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ASPEN PLUS simulation model for CO_2 removal with MEA: Validation of desorption model with experimental data

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ABSTRACT

The chemical absorption process has been extensively studied as one of the main carbon capture and separation technologies. This process comprises two stages: The absorption of CO_2 into the solvent and the desorption, to regenerate the solvent and produce the high concentrated CO_2 gas.

Validated simulation models are essential for the scale-up of the chemical absorption process and they are typically validated using only data from one pilot plant. In this work, a simulation model of the desorption column built in ASPEN PLUS v8.6 was validated using four experimental pilot campaigns using 30 wt% MEA. The desorbers in the different campaigns varied in the diameters, structured packing heights and packing types.

A good agreement is observed between experimental data and the simulation results of the chemical absorption process presented here. The model shows an AARD (average absolute relative deviation) of 9.2% for the CO_2 stripped (kg/h) for the tested 78 experimental runs. The simulated temperatures of the liquid flux leaving the reboiler show a deviation of 3.3% compared with the experimental data. The deviations on the estimation of the CO_2 stripped show some dependency on the CO_2 loading in the rich amine flux entering the desorber. However, the deviations are independent on the temperature of the rich amine.

1. Introduction

Chemical absorption is a well-known process that has been proposed as the most dominant technology for CO_2 capture in power plants before 2030. As in the case of the desulphurization process, both process [1] and solvent improvements [2,3] are needed to make the CO_2 capture by chemical absorption economically feasible [4].

The chemical absorption process can be divided in two phases: absorption and desorption. The flue gas from a power plant (typically with emissions of 300–700 g CO_2/Kwh), enters the bottom of a packed column, flows upward and meets a CO_2 absorbing solvent circulated countercurrently. The CO_2-rich solution, leaving the bottom of the absorber, is then pumped to a cross heat exchanger and then to a desorber column for its regeneration at high temperature. In the regeneration, the reactions between CO_2 and the solvent are reversed using heat, and gaseous CO_2 and water vapour are produced. The gases are sent to a condenser, where gas rich in CO_2 is obtained. The regenerated solvent, now with low concentration of CO_2 (lean solution), is returned to the absorber. In the regeneration, one of the main factors to consider for the process optimization is the energy invested.

The use of validated simulation tools is of high importance to predict the CO_2 purification performance and consequently design the entire absorption/desorption process. Numerous experimental and simulation studies on desorption of CO_2 in 30 wt.-% MEA have been carried out over the years and an overview of the published work in the last 5 years is given below. The literature review shows that only very few previous studies [5,6] included simulation models validation with two pilot plants and that most of the previous work was based on fitting the model with very few experimental runs of one campaign and using the rest of the runs from the campaign to test the model. Furthermore, the models are typically fitted using parameters (like kinetic constants) that would have to be refitted when those models are used to simulate another pilot.

The current work had two main objectives. Firstly, we tested how an ASPEN PLUS v8.6 rate-based simulation model was able to predict data from different pilots. We used one pilot campaign to validate the model and the model was then further used to predict the three other pilot campaigns without any additional fitting. Secondly, since the same simulation model was used for each pilot campaign, the results showed how well the experimental runs from the different campaigns and pilots agreed with each other. This study highlights that a rigorous model is able to predict the desorber performance as long as the packing

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Table 1
Review on simulation models of desorption of CO_2 in MEA solutions between the years 2012–2017.

Source	Desorber Validation parameters	Pilot plant Data	Modelling type	Framework	Objective
[13]	Temperature; Loading; Regeneration energy	1 pilot plant (39 runs)	ASPEN PLUS	ENRTL	Re-fitting
[14]	Temperature; CO_2 Loading	1 pilot plant (19 runs)[15]	gProms	SAFT-VR	Prediction of desorber runs
[16]	Reboiler duty; CO_2 concentration; Temperature	1 pilot plant (19 runs)	ASPEN PLUS	ENRTL	Comparison of rate/based and equilibrium models and re-fitting
[5]	CO_2 desorbed; Reflux flow rate; Loading	2 Pilot Plants	MATLAB	NA	Validate an in-house model
[17–19]	Temperature; Composition; CO_2 Loading	1 Pilot Plant (2 runs)	gProms SuperTRAPP merhod Stadistical Associating Fluid Theory	SAFT-VK	Integration of theoretical CO_2 capture in a power plant
[20]	Reboiler duty	NA	Aspen Plus Aspen Hysys	ENRTL	Validate heat consumption reduction by changes on absorption configuration
[21]	Loading; Desorbed CO_2; Solvent flow rate	1 Pilot Plant	K-Spice + InfoChem + CO2SIM	InfoChem	Dynamic changes
[6]	Reboiler duty; CO_2 loading	2 pilot plants	ASPEN PLUS v7.3	NA	Validate two packings and two scales
[22]	Reboiler temperature	1 pilot plant	Dymola + Modelica + Optimica	NA	Represent dynamic changes
[23]	Heat of regeneration; Temperature; CO_2 loading	1 Pilot Plant (2 runs)	In-House	ENRTL	Validate an in-house model for different CO_2 concentration in the fluegas
[24]	Temperature; Vapour composition	1 pilot plant (1 run from [25])	ASPEN PLUS v8.0	ENRTL-RK	Enhancement of existing model
[26]	Temperature; Reboiler duty	1 pilot plant (5 runs)	Aspen Hysys	ENRTL	Evaluation of performance of Exhaust Gas recycle and validation of simulation model
[27]	Lean temperature; CO_2 concentration on the top of the stripper; Flow rate	1 pilot plant with variation of operation parameters	Dynamic, Mathamatical (NLARX) model + Simulink	NA	Evaluation of dynamic predictions
[28–30]	Loading; Reboiler duty	1 pilot plant with variation of operation parameters	ASPEN PLUS + dCAPCO2 MATLAB + dCAPCO2	UNIQUAC UNIQUAC + GM enhancement factor model	Operation and comparison of MEA and PZ through transient response
[31]	Temperature; Loading	1 pilot plant	ASPEN PLUS + ASPEN PLUS DYNAMICS + ASPEN PLUS GUI + FORTRAN	ENRTL	Prediction of dynamic changes
[32]	NA	1 pilot plant [25]	Aspen Custom Modeller	ENRTL	Comparison with new solvent

performance can be correctlty predicted. The solvent used is 30 wt.-% MEA and 78runs were simulated, which represented multiple conditions and configurations.

2. Literature review

Commercially available process simulation software as ASPEN HYSYS, ASPEN PLUS, gPROMS, ASPEN, Custom Modeler, liean with Tsweet, Protreat have been extensively used for steady and dynamic simulations AspenAspen Plus[7]. Over the years, also in-house simulation tools have been used [6,14]. For example, Pinto et al. [8] used Procede Process Simulator (PPS) and discussed the performance of their simulation model compared to experimental liquid loading, temperatures and CO_2 captured. Furthermore, they compared the experimental mass transfer coefficients to the simulated one separating this study from the other studies listed in Table 1. However, Pinto et al. [8] did not include the desorber.

Because chemical absorption has reached a TRL9 (Technology Readiness Level), most recent simulation studies are related to process dynamics to study the flexibility on the CO_2 absorption/desorption operation. A review on dynamic models previous to 2013 can be found in Bui et al. [7].

Overall, in the simulation models, kinetic constants, effective absorption area or heat loss (desorber) are often adjusted to make the simulations fit the experimental data [4,5]. Often the data is fitted to very few experimental runs and the rest of the runs from the same campaign are thereafter simulated using the adjusted model. Finally simulations of industrial size plant are made [10]. However, when the fitted model is used to simulate other pilot data, considerable deviation might be seen [11]. The literature clearly shows that the choices related to the equilibrium model, mass transfer coefficients, and kinetic parameters influence the model predictions heavily making important to validate the simulation model using data from several pilot plants, with various operating conditions before using the model for process design or optimization [6,9,12].

As seen in Table 1, ASPEN PLUS is a commonly used software. Zhang & Chen [16] validated their ASPEN PLUS model with one pilot plant under different operation conditions (reproduced 19 runs). The thermodynamic, kinetic and transport property parameters were adjusted. The validation parameters used for the desorber were the reboiler duty, temperature and concentration profiles. Their model predicted the reboiler duty in a good agreement with the experimental data, with some deviations at high reboiler duty. Some slight underprediction was observed in the CO_2 concentration, while the temperature reproduced well the experimental results. Lim et al. [13] also used ASPEN PLUS to represent one pilot plant. They obtained a representation of loading and temperature, in good agreement with experimental data, while the regeneration energy was over-predicted. Li et al. [24] used ASPEN PLUS to predict one pilot plant run. They adjusted the water wash section and obtained lower errors in the prediction of temperature and loading than the basis model. Von Harbou et al. [6] used ASPEN PLUS v7.3 to simulate two pilot plants with different scale and packing. The mass transfer correlations and CO_2 solubility were adjusted. The reboiler duty and loading results were mostly under 5% of error. Also Oi & Pedersen [20]used ASPEN HYSYS and compared it to ASPEN PLUS. Both modelled used the ENRTL framework. Their work aimed to validate a reduction of heat consumption by changes on the absorption process configuration. The temperatures were in good agreement with experimental results. Gaspar et al. [28–30] used ASPEN PLUS in combination with other software (dCAPCO2) to measure the transient response to step changes on compositions and flows using separately MEA and PZ.

In addition to ASPEN PLUS, other simulation packages from ASPEN have been used in the literature to simulate the dynamic response in carbon capture pilot plants. Huser et al. [32] and Posch and Haider [33] used the ASPEN Custom Modeller and the ENRTL framework for the validation of the absorber with one pilot plant. However, the validation with data from Notz et al. [25] in Huser et al. [32] was only done with data from the absorber. Akram et al. [26] used ASPEN HYSYS. The reboiler duty was under-predicted and the desorber temperature was in a good agreement with the experimental data. Chinen et al. [31] also used ASPEN software but to study dynamically the response of the system at steps in the key variables. They obtained some deviation of the temperature at medium height and small variations on the loading.

In the literature other software has also been used to simulate the dynamic performance of absorption and desorption [21,22]. For example, Enaasen et al. [21] used dynamic K-Spice modelling, with multiflash provided by InfoChem and thermodynamics from CO2SIM. An over-prediction on loading was observed, potentially due to K-Spice configuration or due to inaccuracies in the analytical procedures during the pilot campaign. Additionally, although dynamic results were in good agreement with experiments, steady state results had a strong deviation.

In-house codes are also extensively used, as in Nagy & Mizsey [23]. In their work two experimental runs were represented to simulate coal and gas natural combustion (with high and low CO_2 content in the fluegas). In their work, the reboiler duty was represented, obtaining under-predicted values at high reboiler duty conditions. The main reason highlighted in their work is that the heat of absorption taken from ASPEN has some deviations. Additionally, the temperature and loading along the desorber were both over-predicted. Saimpert et al. [5] represented the desorber with an in-house MATLAB model, validated with two pilot plants, what is different to most of the studies. However, the model did not represent the two pilot plant campaigns with similar accuracy. Considering one pilot plant, the model showed under-prediction of the flow rate (with absolute deviation of 32%) and over-prediction of temperature (1–5 °C), mainly due to considering adiabatic conditions in the desorber. For the second pilot plant, the model agreed on temperature and CO_2 desorbed, with only slight deviations. This means that the developed simulation model was either not flexible enough to simulate these two different pilot plants or the data from the pilots were contradicting or too inaccurate. Also GarÐarsdóttir et al. [22] simulated the flexible operation at part-load and peak-loaded scenarios using Dymola, Modelica and Optimica software. Although this study did not include experimental validation, the results showed the process control strategy as tool to decrease the time response of the absorption system in both scenarios.

Many authors have based their work on the use of gProms to represent the absorption/desorption process over the years. Brand [34] used gProms without adjusting any model parameter. The model represented fairly well the data with some over-prediction of temperature and loading at the top and on the bottom of the desorber and some under-prediction at low temperature and on the bottom. In the works of Mac Dowell et al. and Mac Dowell & Shah [17–19], a more complex combination of software was used for the parameters prediction using one pilot plant. They combined gProms with superTRAPP method to predict viscosity and thermal conductivity, while statistical associating fluid theory was used to predict the potentials of variable range and SAFT-VK framework was used for the remaining parameters. Additionally, only two runs were used in Mac Dowell et al. [17] for the validation of the model and this provided the basis for the prediction of the theoretic optimum operation and CO_2 capture system integration in the works of Mac Dowell & Shah [18,19]. As done by many authors, they also regarded the desorber as an adiabatic column [17,18], what will be commented further below. Ahn et al. [14] used gProms to find the optimum configuration for the highest reboiler duty reduction.

The desorption step has been found indeed more complex than the absorption process. More than 30 years ago, the simulation of the desorption process was discussed by Weiland et al. [35], where the modelling of the desorption process was recognised of being more complicated due to the reversibility of the chemical reactions. The thermodynamic calculations consequently had strong influence in the

process simulation. Weiland et al. [35], with a model based on physico-chemical data, expressed the overall mass transfer coefficients along the stripper. The concentrations of MEA varied between 0.5 and 5 Kmol/m^3, with loadings between 0.313 and 0.325, exhibiting errors of 25%, expressed as root mean square deviations. Later, Escobillana [36] modified the interphase area and the bubble diameter to fit the simulation models to experimental data and proposed to fit the enhancement factor, obtaining a good representation of the CO_2 concentration and temperature along the sieve tray stripper.

Unlike the other works presented above, Luo et al. [11] simulated four pilot plants using ASPEN PLUS v2006.5 and compared to other three commercial software and two in-house codes. In their work, there were not significant differences between the results from the different software. The reboiler duty was used as output while the rich and lean loadings were inputs in the simulation model. The predicted reboiler duty showed some over-prediction compared to experimental results. These results mean that a higher energy investment was predicted to reach the concentrations of the lean flux. However, there was also an over-prediction of the temperature along the stripper, what indicated that the kinetics of the reversible reaction for the solvent regeneration could had some deviations compared to the reality.

3. Methodology

Vapour-Liquid-Equilibrium (VLE) of the system CO_2-MEA-H_2O is of high importance to predict the desorption [35,37]. Greer et al. [38] validated the simulation results from their Matlab model with VLE results, where temperature dependent variables were modelled to obtain the dynamic performance of the desorber, at rich loading of 0.46 mol CO_2/mol amine. In this work, the ENRTL-RK rate-based model, available in ASPEN PLUS v8.6 for MEA, was used as a basis for the simulations and the discretization of the film was considered only on the liquid phase, along 10 segments. No film was considered in the gas phase, as there is not reaction in the gas phase. The VLE model in ASPEN PLUS was found to be valid by comparing the simulated partial pressure of CO_2 to experimental VLE data [39]. The temperature, composition and flow rate of the rich amine solution were used as inputs and the rich flux was considered one phase solution entering the desorber for all the cases. Similar approach was used in Tobiesen et al. [14] who, in simulations, assumed that the rich solution was one liquid phase. In many of the pilot campaigns the reality is that at high loading, the solution could flash before going into the desorber. This would give differences in the enthalpy of the solution, what would cause under-predicted values of temperature and deviations in CO_2 mass transfer [14]. The reboiler duty, pressure at the top of the desorber and pressure drop were used to define the operation conditions. The composition, temperature and flow rate of the lean solution as well as the CO_2 concentration and gas flow at the top of the desorber and reboiler temperature were obtained from the simulations.

The data used in this work is collected in Table 2. A simulation model in ASPEN PLUS was validated with the data in Tobiesen et al. [15] and then used to represent data from Enaasen et al. [41], Pinto et al. [42] and Notz et al. [25], using the desorbed CO_2 and the temperature of the lean flux in the reboiler as performance parameters.

As seen in Table 2, the pilot plant campaigns have different desorber diameters, packing heights and different structured packings. Moreover, the runs were performed under different conditions of CO_2 loading, temperatures and rich solvent flow. Due to this variability, the results allowed a comprehensive understanding of the desorption process and its representation. Table 2 shows that data sets covers in CO_2 loadings from 0.15 to 0.53 mol_{CO2}/mol_{MEA}. In full height pilots the lean loading is typically 0.2–0.25 mol_{CO2}/mol_{MEA} and with rich loadings around 0.45–0.48 mol_{CO2}/mol_{MEA}. Thus, the data from the pilot plants used here covers the full range of loadings. This is important since the pilot don't have enough packing heights to allow full recovery of the solvent in one run (from loading 0.48 to 0.2 mol_{CO2}/mol_{MEA}). Similarly, the lean solvent temperature (temperature of the liquid in the reboiler) and the rich solvent temperature vary more than 20 °C between the runs. The liquid flow rate is relatively contant in the works of Pinto et al. [42] and Enaasen et al. [41]. However, in Tobiesen et al. [15] and Notz et al. [25] the largest liquid flow is up to 4.5 times higher than the smallest flow used covering very different operating conditions for the packing.

The results in Zakeri [43] were incorporated through the Stilmchair correlation to characterize the packing Mellapack 250Y, used in Tobisen et al. [15] and Notz et al. [25]. Same behaviour as reported by Zakeri [43] in case of Mellapack 250Y was assumed in the case of Sulzer 2× packing (used in Pinto et al. [42] and Enaasen et al. [41]).

In this work, the deviations between experimental data and simulation results are given by the percentage of average absolute relative deviation (%AARD):

$$ARD = \frac{|x_{sim} - x_{exp}|}{x_{exp}} \quad (1)$$

$$\%AARD = \frac{\sum_1^n ARD}{n} * 100 \quad (2)$$

As mentioned by Weiland et al. [35], the heat effects cannot be ignored in the stripping process. Tobiesen et al. [15] carried out few runs with pure water to check the heat balance and estimate the heat loss, stayed as 0.5 kW along the stripper. In this work, these heat losses were incorporated as liquid losses. Enaasen et al. [41] and Pinto et al. [42] did not mention explicitly the numerical quantification of the heat loss along the column. Although the experiments were carried out in the same facilities used by Tobiesen et al. [15], the insulation of the pilot plant was improved. Since Enaasen et al. [41] and Pinto et al. [42] did not give a value of the heat losses, the results are given based on simulations without heat loss. However, at the end of this work, the effect of heat loss is presented. Notz et al. [25] reported that the heat losses varied from −0.247 (adding heat from outside instead of losing it) to 1.05 KW, with dependence on the running conditions, and those

Table 2
Overview of the literature data used in this work.

Resources	[15]	[41]	[42]	[25]
Desorber Diameter (m)	0.1	0.1	0.15	0.125
Packing height (m)	3.89	3.57	3.57	2.52
Packing type	Sulzer Mellapak 250Y	Sulzer Mellapak BX 500	Sulzer Mellapak BX 500	Sulzer Mellapak 250Y
Rich solution Loading (mol CO_2/mol MEA)	0.30–0.45	0.41–0.49	0.25–0.53	0.31–0.51
Lean solution Loading (mol CO_2/mol MEA)	0.18–0.45	0.22–0.34	0.21–0.34	0.146–0.36
Temperature Rich Solution (°C)	105–115	98–110	99–112	97–117
Temperature Lean Solution (°C)	101–121	106–119	112–118	102–125
Flux Rich solution (L/min)	3.0–9.0	2.43–4.1	3.3–3.43	1.32–6
Condenser temperature (°C)	15	15–25	15–34	14–20
Reboiler Duty (KW)	3.9–13.8	6.13–10.35	4–8.4	5.95–17.5
Runs	19	8	7	47

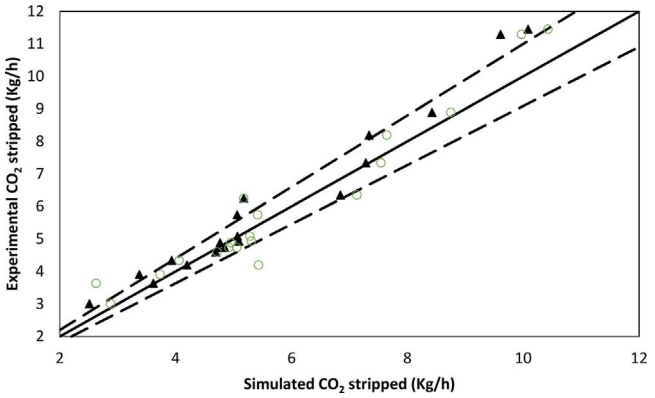

Fig. 1. Experimental values of CO_2 absorbed [15] vs simulated values obtained in this work (▲) and with the ASPEN PLUS ENRTL-RK template (○). Dotted lines represents the ± 10% prediction of experimental values and on the black the experimental and simulated desorbed CO_2 (kg/h) are equal.

values were incorporated in this work and are commented below.

4. Results

4.1. Desorbed CO_2, lean loading and temperature

Firstly, the standard ENRTL-RK ASPEN PLUS model available in ASPEN PLUS v8.6 was used to simulate the data from Tobiesen et al. [15]. The results are shown in Figs. 1 and 2. As seen in the figures, the model predicted the desorbed CO_2 well, with AARD of 8.7%. The lean loading was predicted with AARD of 6.0%. The model was modified by taking into account the packing characterization obtained experimentally in Zakeri [43] and simulations were performed to see if the experimental data representation was improved. The enhanced model showed AARD% of 6.9% and 1.9%, for desorbed CO_2 and lean loading, respectively. As seen in Fig. 1, most of the represented values were within the 10% of error with the current model while the base case had three additional points with higher error. Fig. 1 shows that the highest deviations were observed in the cases of high stripped CO_2, while at low stripped CO_2, below 6 kg/h, a good fit was observed. Fig. 2 shows a consistent prediction of the lean loading with AARD below 6%, with exception of one of the runs done with the standard ENRTL-RK ASPEN PLUS at low lean loading. The standard ENRTL-RK ASPEN PLUS model showed some under-prediction of the lean loading, what means that this model predicted a higher CO_2 absorption than the reality.

The developed model was used for the campaigns from Enaasen et al. [41], Pinto et al. [42] and Notz et al. [25]. The results from the

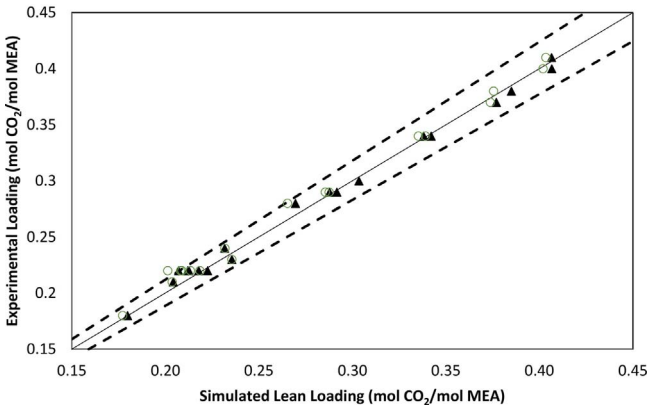

Fig. 2. Experimental values of Lean Loading [15] compared to simulated values obtained in this work (▲) and with the ASPEN PLUS ENRTL-RK template (○). Dotted lines represents the ± 6% prediction of experimental values and on the black line the experimental and simulated lean loadings (mol CO_2/mol MEA) are equal.

simulations with the model from this work are shown in Fig. 3 and 4 . Fig. 3 shows that the best fit with the new model was seen for loadings below 0.39 mol CO_2/mol MEA with an AARD% of 10%. The better prediction of the desorbed CO_2 automatically improved the prediction of lean loading because the CO_2 entering the stripper was taken from the experimental data and what is not desorbed leaves with the lean solvent. As seen in Fig. 3 and Table 3, for the campaign of Tobiesen et al. [15] and Pinto et al. [42], there was a good agreement at low loadings and under-prediction at high loadings. Tobiesen et al. [15] also simulated the desorption at a wide range of CO_2 loadings and temperatures of the rich solvent. Their in-house model was able to represent the CO_2 concentration and temperature along the stripper column. The in-house model was able to represent the CO_2 concentration and temperature along the stripper column. At low loadings (0.29–0.32 mol CO_2/mol MEA) the simulations showed good agreement in loading and temperature compared to experimental data, while under-predicted lean loadings were observed at medium (0.33–0.39 mol CO_2/mol MEA) and high loadings (0.4–0.46 mol CO_2/mol MEA).

However, the best agreements were observed at high loadings (0.4–0.45 mol CO_2/mol MEA) in the simulation of the campaign of Enaasen et al. [41], with exception of two runs, while some under-prediction was shown at low loadings. Moreover, the CO_2 stripped was over-predicted for the campaign of Notz et al. [25], at loading over 0.4 mol CO_2/mol MEA. The AARD for all the four pilot campaigns (in total 78 experimental runs) was 9.2% and 4.9% for stripped CO_2 and lean loading, respectively. This is a good result considering that, for example, the physical properties as Henrýs Law constant and diffusion for the CO_2 into the solutions are typically not measured at the stripper and reboiler temperatures but the behaviour is extrapolated [40,44].

In this work, it was found that there is no dependency of the prediction of the CO_2 desorbed on the temperature or flux of the rich solution in the cases of Pinto et al. [42], Enaasen et al. [41] and Tobiesen et al. [15]. However, the simulation model predicted the data of Notz et al. [25] better at rich flux temperatures above 115 °C, as seen in Fig. 3.

In addition to the desorbed CO_2, the temperature of the lean solvent leaving the desorber was checked with the experimental data and the results of each pilot plant campaign were analysed separately by values of AARD. Overall, the simulation model slightly over-predicted the reboiler temperature. The simulation results in Tobiesen et al. [15] showed some over-prediction of the lean temperature (3.29% of AARD). This general over-prediction could indicate that the heat losses were even higher than it was reported in the experimental data. However, at the same time the simulation model of Tobiesen et al. [15] under-predicted the temperature along the stripper, which could be attributed to the presence of two phases, gas-liquid, in the rich amine entering the stripper. In the current work, however, the over-prediction together with the under-predicted stripped CO_2 could indicate deviations on the desorption kinetics. Nevertheless, the simulated temperature results agreed well with the other pilots campaigns. In the case of the campaign from Pinto et al. [42], the temperature in the reboiler was slightly under-predicted (2.3% of AARD). Additionally, the experimental reboiler temperatures in Enaasen et al. [41] and Notz et al. [25] were well predicted. The AARD were 0.7 and 1.5% for Enaasen et al. [41] and Notz et al. [25] respectively, even though there were four experimental runs Notz et al. [25] that showed a greater deviation, up to 14% of AARD.

For further study, the temperature profile along the desorber was studied in this work and compared to the experimental data. Typical results are showed in Fig. 6, where data from Notz et al. [25] are represented. Overall, the temperature profiles were well predicted. The runs with the highest temperature deviations were the ones with the highest ratio between simulated and experimental values in Fig. 5 and Fig. 10.

In order to check the performance of the pilots, Fig. 7 shows the

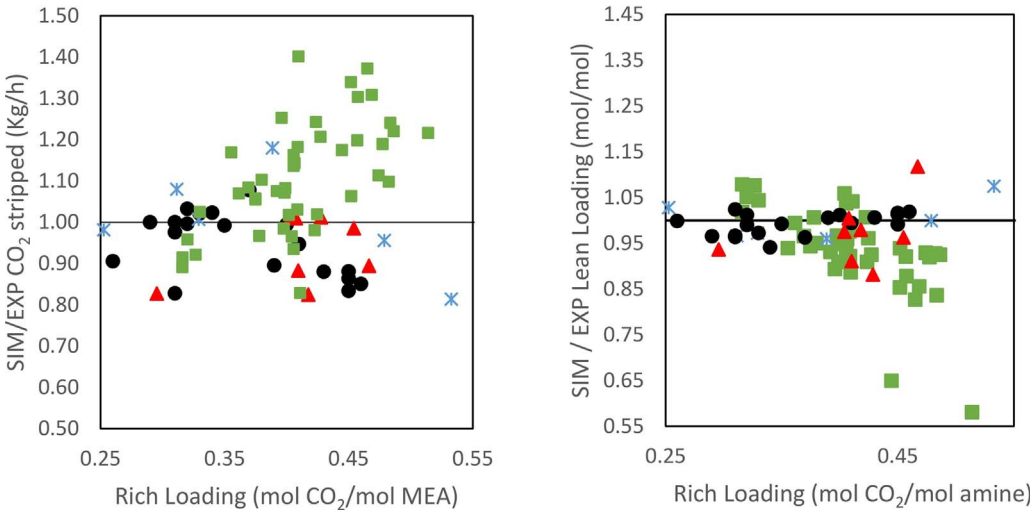

Fig. 3. (Left) Ratio Simulated/Experimental CO_2 stripped (Kg/h) vs Rich Loading (mol CO_2/mol MEA) and (Right) Ratio Simulated/Experimental Lean Loading (mol CO_2/mol MEA) vs Rich Loading (mol CO_2/mol MEA) from the campaigns: from Enaasen et al. [41] (▲)), Pinto et al. [42] (*),Tobiesen et al. [15] (●) and Notz et al. [25] (■). Line represent the case in which simulated and experimental values of CO_2 stripped are equal.

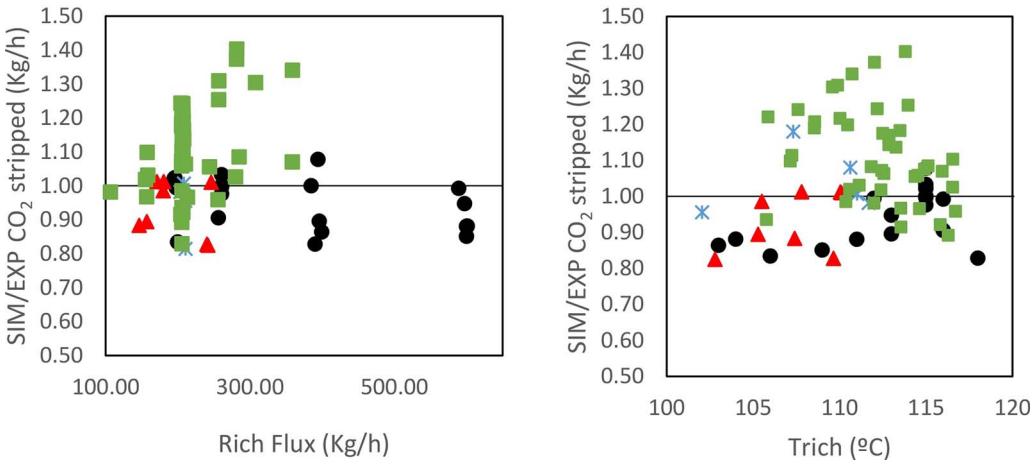

Fig. 4. Ratio Simulated/Experimental CO_2 stripped (Kg/h) vs Rich Flux (Kg/h) from the campaigns: from [18 et al. [41] (▲), Pinto et al. [42] (*), Tobiesen et al. [15] (●) and Notz et al. [25] (■). Line represent the case in which Simulated and Experimental values of CO_2 stripped are equal.

Table 3
AARD (%) of the simulation (from this work) compared to the experimental campaigns.

	AARD (%)							
	[15]		[42]		[41]		[25]	
Loading Range	Stripped CO_2 (Kg/h)	Lean Loading (mol/mol)	Stripped CO_2 (Kg/h)	Lean Loading (mol/mol)	Stripped CO_2 (Kg/h)	Lean Loading (mol/mol)	Stripped CO_2 (Kg/h)	Lean Loading (mol/mol)
0.25–0.32	4.7	2.2	4.9	3.1	17.2	6.3	7.8	5.6
0.33–0.4	4.0	2.5	9.4	3.4	–	–	11.8	5.6
0.41–0.55	12.4	1.2	11.5	3.8	6.4	5.9	18.9	12.0
Overall	6.9	1.9	8.6	3.4	7.7	5.9	13.9	8.2

experimental specific reboiler duty in all the campaigns as a function of rich loading. As expected, a linear trend was observed between the net reboiler duty and the CO_2 loading of the rich amine flux from 0.3 to 0.5. This similar trend between the four pilot campaigns strengthened the reliability of the experimental data. However, there were three runs from the campaign of Notz et al. [25], with rich loading approximately 0.3, 0.42 and 0.44, that were above this trend. These runs did not converge in the simulations and thus they are not shown in other figures. Additionally, three runs, one from Pinto et al. [42] (at loading 0.44 mol CO_2/mol MEA) and two from Notz et al. [25] at high loading (0.51 and 0.53 mol CO_2/mol MEA), were also out of the trend. The runs with rich loadings 0.51 and 0.53 mol CO_2/mol MEA from Notz et al. [25] showed the highest error in the loading on the lean amine (see Fig. 3). At low rich loading, 0.25-0.26 mol CO_2/mol MEA, the runs had a large scatter.

4.2. Effect of heat loss

As mentioned earlier, Enaasen et al. [41] and Pinto et al. [42] did not specify the heat loss along the column. Although the experiments were carried out in the same facilities used by Tobiesen et al. [15], the insulation of the pilot plant was improved over the years. To investigate the effect of heat losses, simulations were carried out with and without 0.5 KW of heat loss (Figs. 8 and 9). The deviations of both scenarios are shown in (Table 4) as AARD results of the loading in the lean amine, temperature of the lean amine and CO_2 stripped.

In this study, it was found that generally, the temperature profile of the desorber was over-predicted, with exception of two runs in Pinto et al. [42]. This over-prediction was also observed by Luo et al. [11]. Typical profiles from Pinto et al. [42] and Enaasen et al. [41] are included in Figs. 8 and 9. The temperature profile in Enaasen et al. [41]

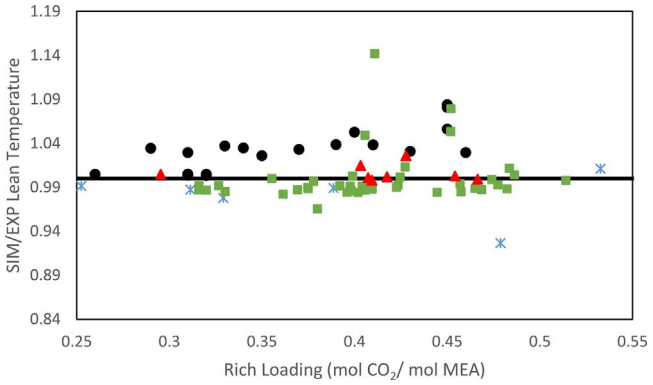

Fig. 5. Ratio Simulated (in this work)/Experimental values from the campaigns: from Enaasen et al. [41] (▲), Pinto et al. [42] (*), Notz et al. [25] (■), Tobiesen et al. [15] (●). Line represent the case in which Simulated and Experimental values of Lean Temperature are equal.

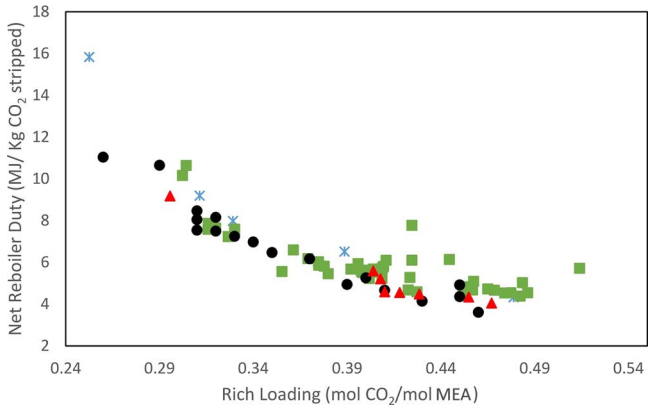

Fig. 7. Evolution of Net Reboiler Duty (MJ/kg stripped CO_2) with the CO_2 Loading in the Rich flux (mol CO_2/mol MEA) from [41] (▲); [42] (*); [15] (●); and [25] (■). Line represent the case in which simulated and experimental values of CO_2 stripped are equal.

improved with the addition of 0.5 KW of heat loss (Fig. 8). Additionally, the loading and temperature of the lean amine improved by 1.8 and 0.11% of AARD respectively. However, the CO_2 stripped had a 4.6% higher AARD than not considering heat loss. The temperature profile in Pinto et al. [42] improved for three runs (Fig. 9). The loading of the lean amine is also enhanced by 0.34% of AARD. However, the temperature of the lean amine and the CO_2 stripped had a higher AARD, 3.8 and 0.16% respectively, than the case without considering the heat loss. These results can be explained with Fig. 3, where an under-prediction in the lean amine loading is shown. Including 0.5 KW of heat loss decreased the desorption of CO_2 and the lean amine loading was higher, compensating this under-prediction observed in the scenario without heat loss (Table 4). However, the CO_2 stripped was also under-predicted and including the heat loss decreased the predicted amount of CO_2 stripped and increased this under-prediction. Regarding these results, the values presented in this work did not include heat loss in the campaigns of Pinto et al. [42] and Enaasen et al. [41]. Overall it can be said, that an estimation of heat loss should be reported together with the experimental values. The simulation results improve when heat loss is taken into account in Tobiesen et al. [15] whereas for Pinto [42] and Enaasen [41], estimating the same heat loss does not give an overall improvement of the simulation results as seen from Table 4. This indicates that the in well insulated pilots, the heat loss is not influencing the results.

Notz et al. [25] indicated the heat losses in each run varying from −0.247 (adding heat from outside instead of losing it) to 1.05 KW. The heat loss was assumed to be heavily dependent on the running conditions. To see if this large variation in heat loss correlated with model predictions, the simulated temperature of the lean amine was plotted as a function of heat loss in Fig. 10. The figure showed that, overall, there was no correlation between the reboiler temperature and heat loss. However, four runs showed strongest deviation. The error of the simulated lean loading showed some dependency on the heat loss and increased as the heat losses increased. At heat losses between 0.6 and 1 KW, the simulated loading on the lean amine agreed with the experimental values. This could indicate that the heat loss is less dependent on the experimental conditions than what Notz et al. [25] reported.

5. Conclusions

In this work the performance of the ASPEN PLUS software to represent experimental pilot data from four different pilots using 30 wt% MEA was tested. In total 78 experimental runs were simulated. The desorbers in the different campaigns varied in the diameters, structured packing heights and packing types. The adjustments done to the existing ASPEN model were tocharacterize the packing, based on experimental data measured with 30 wt% MEA, modify the flow model and refine the film discretization. The simulation model is able to predict the experimental stripped CO_2 from 4 different campaigns with AARD% of 9.2%. The loading and temperature of the lean amine solution were predicted with an AARD of 4.9 and 3.3% respectively. The deviation of the model has shown some dependency on the loading of the rich solution, while this does not depend on the temperature or flux of the rich solution. Based on the simulations, it would be important to have an estimation of the experimental heat loss for each campaign. The results further indicate that the heat loss is not very dependent on the flow rates and reboiler duties used, but dependent on the pilot and the level of insulation. Since the same model without any fitting was used to simulate experimental runs from four different campaigns it is

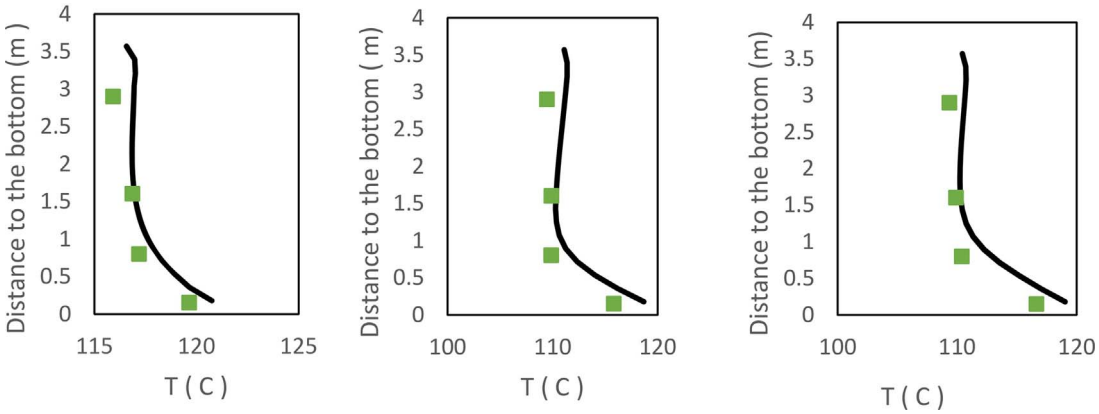

Fig. 6. Runs 3, 13 and 23 from Notz et al. [25]: Experimental results from Notz et al. [25](■); results from this work (−).

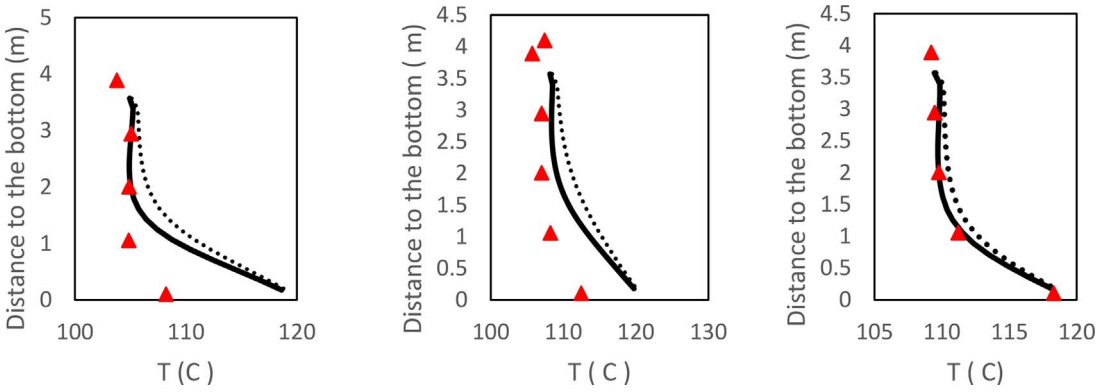

Fig. 8. Runs 2,4 and 5 from Enaasen et al. [41]: Experimental results from Enaasen et al. [41](▲); results from this work without heat loss(▪▪▪) and incorporating heat loss (−).

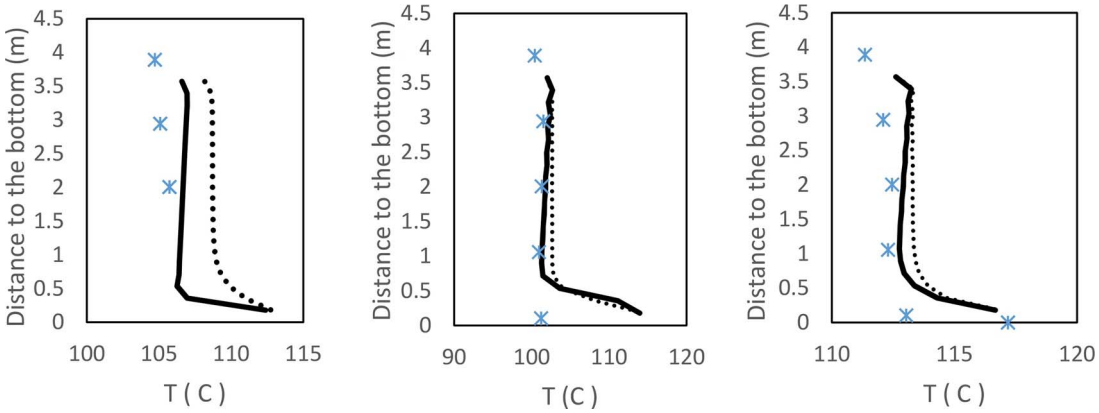

Fig. 9. Runs 1,2 and 7 from Pinto et al. [42]: Experimental results from Pinto et al. [42](*); results from this work without teat loss(▪▪▪) and incorporating heat loss (−).

Table 4
Simulation results of incorporating heat losses (0.5 KW) in Pinto et al. [42] and Enaasen et al. [41] compared with simulations without heat losses.

	AARD (%)			
	Without Heat loss		With heat loss (0.5 KW)	
	[42]	[41]	[42]	[41]
Lean Loading	3.4	5.9	3.0	4.1
Lean Temperature	2.3	0.8	6.2	0.6
CO_2 stripped	11.9	7.7	12.0	12.3

clear that the different pilot campaigns agreed with each other. Finally, the work demonstrates that the ASPEN PLUS simulation tool can be used to simulate the regeneration of CO_2 in the capture process based on 30 wt% MEA if the parameters for the Stilmchair correlation for the solvent used are defined.

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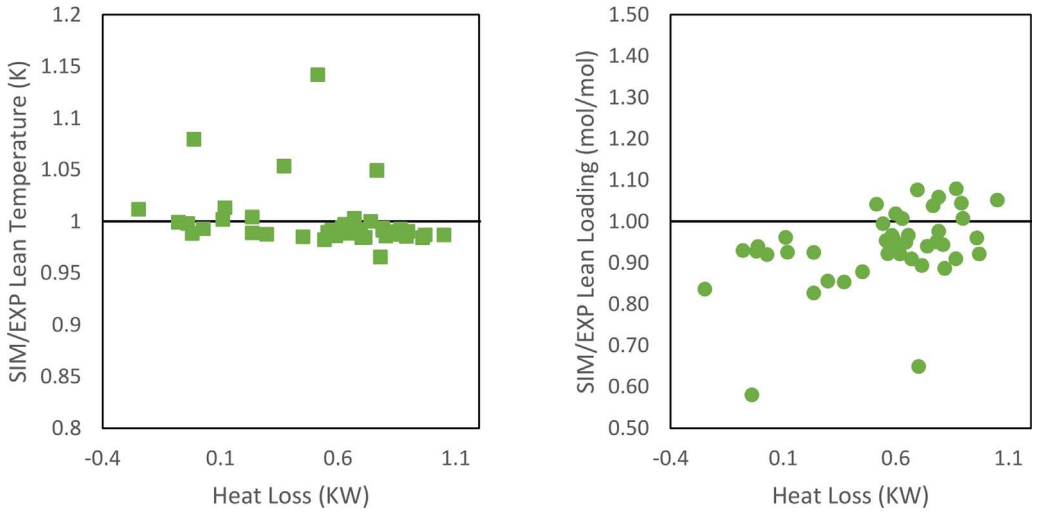

Fig. 10. Evolution of the Ratio SIM/EXP Lean temperature (left) and lean loading (right) with the heat loss reported in Notz et al. [25].

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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