2371}{T_L} \right) \] \[ D_{CO_2}^\text{N}_{20} = 2.35 \times 10^{-6} \exp \left( \frac{-2119}{T_L} \right) \] \[ D_{N_{20},L} = (5.07 \times 10^{-6} + 8.65 \times 10^{-7} C_{\text{MEA}} + 2.78 \times 10^{-7} C_{\text{MEA}}^2) \times \exp \left[ \frac{-2371-9.34 \times 10^6 C_{\text{MEA}}}{T_L} \right] \] \[ D_{CO_2,L} = D_{N_{20},L} \left( \frac{D_{CO_2}^\text{N}_{20}}{D_{N_{20}}} \right) \] |
| Jamal (2002)        | \[ D_{N_{20}} = 5.2457 \times 10^{-6} \exp \left( \frac{-2255.9}{T_L} \right) \] \[ D_{CO_2} = 3.7191 \times 10^{-6} \exp \left( \frac{-2255.9}{T_L} \right) \] \[ D_{N_{20},L} = (5.2457 \times 10^{-6} + A_1 \times w_{\text{MEA}} + A_2 w_{\text{MEA}}^2) \times \exp \left[ \frac{-2388.9}{T_L} \right] \] \[ A_1 = 1.4196 \times 10^{-5} - \frac{4.4299 \times 10^{-3}}{T_L} \] \[ A_2 = -3.2060 \times 10^{-6} - \frac{9.8151 \times 10^{-4}}{T_L} \] \[ D_{CO_2,L} = D_{N_{20},L} \left( \frac{D_{CO_2}^\text{N}_{20}}{D_{N_{20}}} \right) \] |
| Ying and Eimer (2012)| \[ D_{N_{20}} = 5.07 \times 10^{-6} \exp \left( \frac{-2371}{T_L} \right) \] \[ D_{CO_2} = 2.35 \times 10^{-6} \exp \left( \frac{-2119}{T_L} \right) \] \[ D_{N_{20},L} = (5.07 \times 10^{-6} - 3.5443 \times 10^{-7} C_{\text{MEA}} + 3.4294 \times 10^{-9} C_{\text{MEA}}^2) \times \exp \left[ \frac{-2371+0.3740 \times C_{\text{MEA}}}{T_L} \right] \] \[ D_{CO_2,L} = D_{N_{20},L} \left( \frac{D_{CO_2}^\text{N}_{20}}{D_{N_{20}}} \right) \] |