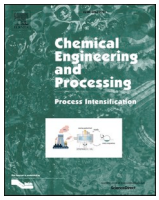
Chemical Engineering & Processing: Process Intensification 194 (2023) 109588

Contents lists available at ScienceDirect

Chemical Engineering and Processing - Process Intensification

journal homepage: www.elsevier.com/locate/cep



Model validation and simulation issues for carbon dioxide reactive absorption with mixed amines

Antonio Tripodi, Renato La Pietra, Matteo Tommasi, Ilenia Rossetti *

Chemical Plants and Industrial Chemistry Group, Dip. Chimica, Università degli Studi di Milano, CNR-SCITEC and INSTM Unit Milano-Università, via C. Golgi 19, 20133, Milano, Italy

A R T I C L E I N F O

Keywords:
CO_2 capture
Absorption
Stripping
Mixed amine solvent
Absorption-desorption modeling

A B S T R A C T

Capture of CO_2 form point emission sources is a dramatically urgent task to limit the current impact of the power generation sector and of industrial fields classified as "hard to abate". Many challenges are still present from the design point of view to define correctly the properties (chemical, physical, rheological) of the used solvents. These affect the sizing and rating of absorption devices and the regeneration systems. In turn, this jeopardises the prediction of feasibility of capture plants and the relative economics.

In this work, the modeling steps commonly applied to calculate the CO_2 absorption into a mixed amine-water solvent have been exemplified starting from ground data. First, several open datasets of equilibrium and rheological quantities have been reviewed. This allowed the selection of the thermodynamic parameters that give the best compromise between physical and chemical equilibria. Then an adsorption tower was dimensioned, checking the impact that different tunable parameters have on the calculation outcome. Furthermore, two absorber-stripper tandem columns have been simulated in order to reproduce available plant data. The performed rate-based simulations find a convergence point only for proper liquid/gas ratios, and are significantly slowed-down as the number of kinetic reactions increases respect to instantaneous equilibrium ones.

Results demonstrate that the CO_2 loading into a solvent depends crucially on the partial pressures of all the species and on setting the mixture at fixed volume or pressure. This data collection and validation was exemplified following the whole procedure, as a guidance for technicians in the field. An example of gas flowrate up to 160 kg/h, with CO_2 content 15 – 20 vol% and for CO_2 capture efficiencies up to 90%.

1. Introduction

Post-combustion absorption with regenerated basic solvents is still the leading technology to decrease CO_2 emissions from combustion gasses on large scales [1]. Its main advantages are the capability of treating large flows, even at moderate pressures, though the solvent regeneration is energy intensive. Chemical absorption is generally more efficient than physisorption, leading to smaller towers and regeneration duties, but this aspect depends crucially on the choice of the reactant selected for CO_2 capture. Data from bench scale and full size plants are then continuously made available for different amines (the preferred weak bases for this application) [2–4].

As other mature technologies used in large-size plants (i.e. oil refining, gas-compression), also carbon absorption is provided as a default package in most commercial simulation suites [5–10], both for design and rating purposes. Nonetheless, following the ongoing research on new solvents, thermodynamic models need to be implemented and benchmarked [11–13]. The use of different amine solutions for this application has been recently reviewed [14] and experimental laboratory data on the absorption and VLE data for mixed basic solvents are available in the literature [15,16].

This work comprises a review on data and the corresponding simulation of the CO_2 capture with the "CESAR1–2″ [17] solvent, a mixture of 2-Amino-2-Methyl-1-propanol (AMP) and Piperazine (PZ) in water that is a good compromise between equilibrium loading and fast absorption kinetics [18]. Among the latest works available on this mixture [18–29], a selection has been made, privileging those already oriented as a basis for process modeling [30,31].

Some issues are specifically considered to try to fill the gaps in the current knowledge:

* Corresponding author.
E-mail address: ilenia.rossetti@unimi.it (I. Rossetti).

https://doi.org/10.1016/j.cep.2023.109588
Received 20 August 2023; Received in revised form 6 October 2023; Accepted 23 October 2023
Available online 28 October 2023

a) Insufficient plant tests are available in the open literature for CESAR solvent [32–35], and some simulation studies are not systematically benchmarked against field data [36,37].
b) Thermodynamic models and parameters for the mixture have not been univocally chosen and validated. This makes any calculation too much dependent on the selected references [4].
c) The process simulations have many degrees of freedom, often fixed with arbitrary choices, without a systematic evaluation of the impact of each parameter (see for example the very interesting work of Zhang et al. [38]).

To screen the impact of simulation parameters on a test-absorber, an approach similar to that of Afkhamipour and Mofarahi [39] was followed.

Review, revision and summary of the properties and data of a mixed amine solvent for CO_2 capture has been carried out in the present work. Starting from the verification of the VLE of the pure components and the speciation predicted by the default parameters implemented in Aspen Plus, correction were made. Specifically, a revision was needed for the Antoine parameters of PZ and the formation enthalpy and Gibbs free energy. The vapor liquid equilibria for the binary and ternary systems has bee also verified, together with the assessment of the differences between equilibria when pure CO_2 or gas mixtures are used over a wide pressure range.

The absorber-regenerator complete system has been simulated and benchmarked against the well reported pilot-plant data of Mangalapally et al. [40,41] and Artanto et al. [32,33,42]. This activity constitutes the basis for further full-scale plant simulations and economic evaluations. We selected a specific solvent because it represents a good benchmark and compromise between kinetics and thermodynamic considerations. However, besides this very specific choice, the overall approach and criticalities described in this paper can be adopted to treat and interpret the data for other solvent mixtures.

2. Methods

Beside the thermodynamic data for the quaternary mixture AMP-PZ-CO_2–H_2O already introduced, works on the ternary systems (without one of the two amines) were reviewed. This allowed to fill some gaps and to ascertain the coherence of some quantities. The calculations were made using Aspen Plus v10 and v11 (Aspen Technology, Inc., Bedford, MA, USA).

The operating methodology was as follows:

a) Check of the AMP-Water and PZ-Water binary Vapor Liquid Equilibria (VLE).
b) Addition of CO_2 (treated with Henry constant) and of the relative equilibrium reactions: together with the VLEs of point a), this determines the overall loading.
c) Check of AMP and PZ speciation according to literature data. Notice that we did not adjust the electrolyte parameters aiming only for a good loading fit. Some investigations only adjust fitting without considering the effect on speciation [19,22,25]. Joint analysis of the amines loading and speciation are available for AMP [43] and PZ [44], but data for their blend are not available, at least to our best knowledge. In particular reference [44] determines the speciation for PZ based on NMR experiments on different mixtures. On the contrary, an extensive revision of many literature data for the AMP solvent is retrievable in reference [43], divided by experimental method, e.g. VLE under different measurement conditions (isothermal or isobaric), Solid Liquid Equilibria or calorimetry. The original references there reported can be used to retrieve the experimental methods through which the speciation was investigated, typically by NMR, refractive index and titration.
d) If the tests in points a)-c) did not yield binary VLEs, CO_2 loading and amine speciation in accordance with the available data, the electrolytes interaction parameters from the Aspen databases were tentatively substituted with different ones found in the literature [25].
e) A further adjustment of CO_2 Henry parameters was made when needed: this influenced, at fixed loading, the PZ partial pressure in the vapor, which was actually fairly dispersed in the reviewed datasets ([45] and references therein), leaving this issue still open to further investigations.
f) If modifications in points d) and e) were not sufficient, also the formation energies of some species were *slightly* modified to shift the equilibrium constants. The modification was done adjusting the parameters until checks a)-c) were satisfactory. Properties environment on ASPEN Plus and the calculation mode of the equilibrium constants was selected. After different trials with different sets of equilibrium constants found in literature [25], the most correct description was assessed by letting the software compute the equilibrium constants from the standard Gibbs free energy variation [46]. In particular, the parameters DGFORM and DHFORM for PZ, H_2O and CO_2 were obtained by Hilliard work [19] while those for AMP were obtained by ASPEN Plus data bank.
g) Finally, the mixture density and viscosity were fixed.

3. - Thermodynamic properties review

3.1. Amines loading

There are two ways to calculate the loading with common computer tools, one close to lab experiments (pure CO_2 in the vapor phase), one closer to real process conditions (CO_2 into a N_2-rich stream), and the simulation results were appreciably different. In any case, many experimental works did not specify how a certain partial pressure of CO_2 was achieved. Indeed, if an inert was present, the high pressure zone of the calculation was affected. In the low-pressure part, the VLE equilibrium of PZ interferes, so the CO_2 loading was not independent from the amine vapor fraction. Moreover, in Aspen Plus the saturation condition of a mixture is calculated imposing a vapor fraction of 0, but this condition is never actually achieved in lab experiments. Significant values of vapor fractions ranging from 0.1 to 1% (vol/vol) leave the mass balances virtually unaffected but play a role in the high-pressure part of the diagram. Figure S1 and Table S1 let understand the role that the calculation constraints have on the loading. Commonly adopted process conditions foresee a CO_2 partial pressure lower than 20 kPa, but in presence of N_2 (a condition not encountered in any of the reviewed laboratory tests). This may significantly change the predicted loading in the solvent when basing the simulation on laboratory data not strictly reproducing process conditions.

Other data for the loading into the single amines can be found in the papers by Hartono et al. [43], Pahlavanzadeh et al. [47] and Hu et al. [48] for AMP or by Bishnoi et al. [49] for PZ.

3.2. Speciation

Another important feature that may bring to unreliable predictions is the reactive behavior of the solvent and most of all its relative modeling. Speciation is strongly affected by formation energies and saturation pressures, which determines the overall carbon content of the liquid, It is not much affected by interaction parameters. Many processes or experimental papers aim at reproducing the loading into the mixed solvent [23,25,37], but do not account for speciation details in relation to available data. The latter, in turn, are treated most often referring to the behavior of the pure amines. Also the speciation has a role on the loading, so that the CO_2 solvation in the mixture and the speciation of both amines should be reviewed at the same time, not separately, as instead is most commonly done in the literature.

In relation to AMP (Fig. 1), the reproduced data are from Hartono [26,43], while those for PZ (Fig. 2) are from Ermatchkov et al. [44].

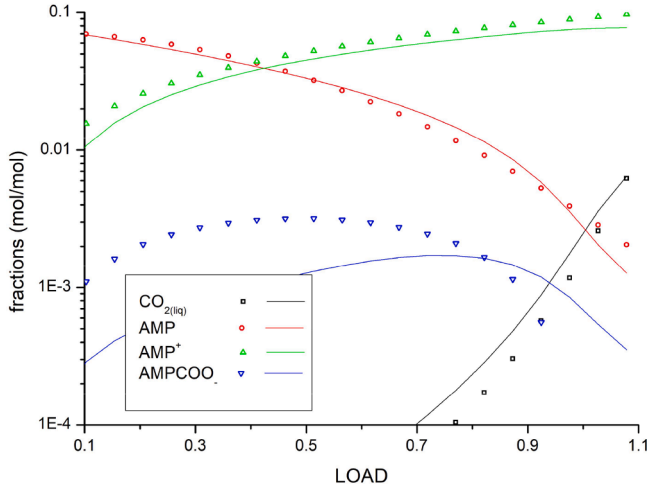


Fig. 1. Distribution of the AMP moles between the AMP and $AMPH^+$ forms, and concentration of the CO_2 / HCO_3^- species in a solution of AMP in water (8% mol). Data from [26,43].

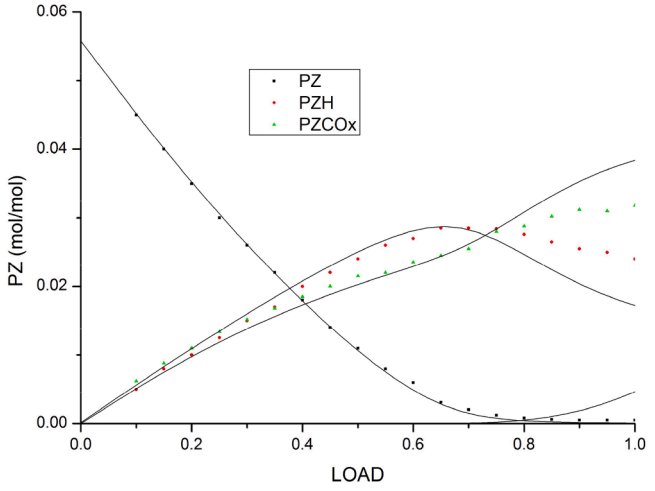


Fig. 2. Main species for Piperazine in water vs. CO_2 loading (original solution: PZ 1 M). Data from [44].

The corrections implemented in the ΔG and ΔH of formation are reported in Table S2.

3.3. Vapor liquid equilibrium

Partial pressure of PZ in water is differently accounted for in the literature [19,21,25,26,50,51]. This point is crucial, because it has a non-negligible impact on the linked CO_2—HCO_x equilibria at low CO_2 partial pressures.

A list of reviewed Antoine-equation parameters is in Table S3 and in Table 1. The Henry constant for the CO_2 in water is expressed as: $\ln\left(\frac{P}{Pa}\right) = A + \frac{B}{C+T} + DT + ElnT + FT^G$.

The following graphs (Figs. 3-5) represent: a) the VLE of PZ-H_2O (saturation @ 333 K), b) the CO_2 loading in the mixed solvent (saturation @ 328 K), and c) in the PZ only (saturation @ 328 K), using the parameters of set 1 and 3 respectively and other conditions as specified. It has to be noted that the regression of the electrolyte parameters can alter the species distribution, but not the maximum loading achieved before free CO_2 is solvated. On the other hand, fixing the PZ-H_2O VLE and the CO_2-PZ loading at the same time, requires the adjustment of the CO_2—H_2O Henry constant. The latter then becomes specific for the ternary mixture (rather than independent) and, moreover, jeopardizes the CO_2 loading into AMP-water solutions. Since this latter calculation did not show any issue and it was in accordance with the reviewed literature, the CO_2-water solubility was not modified.

This may be a conceptual issue, since Antoine and Henry parameters have been validated in the literature and their possible adjustment (whenever needed) may be criticized. Different approaches, which download the non-ideality definition in new models such as e-NRTL, e-UNIQUAC or related approaches have been proposed over the years and are equally valid. The key point remains the dependence on the specific mixture and speciation of the electrolyte definition. This, in practical terms, often ends in missing convergence of the calculation algorithms. Overall, the correction of Henry's constant responds, when needed, to the same concept, i.e. the adaptation of the simulation parameters to the specific solubility conditions determined by the solvent mixture in use. The mathematical form of the equation however leads to negligible computational problems in the case of Henry's constant adjustment instead of the e-NRTL approach. For this reason we have followed this pathway when necessary.

In the CO_2 gas-liquid absorption processes, the washing column deals with the full chemical system, while the stripper condenser treats

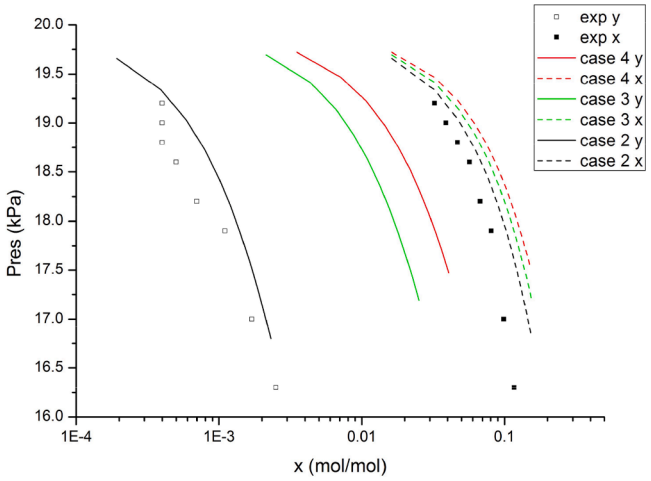


Fig. 3. P-xy diagram for the PZ-water system. Calculations according to constraints of Table 1, data from [26].

Table 1
Thermodynamic constraints for the PZ-water VLE, the PZ-water-CO_2 loading and CO_2-PZ-water-AMP loading of Figs. 3-5.

Case	T	Vapor Fraction	P	Water	PZ	Antoine-equation coefficients for Piperazine			
	(K)	mol/mol	kPa	mol/mol		A	B	E	F
Base	328	0	Sat	0.944	0.056	Taken from Aspen Plus database			
1	333	0	Sat	0.965	0.035	71.0	−7914.5	−6.646	5.2
2	328–333	0	Sat	–	–	77.0	−10,894	−6.646	5.21
3	328–333	0	Sat	–	–	70.5	−7914.5	−6.646	5.21
4	328–333	0	Sat	–	–	71.0	−7914.5	−6.646	5.2
5	333	0	Sat	0.965	0.035	71.0	−7914.5	−6.646	5.2

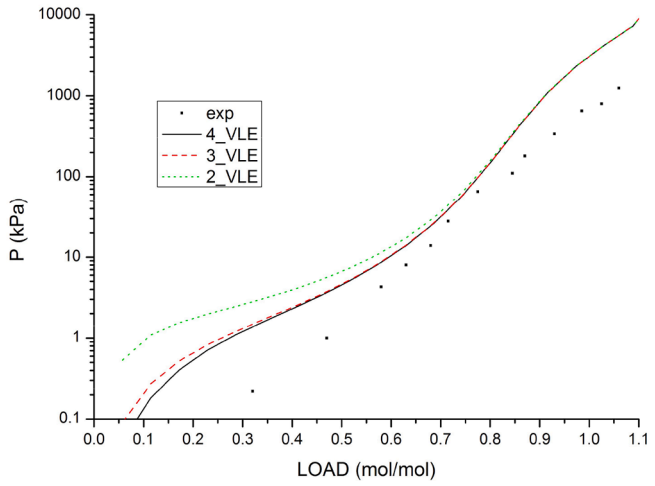


Fig. 4. P-LOAD diagram for the AMP-PZ-CO_2-water system. Calculations constraints in Table 1, data from [25].

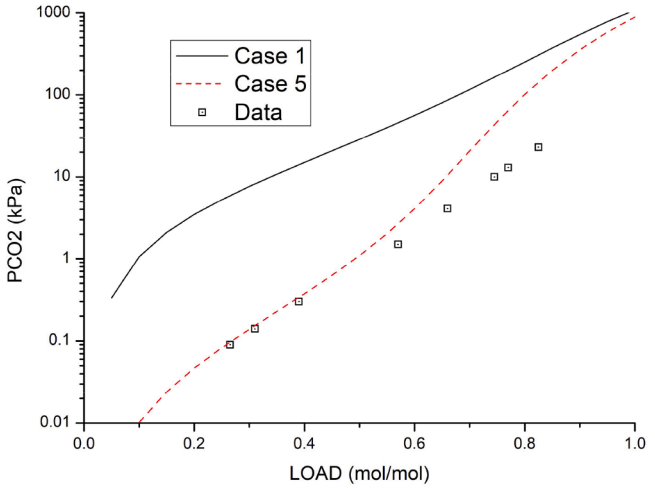


Fig. 5. P-LOAD diagram for the PZ-CO_2-water system. Calculations constraints in Table 1, data from [45].

essentially a binary CO_2—H_2O mixture. Therefore, separate thermodynamic systems should be validated and loaded in the whole process simulation. Moreover, the stripper still deals with the amines in its bottoms. So its condenser and top stages should be detached and the columns split into two blocks, to which different thermodynamic packages were assigned. This would result in a too complex and involved simulation framework.

The check of the AMP-H_2O VLE did not show any issue and we found all the reviewed works plus the Aspen templates in accordance between each other.

3.4. Density

When rate-based rigorous calculations are involved, rheological properties become as important as equilibrium concentrations, because they determine the interphase transfer coefficients. Beside this aspect, density is of primary importance because it determines the hydraulic design of a column even in equilibrium calculations.

Fig. 6 reports the good correlation between the Aspen Plus default calculation (Rackett model for liquid mixture molar volume) and the experimental data [25,28,29] for a heavy loaded amine solution.

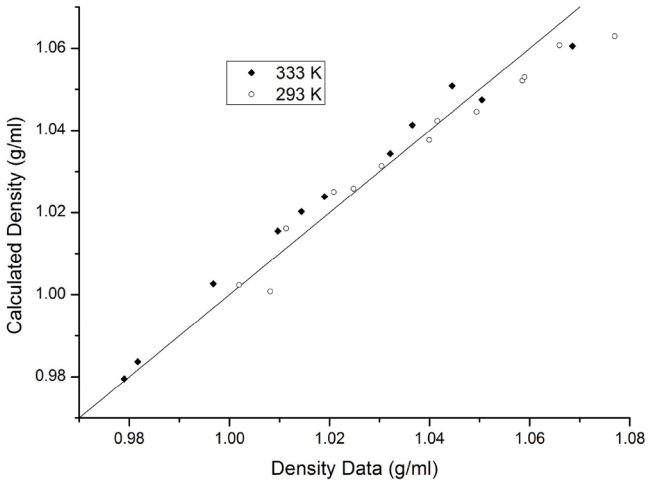


Fig. 6. Calculated and experimental densities at different temperatures for a mixture of Water, AMP and PZ.

3.5. Viscosity

Though literature reports are available [29], to the authors best knowledge, a systematic test for this parameter description has not been made yet. Viscosity deeply influences the estimate of all the transport parameters, therefore accurate predictions are needed. Aspen basic parameters (Andrade liquid mixture viscosity model implemented in the NRTL package) yielded a poor fit, so an adjustment was needed, as reported synthetically in Fig. 7. The refitted data here below were used.

3.6. Reaction parameters

The equilibrium constants used in this work are calculated from the Δ_fG^0 and Δ_fH^0 of the involved species, which were adjusted in order to satisfy at the same time the AMP, PZ and CO_2 speciation.

PZ has two basic sites whose equilibrium constants for CO_2 absorption in aqueous solution are reported e.g. in [49]. Such data suggest that the equilibrium constant for the formation of the mono-carbamate species is one order of magnitude higher than the one for the formation of the di-carbamate, that should be therefore considered as a minor component.

The kinetic and equilibrium constants for the listed reactions are variously reported in the literature [52–57]. According to the model of

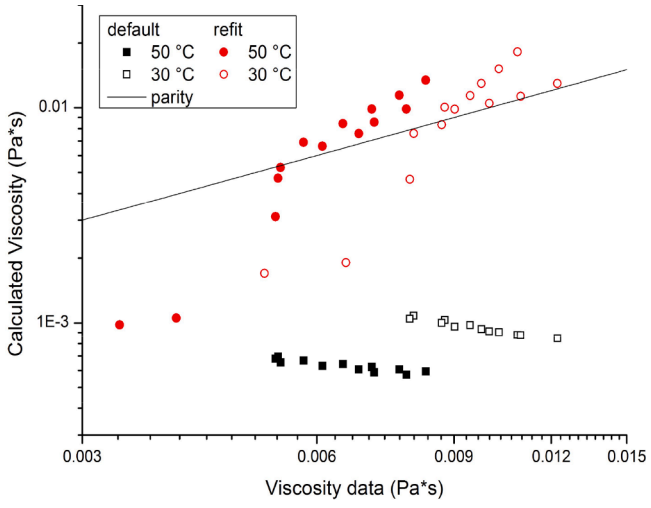


Fig. 7. Calculated and experimental viscosities for a mixture of Water, AMP and PZ.

Dash et al. [19], the AMP carbamation [43] need not to be modeled, so this simulation uses reactions from Table S4 and Table S5 with data elaborated from [20] and [49].

3.7. Methyl-Ethanol-Amine model

The thermodynamic properties for a benchmark MEA-absorption simulation were loaded directly from the Aspen Plus template, which is built upon a consolidated literature body (see [58] and the list of references therein) and validated against plant data [59]. This reference case has been used for comparison purposes.

4. - Absorber model validation

This simulation takes as a reference the works of Mangalapally et al. [34,40,59,60]. Generally, the stage number and vapor mass-transfer coefficient (MTC) showed to be determinant. Nevertheless, an open-circuit absorber behaves very differently from a closed-circuit one. The issue may be due to the transfer of water and PZ between the phases. This is suggested by the fact that, with an already partially carbonated lean solvent, the absorber performance is not decreased and can satisfactory reproduce the data even without increasing the MTC.

Table 2 summarises the chosen packing, Mellapack 125Y, and operating parameters. Tables 3 to 5 compare different simulation cases. In particular Table 3 considers an equilibrium simulation of the absorber, not considering the kinetics of reactions, at variable L/G ratios or number of stages. 100% CO_2 removal rate is always predicted except at low L/G proportion. The number of stages was less determinant as shown by case *d* in Table 3.

Table 4 reports rate-based simulations with variable mass transfer coefficients, area and number of stages. All these parameters were affecting the CO_2 removal rate.

Table 5 includes also the reaction kinetics in the rate based model of the absorber. Different cases are reported manipulating the mass transfer coefficient, the area correction factor and the number of stages, resulting in widely different CO_2 removal rate.

The rate-based simulation required additional parameters to be fixed. For instance, the film and fluid discretization ratio are the ratio of the thickness of the adjacent discretization regions, where rate calculations are performed. The area correction factor is instead a corrective parameter that is multiplied by the value of the simple interfacial area. The removal rate increased as reasonable when increasing the number of stages, the interfacial area and mass transfer coefficient.

The first evident conclusion is that equilibrium calculations, with limited discretization of the absorber column, return in almost every case full CO_2 capture and the same is achieved when considering rate-based systems without kinetic equations (Tables 3 and 4). By contrast, removal rates between 77.9 and 89.3% are predicted when implementing the kinetics of reaction, which demonstrates fundamental for reliable performance predictions.

The model is able to capture the temperature profile (Fig. 8), while the CO_2 fractional capture trend is not uniformly correlated all over the column profile (Fig. 9).

Table 2
General reference data for the absorber validation.

Unit - packing	Height (m)	Diameter (m)	L/G (kg/kg)	removal ratio (vs. feed)	CO_2 in (m^3/m^3)	amines load (kg/kg)
absorber – Mellapak 125Y	4.25	.140	2.9	–	15% vol	30% wt
Washing section – Mellapak 125Y	0.42	.125	–	88%	–	–

Table 3
Equilibrium simulation, without kinetic reactions and with Mellapak 125Y packing.

Case	L/G	Calc. stages	Vapor Mass Transfer	Area correction	Removal rate
a	3	10 + 5	1	.5	100%
b	1	7 + 5	1	.5	90.8%
c	3	10 + 10	1	.5	100%
d	3	4 + 5	1	.5	100%

Table 4
Simulation rate-based, without kinetic reactions and Mellapak 125Y packing.

Case	L/G	Calc. stages	Vapor Mass Transfer	Area	Removal rate
a	3	10 + 5	1	1	97.7%
b	3	10 + 5	.72	0.7	90.1%
c	3	20 + 10	1	1	100%

5. System simulations

For the complete absorber-stripper systems, three solvents and process conditions were simulated:

A CESAR solvent ([60] and other references as for the absorber validation);
B MEA solvent as benchmark [32,42];
C CESAR solvent (different data) [33,42,61].

The plant layouts were slightly different, and reported in Figs. 10 and 11.

We obtained simulations results in line with the data reported in the cited references for each system. In particular, Table 6 reports CO_2 capture efficiency, reboiler duties, L/G ratio and solvent composition. The corresponding absorber and stripper specifications are detailed in Tables 7 and 8.

According to the three cases, the simulation results are exemplified in Figs. 12-15, which detail the flow patterns and the temperature profiles through the absorber and the stripper. Accordingly, Tables 9–11 report the composition of the material streams (refer to the pertinent flowsheet for each case, as indicated in each caption). The comparison with the reported literature data for both the mixed solvent and the MEA reference case is satisfactory.

However, the column calculation is considered “accomplished” if the mass out-balance is within 0.001, the charge unbalance within 0.001 and the hydraulic plot is consistent with low pressure drops. The stripper is not going to “converge” in a computational sense unless the stages are reduced.

Sizing of the absorber as standalone needed at least 100 stages, otherwise the MTC correction became too large.

When considering close-circuit sizing the stripper convergence was troublesome. This is because water must be present in the bottoms, to solvate the electrolytes, and in the distillate to carry the CO_2 in equilibrium with the needed vapor flow. This requirement imposes a double bound on the VLE and electrolyte balance, that is directly linked with the reflux ratio (which, in turn, determines the column hydraulics). Apart from this intrinsic difficulty, the result is a rigid CO_2 residue in the lean solvent, which is not accounted for in the reviewed literature but is CRUCIAL for the absorber. Most likely, this is due to the fact that the driving force for CO_2 absorption and speciation is reduced at every stage, so the calculation is already nearer to the reaction equilibrium condition (provided there is enough amine) and the kinetic aspect less important. Also, the temperature bulge is less pronounced and so the equilibrium more favorable in any stage.

Table 5
Simulation rate-based, with kinetic reactions and Mellapak 125Y packing. Case i: $F = 1.99$ Pa$^{0.5}$.

Case	L/G	Calc. stages	Vapor Mass Transfer	Fluid Discretization	Film Discretization	Area correction	Removal rate
A	3	10 + 5	1	2	5	1	77.9%
B	3	10 + 5	1.1	2	5	1	78.6%
C	3	20 + 10	1	2	5	1	79.8%
D	3	20 + 10	1.2	2	5	1	80.4%
E	3	40 + 20	1	2	5	1	79.8%
F	3	40 + 20	1.3	2	5	1	81.6%
G	3	40 + 20	2.2	4	10	1	88.8%
H	3	40 + 20	2.5	4	15	1	89.3%
I	3	80 + 40	1.5	2	5	1.2	88.1%

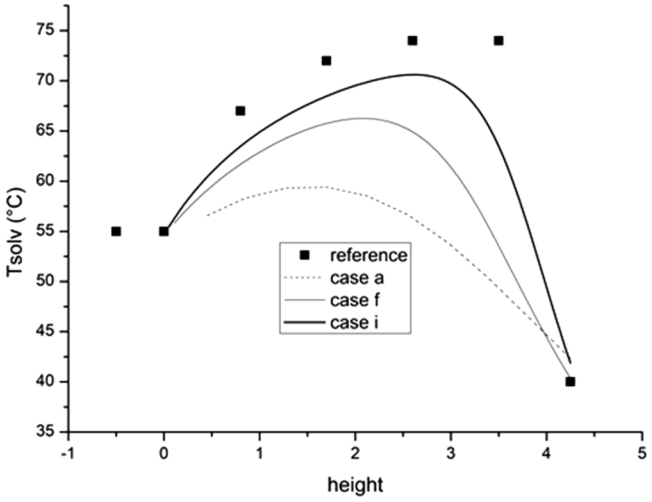


Fig. 8. Absorber temperature according to the different validation cases (Table 5).

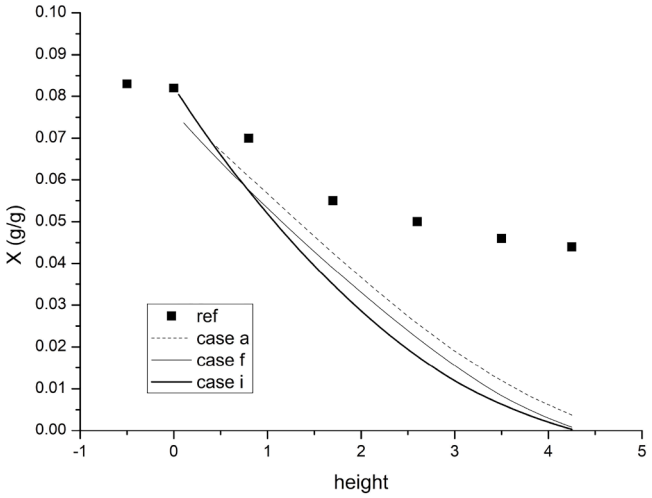


Fig. 9. Fractional carbon capture along the absorber height in several cases (Table 5).

As a comparison with previously published data, Afkhamipour and Mofarahi considered a rate-base simulated packed column for CO_2 capture with MEA [39]. The authors compared equilibrium and rate-based results and provided parameters for mass transfer. Experimental CO_2 removals between 52 and 100% were achieved under variable gas and liquid flow rates and different packings and the fit of available experimental data was satisfactory. Mixed amine solutions were instead tested by Artanto et al. [32], who tested MEA and AMP and their mixtures experimentally. Besides providing data on the effect of

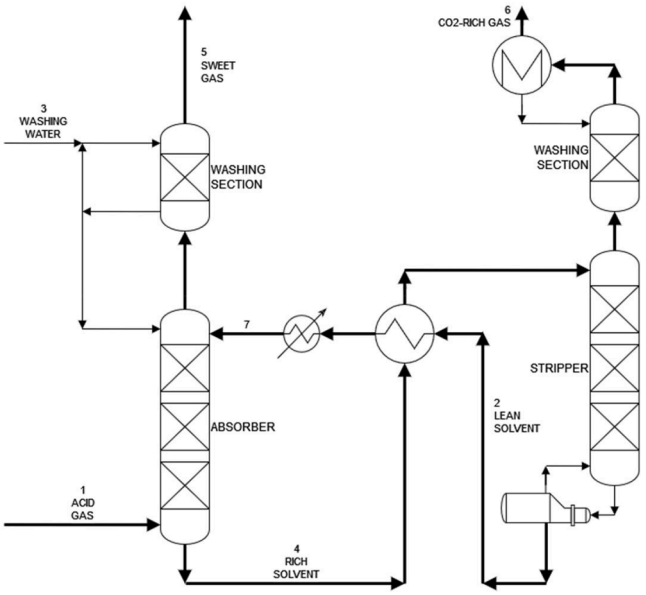


Fig. 10. Process scheme for case A.

L/G and loading on the CO_2 recovery, interesting data on the heat duties of the different components were presented. As for modeling studies, van der Spek et al. [30] developed a process simulation model for post-combustion CO_2 capture with AMP/PZ mixture. This includes the regression of AMP–PZ binary interaction parameters. The rheological properties of the mixture were not modified, which has an impact of the estimation of the transport properties. The techno-economic performance of AMP/PZ was also considered [62,63], but not including in the process simulation reaction kinetics and mass transfer limitations, as well as thermodynamic interactions between AMP and PZ [30]. Therefore, the present work can add further refinement to the existing literature on mixed amine solvents.

6. Conclusions

The analysis performed in this work once more show how the CO_2 absorption depends on the careful definition of VLE conditions, for any component of both the liquid and gas phases. This is particularly critical when mixed solvents are used. In such cases, a careful definition of properties is often not available and not always reliably reconstructed from data of single solvents. Furthermore, it is underlined that when laboratory experimental conditions are not fully specified, the data-calculation comparison is not trivial, and some arbitrary choices must be made with significant impact on the results. This is particularly evident considering fixed-volume systems compared to fixed-pressure ones. Many thermodynamic parameters are then evaluated or regressed in conditions different from the ones of the industrial process, yet this is an issue seldom considered when simulation programs are

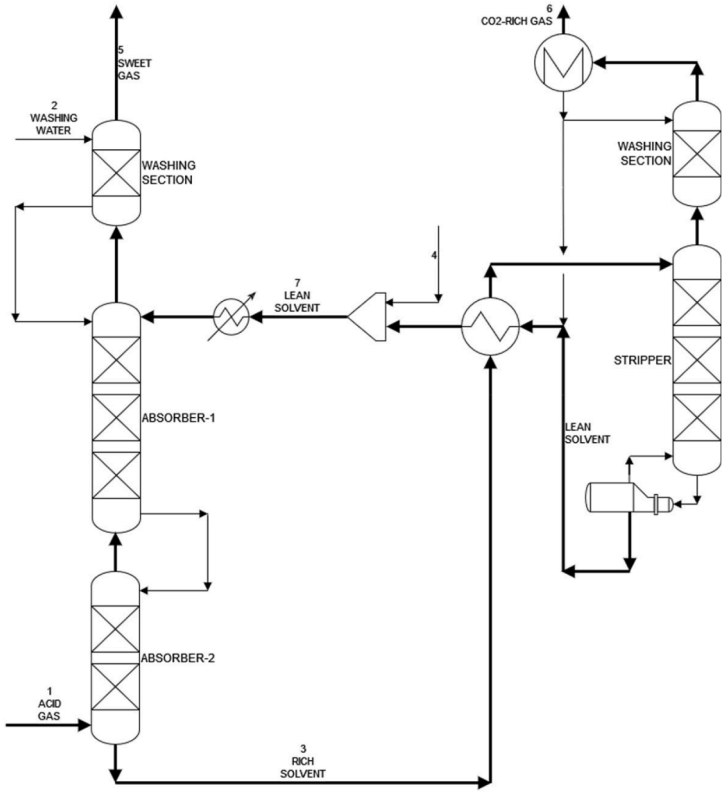


Fig. 11. Process scheme for cases B-C.

Table 6
General outputs for the process simulations; (*) feed preconditioned at 100 °C.

Case	Solvent	Total gas flow	CO_{2in}	CO_{2out}	L/G	Load	Reboiler duty
	(wt.%)	(kg/h)			(kg/kg)	(kg/kg)	(kW)
A	AMP-PZ (28–17%)	80	12.0	1.28 – 1.24	3.16	0.015 – 0.11	43.1*
B	MEA (33%)	75	12.7	1.66 – 0.21	3.20	0.13 – 0.24	120
C	AMP-PZ (22–8%)	156	24.1	3.16 – 3.16	2.56	0.13 – 0.30	121

Table 7
Absorber specifications.

Case	Stages / height / diameter (m)	Packing	MTC-area correction
A	80 / 4.25 / 0.140	Mellapak 125Y	1.0 – 1.0
B	80 / 3.7 / 0.21 80 / 3.7 / 0.21	PALL X2	1.0 – 1.0
C	70 / 5.4 + 1.35 / 0.2	PALL X2	1.0 – 1.0

used.

For amines and carbonates speciation, it has been found heuristically that adjusting the formation energies is a more straightforward method, to obtain a general agreement, than to fix the reaction constants. This is due to the fact that multiple equilibrium constants depend on the same free energies, and that the activity coefficients are de-coupled, so the parallel adjustment of the constants' values and electrolyte interaction parameters leave too many degree of freedom to interplay.

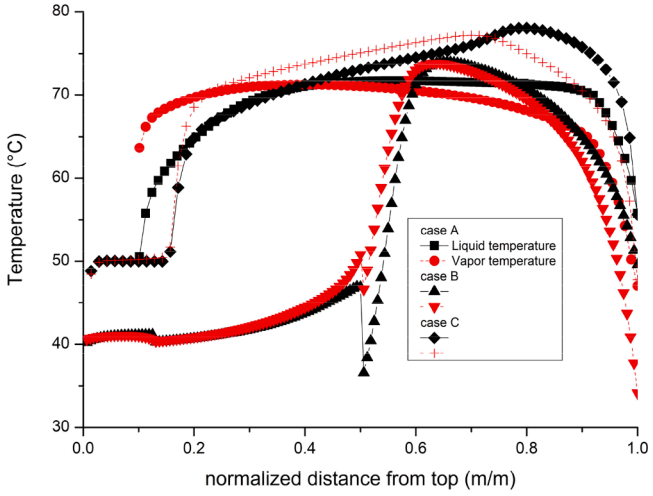


Fig. 12. Temperature in the absorbing column.

Table 8
Stripper specifications.

Case	Stages / height / diameter (m)	Packing	MTC-area correction	Total distillate (kg/h)	Reflux Ratio	Feed Stage / total	Pressure (Pa)	Reboiler Duty (kW)
A	60 / 2 + 4 / 0.12	PALL X2	1.0 – 1.0	29	2.0	20/60	$1.01\ 10^5$	43.1
B	80 / 3.9 / 0.18	PALL X2	1.0 – 1.0	62	1.4	2/80	$1.01\ 10^5$	120
C	20 / 4.25 / 0.2	Mellapak 125Y	1.0 – 1.0	200	–	1/20	$1.01\ 10^5$	121

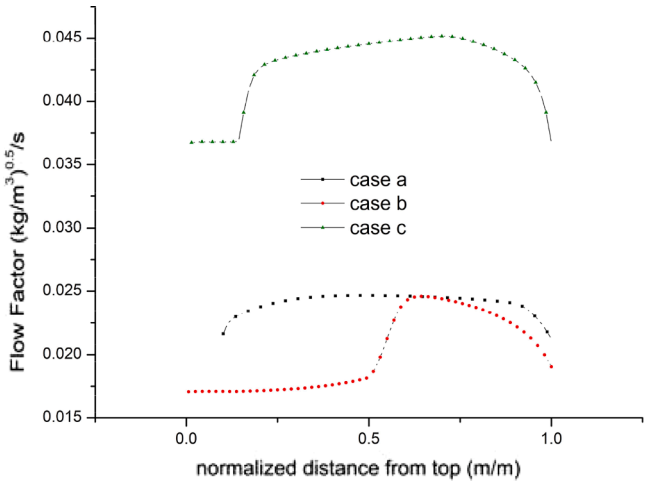


Fig. 13. Flow factor in the absorbing column.

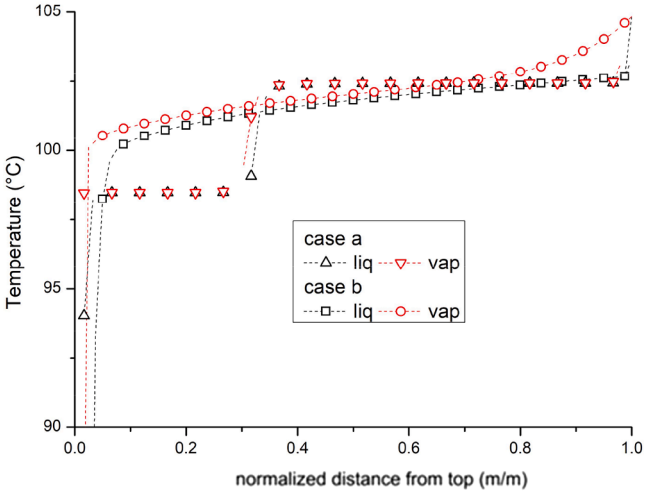


Fig. 14. Temperature in the stripping column.

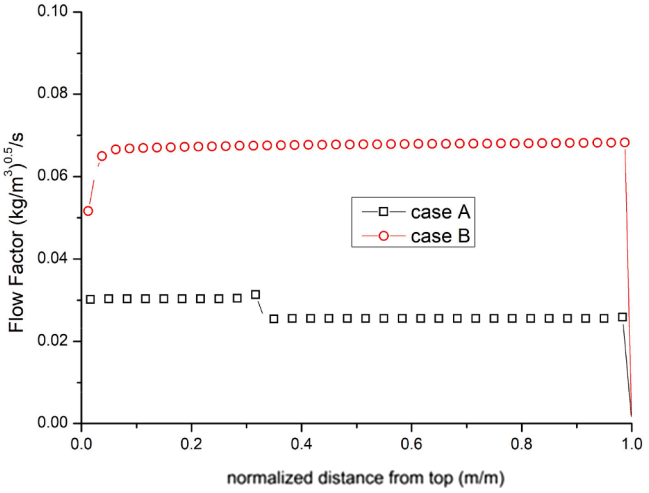


Fig. 15. Flow factor for the stripping column.

PZ Antoine parameters were not fully consistent with data. If PZ VLE and CO_2-PZ loading were fixed acting on both Antoine constants for PZ and Henry constant for CO_2, then CO_2 solubility in AMP was no more correct. Yet AMP Antoine coefficients were already appropriate, without need of corrections. So the binary amines-water equilibria, the ternary CO_2-amine-water equilibria, and the quaternary equilibrium could not be represented with the same ensemble of parameters. The issue was not solved manipulating the electrolyte interaction parameters, because the reviewed literature covers only the AMP-PZ ELECNTRL parameters, not the full AMP-PZ-CO_2 set. Moreover, this approach would solve only the full mixture range (just tackling the problem of the activity coefficient from the liquid side, rather than from the vapor side), leaving open the fact that the ternary and binary mixture representation would be affected, too. Our calculation is nevertheless in general accordance with data at similar temperature. Moreover, also this calculation was affected by the kind of VLE condition assumed in the calculator.

Viscosity has a big impact on the column rate-based calculation, yet we did not find AP simulations in the literature, that account for the refit of the viscosity parameters. In case this step is not performed, the simulation may as well be done with an empirically adjusted equilibrium model. This poses a serious problem, however, to the reliability of packing scale-up.

Overall, when properly addressing all these issues a reliable sizing of the absorber and stripper unit can be achieved, including the estimation of reboiler duties. The simulations for a mixed CESAR solvent and for a MEA reference case have been successfully validated against the cited literature.

In conclusion, to correctly compute the rate-based model of an absorber and stripper through Aspen Plus, some of the parameters should be manipulated. In particular, the revised parameters of the Antoine equation are collected in Table S3 and Table 1, ΔG and ΔH of formation (to better fit the speciation and equilibrium partition of the

Table 9
Material streams report for case A (scheme of Fig. 10).

Stream	H_2O (kg/h)	AMP	PZ	CO_2
1	4.00	0.00	0.00	12.0
2	138	70.3	42.7	1.76
3	19.0	0.00	0.00	0.00
4	155	70.3	42.6	12.8
5	6.17	0.0900	0.205	0.978
6	18.0	0.00	0.00	11.0
7	137	70.3	42.6	1.74

Table 10
Material streams report for case C (scheme of Fig. 11).

Stream	H_2O (kg/h)	AMP	PZ	CO_2
1	12.8	0.00	0.00	24.1
2	60.0	0.00	0.00	0.00
3	289	83.3	16.7	33.4
4	0.980	0.0100	0.0100	0.00
5	10.2	0.0367	0.00	4.07
6	57.8	0.287	0.0858	19.1
7	243	84.1	16.9	13.9

Table 11
Material streams report for case B (scheme of Fig. 11).

Stream	CO_2 (kg/h)	H_2O	MEA
1	12.5	1.50	0.00
2	–	–	–
3	21.8	196	90.2
4	0.00	36.0	21.0
5	0.21	2.66	0.0172
6	6.84	0.116	0.00
7	9.23	161	69.2

reacting species) are reported in Table S2.

PZ equilibrium data were revised as indicated in the same Tables, while AMZ data already present in the software database were in generally good agreement with the reviewed literature, so they were not changed. Density calculation by Aspen was in agreement with the experimental data, as reported in Fig. 6, so no change was done. On the contrary, viscosity calculation through Aspen default settings was not correctly fitting the experimental data, so the available literature values were refitted as reported in Fig. 7.

Overall, CO_2 removal rates higher than 85% and reaching 98% were possible with lower duty consumption with respect to the MEA benchmark.

Dedication

This paper is dedicated to the memory of Prof. Lucio Forni, formerly professor at Università degli Studi di Milano, passed away at the end of December 2022. I. Rossetti, as former student and colleague, gratefully remember all the teachings and the moments spent together.

Authors contribution statement

Antonio Tripodi: Junior researcher who wrote the first draft and revised data and calculations

Renato La Pietra and Matteo Tommasi: Graduating student and PhD who performed the simulation

Ilenia Rossetti: Full professor, team leader, fund raising, coordinator of the whole activity and revisor of the draft manuscript.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

All the needed data are reported or cited in the manuscript.

Acknowledgments

A. Tripodi gratefully acknowledges MUR for funding its RTDA position in the frame of the project Programma Operativo Nazionale “Ricerca e Innovazione” 2014/2020 to deliver research on “Green” topics.

I. Rossetti gratefully acknowledges the financial contribution of Fondazione Cariplo through the grant 2021-0855 – “SCORE - Solar Energy for Circular CO_2 Photoconversion and Chemicals Regeneration”, funded in the frame of the Circular Economy call 2021.

This study was carried out within the Agritech National Research Center and received funding from the European Union Next-GenerationEU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) – MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.4 – D.D. 1032 17/06/2022, CN00000022). This manuscript reflects only the authors’ views and opinions, neither the European Union nor the European Commission can be considered responsible for them. I. Rossetti and M. Tommasi acknowledge specifically the participation and funding of Tasks 8.2.3, 8.3.2 and 8.4.1.

I. Rossetti acknowledges Università degli Studi di Milano for support through the grant PSR 2021 - GSA - Linea 6 “One Health Action Hub: University Task Force for the resilience of territorial ecosystems”.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.cep.2023.109588.

References

[1] Ö. Yildirim, A.A. Kiss, N. Hüser, K. Leßmann, E.Y. Kenig, Reactive absorption in chemical process industry: a review on current activities, Chem. Eng. J. 213 (2012) 371–391, https://doi.org/10.1016/j.cej.2012.09.121.

[2] L. Dubois, D. Thomas, Postcombustion CO2 capture by chemical absorption: screening of aqueous amine(s)-based solvents, Energy Procedia 37 (2013) 1648–1657, https://doi.org/10.1016/j.egypro.2013.06.040.

[3] P.D. Vaidya, E.Y. Kenig, CO2-alkanolamine reaction kinetics: a review of recent studies, Chem. Eng. Technol. 30 (2007) 1467–1474, https://doi.org/10.1002/ceat.200700268.

[4] A. Muhammad, Y. GadelHak, Simulation based improvement techniques for acid gases sweetening by chemical absorption: a review, Int. J. Greenh. Gas Control. 37 (2015) 481–491, https://doi.org/10.1016/j.ijggc.2015.03.014.

[5] M. Garcia, H.K. Knuutila, S. Gu, ASPEN PLUS simulation model for CO2 removal with MEA: validation of desorption model with experimental data, J. Environ. Chem. Eng. 5 (2017) 4693–4701, https://doi.org/10.1016/j.jece.2017.08.024.

[6] J. Gervasi, L. Dubois, D. Thomas, Simulation of the post-combustion CO2 capture with Aspen HysysTM software: study of different configurations of an absorptionregeneration process for the application to cement flue gases, Energy Procedia 63 (2014) 1018–1028, https://doi.org/10.1016/j.egypro.2014.11.109.

[7] S. Moioli, L.A. Pellegrini, S. Gamba, Simulation of CO2 capture by MEA scrubbing with a rate-based model, Procedia Eng 42 (2012) 1651–1661, https://doi.org/10.1016/j.proeng.2012.07.558.

[8] X. Wang, Computer simulation and process improvement of CO2 capture by chemical absorption, Chem. Eng. Trans. 59 (2017) 547–552, https://doi.org/10.3303/CET1759092.

[9] S. Hasan, A.J. Abbas, G.G. Nasr, Improving the carbon capture efficiency for gas power plants through amine-based absorbents, Sustain 13 (2021) 1–28, https://doi.org/10.3390/su13010072.

[10] I. Process, S. Engineering, F. Ahmadi, Assessing the Performance of Aspen Plus and Promax for the Simulation of CO2 Capture Plants, Promax, 2012, p. 72.

[11] L.M.C. Pereira, L.F. Vega, A systematic approach for the thermodynamic modelling of CO2-amine absorption process using molecular-based models, Appl. Energy. 232 (2018) 273–291, https://doi.org/10.1016/j.apenergy.2018.09.189.

[12] M. Saimpert, G. Puxty, S. Qureshi, L. Wardhaugh, A. Cousins, A new rate based absorber and desorber modelling tool, Chem. Eng. Sci 96 (2013) 10–25, https://doi.org/10.1016/j.ces.2013.03.013.

[13] M. Afkhamipour, M. Mofarahi, Rate-based modeling and sensitivity analysis of a packed column for post-combustion CO2capture into a novel reactive 1-dimethylamino-2-propanol (1DMA2P) solution, Int. J. Greenh. Gas Control. 65 (2017) 137–148, https://doi.org/10.1016/j.ijggc.2017.09.006.

[14] F. Meng, Y. Meng, T. Ju, S. Han, L. Lin, J. Jiang, Research progress of aqueous amine solution for CO2 capture: a review, Renew. Sustain. Energy Rev. 168 (2022), 112902, https://doi.org/10.1016/j.rser.2022.112902.

[15] F. Meng, S. Han, Y. Meng, T. Ju, L. Lin, J. Jiang, A comparative study of the effects of aqueous mixed amines on biogas upgrading based on 13C nuclear magnetic resonance (NMR) analysis, J. Clean. Prod. 369 (2022), https://doi.org/10.1016/j.jclepro.2022.133288.

[16] F. Meng, T. Ju, S. Han, L. Lin, J. Li, K. Chen, J. Jiang, Study on biogas upgrading characteristics and reaction mechanism of low energy consumption 2-Amino-2-methylpropanol (AMP)/piperazine (PZ)/H2O mixed amines, Sep. Purif. Technol. 310 (2023), https://doi.org/10.1016/j.seppur.2023.123195.

[17] P. Brúder, A. Grimstvedt, T. Mejdell, E.F. da Silva, H.F. Svendsen, CO2 Capture into Aqueous Solutions of the Mixed Solvent Cesar 1, Elsevier B.V., 2010, https://doi.org/10.1016/s1876-0147(10)02004-5.

[18] M.N. Hassankiadeh, A. Jahangiri, Application of aqueous blends of AMP and piperazine to the low CO2 partial pressure capturing: new experimental and theoretical analysis, Energy 165 (2018) 164–178, https://doi.org/10.1016/j.energy.2018.09.160.

[19] S.K. Dash, A.N. Samanta, S.S. Bandyopadhyay, Solubility of carbon dioxide in aqueous solution of 2-amino-2-methyl-1-propanol and piperazine, Fluid Phase Equilib 307 (2011) 166–174, https://doi.org/10.1016/j.fluid.2011.05.009.

[20] A.K. Saha, S.S. Bandyopadhyay, A.K. Biswas, Kinetics of absorption of CO2 into aqueous solutions of 2-amino-2-methyl-1-propanol, Chem. Eng. Sci. 50 (1995) 3587–3598, https://doi.org/10.1016/0009-2509(95)00187-A.

[21] S.K. Dash, A. Samanta, A.N. Samanta, S.S. Bandyopadhyay, Vapour liquid equilibria of carbon dioxide in dilute and concentrated aqueous solutions of piperazine at low to high pressure, Fluid Phase Equilib 300 (2011) 145–154, https://doi.org/10.1016/j.fluid.2010.11.004.

[22] D. Tong, G.C. Maitland, M.J.P. Trusler, P.S. Fennell, Solubility of carbon dioxide in aqueous blends of 2-amino-2-methyl-1-propanol and piperazine, Chem. Eng. Sci. 101 (2013) 851–864, https://doi.org/10.1016/j.ces.2013.05.034.

[23] H. Li, P.T. Frailie, G.T. Rochelle, J. Chen, Thermodynamic modeling of piperazine/2-aminomethylpropanol/CO2/water, Chem. Eng. Sci. 117 (2014) 331–341, https://doi.org/10.1016/j.ces.2014.06.026.

[24] A. Samanta, S.S. Bandyopadhyay, Absorption of carbon dioxide into aqueous solutions of piperazine activated 2-amino-2-methyl-1-propanol, Chem. Eng. Sci. 64 (2009) 1185–1194, https://doi.org/10.1016/j.ces.2008.10.049.

[25] S.K. Dash, A. Samanta, A. Nath Samanta, S.S. Bandyopadhyay, Absorption of carbon dioxide in piperazine activated concentrated aqueous 2-amino-2-methyl-1-propanol solvent, Chem. Eng. Sci. 66 (2011) 3223–3233, https://doi.org/10.1016/j.ces.2011.02.028.

[26] A. Hartono, M. Saeed, A.F. Ciftja, H.F. Svendsen, Binary and ternary VLE of the 2-amino-2-methyl-1-propanol (AMP)/piperazine (Pz)/water system, Chem. Eng. Sci. 91 (2013) 151–161, https://doi.org/10.1016/j.ces.2013.01.015.
[27] G. Puxty, R. Rowland, Modelling CO 2 mass transfer in amine mixtures – PZ - AMP and PZ - MDEA, (n.d.) 1–12.
[28] M. Stec, T. Spietz, L. Więcław-Solny, A. Tatarczuk, A. Wilk, A. Sobolewski, Density of unloaded and CO2-loaded aqueous solutions of piperazine and 2-amino-2-methyl-1-propanol and their mixtures from 293.15 to 333.15K, Phys. Chem. Liq. 54 (2016) 475–486, https://doi.org/10.1080/00319104.2015.1115328.
[29] X. Liu, C. Zhu, T. Fu, Y. Ma, Volumetric and viscometric properties of ternary solution of (piperazine +2-Amino-2-methyl-1-propanol + H2O) at T = (303.15–343.15) K, J. Mol. Liq. 310 (2020), 113187, https://doi.org/10.1016/j.molliq.2020.113187.
[30] M. van der Spek, R. Arendsen, A. Ramirez, A. Faaij, Model development and process simulation of postcombustion carbon capture technology with aqueous AMP/PZ solvent, Int. J. Greenh. Gas Control. 47 (2016) 176–199, https://doi.org/10.1016/j.ijggc.2016.01.021.
[31] Y. Artanto, J. Jansen, E.E.B. Meuleman, P.H.M. Feron, Behaviour of the Mass-transfer coefficient of CO2 absorption in different Solvents at the PCC pilot plant at Loy Yang power, in: 5th Int. Conf. Clean Coal Technol, 2011.
[32] Y. Artanto, J. Jansen, P. Pearson, T. Do, A. Cottrell, E. Meuleman, P. Feron, Performance of MEA and amine-blends in the CSIRO PCC pilot plant at Loy Yang Power in Australia, Fuel 101 (2012) 264–275, https://doi.org/10.1016/j.fuel.2012.02.023.
[33] Y. Artanto, J. Jansen, P. Pearson, G. Puxty, A. Cottrell, E. Meuleman, P. Feron, Pilot-scale evaluation of AMP/PZ to capture CO2 from flue gas of an Australian brown coal-fired power station, Int. J. Greenh. Gas Control. 20 (2014) 189–195, https://doi.org/10.1016/j.ijggc.2013.11.002.
[34] I. von Harbou, H.P. Mangalapally, H. Hasse, Pilot plant experiments for two new amine solvents for post-combustion carbon dioxide capture, Int. J. Greenh. Gas Control. 18 (2013) 305–314, https://doi.org/10.1016/j.ijggc.2013.08.002.
[35] D.-piewak, A. Krótki, T. Spietz, M. Stec, L. Wiêcław-Solny, A. Tatarczuk, A. Wilk, PDU1-scale experimental results of CO2 removal with AMP/PZ Solvent, Chem. Process Eng. - Inz. Chem. i Proces. 36 (2015) 39–48, https://doi.org/10.1515/cpe-2015-0003.
[36] C. Nwaoha, M. Beaulieu, P. Tontiwachwuthikul, M.D. Gibson, Techno-economic analysis of CO2 capture from a 1.2 million MTPA cement plant using AMP-PZ-MEA blend, Int. J. Greenh. Gas Control. 78 (2018) 400–412, https://doi.org/10.1016/j.ijggc.2018.07.015.
[37] S.K. Dash, A.N. Samanta, S.S. Bandyopadhyay, Simulation and parametric study of post combustion CO2capture process using (AMP+PZ) blended solvent, Int. J. Greenh. Gas Control. 21 (2014) 130–139, https://doi.org/10.1016/j.ijggc.2013.12.003.
[38] W. Zhang, J. Chen, X. Luo, M. Wang, Modelling and process analysis of post-combustion carbon capture with the blend of 2-amino-2-methyl-1-propanol and piperazine, Int. J. Greenh. Gas Control. 63 (2017) 37–46, https://doi.org/10.1016/j.ijggc.2017.04.018.
[39] M. Afkhamipour, M. Mofarahi, Comparison of rate-based and equilibrium-stage models of a packed column for post-combustion CO2 capture using 2-amino-2-methyl-1-propanol (AMP) solution, Int. J. Greenh. Gas Control. 15 (2013) 186–199, https://doi.org/10.1016/j.ijggc.2013.02.022.
[40] H.P. Mangalapally, R. Notz, N. Asprion, G. Sieder, H. Garcia, H. Hasse, Pilot plant study of four new solvents for post combustion carbon dioxide capture by reactive absorption and comparison to MEA, Int. J. Greenh. Gas Control. 8 (2012) 205–216, https://doi.org/10.1016/j.ijggc.2012.02.014.
[41] H.P. Mangalapally, R. Notz, S. Hoch, N. Asprion, G. Sieder, H. Garcia, H. Hasse, Pilot plant experimental studies of post combustion CO2 capture by reactive absorption with MEA and new solvents, Energy Procedia 1 (2009) 963–970, https://doi.org/10.1016/j.egypro.2009.01.128.
[42] E. Meuleman, Y. Artanto, J. Jansen, M. Osborn, P. Pearson, A. Cottrell, P. Feron, Co2 Capture Performance of Mea and Blended Amine Solvents in Csiro ' S Pilot Plant With Flue Gas From a Brown Coal-Fired Power Station, in: 6th Int. Tech. Conf. Clean Coal Fuel Syst, 2010. http://linkinghub.elsevier.com/retrieve/pii/S0263876210003345%5Cnhttp://gcep.stanford.edu/pdfs/assessments/carbon_capture_assessment.pdf.
[43] A. Hartono, R. Ahmad, M. Usman, N. Asif, H.F. Svendsen, Solubility of CO2 in 0.1M, 1M and 3M of 2-amino-2-methyl-1-propanol (AMP) from 313 to 393K and model representation using the eNRTL framework, Fluid Phase Equilib 511 (2020), https://doi.org/10.1016/j.fluid.2020.112485.
[44] V. Ermatchkov, Á. Pérez-Salado Kamps, G. Maurer, Chemical equilibrium constants for the formation of carbamates in (carbon dioxide + piperazine + water) from 1H-NMR-spectroscopy, J. Chem. Thermodyn. 35 (2003) 1277–1289, https://doi.org/10.1016/S0021-9614(03)00076-4.
[45] M.D. Hilliard, A. Predictive, Thermodynamic Model for an Aqueous Blend of Potassium Carbonate, Piperazine, and Monoethanolamine for Carbon Dioxide Capture from Flue Gas Dr. Thesis, Tech. Univ., Texas Austin, 2008, p. 1083.
[46] Aspen Technology, Rate-based Model of the CO_2 Capture Process By Mixed PZ and MDEA Using Aspen Plus, 2015.
[47] H. Pahlavanzadeh, S. Nourani, M. Saber, Experimental analysis and modeling of CO2 solubility in AMP (2-amino-2-methyl-1-propanol) at low CO2 partial pressure using the models of Deshmukh-Mather and the artificial neural network, J. Chem. Thermodyn. 43 (2011) 1775–1783, https://doi.org/10.1016/j.jct.2011.05.032.
[48] W. Hu, A. Chakma, Modelling of equilibrium solubility of CO2 and H2S in aqueous amino methyl propanol (AMP) solutions, Chem. Eng. Commun. 94 (1990) 53–61, https://doi.org/10.1080/00986449008911455.
[49] S. Bishnoi, G.T. Rochelle, Absorption of carbon dioxide into aqueous piperazine: reaction kinetics, mass transfer and solubility, Chem. Eng. Sci. 55 (2000) 5531–5543, https://doi.org/10.1016/S0009-2509(00)00182-2.
[50] A.G.T. Rochelle, E. Chen, B. Oyenekan, A. Sexton, J. Davis, M. Hilliard, A. Veawab, CO2 capture by absorption with potassium carbonate third quarterly report 2006, Corrosion (2006) 1–55.
[51] J.A. McLees, Vapor-Liquid Equilibrium of Monoethanolamine/Piperazine/Water at 35 –70 0C, 2006.
[52] B.M.K. Aroua, R.M. Salleh, Solubility of CO 2 in Aqueous Piperazine and Its Modeling Using the Kent-Eisenberg Approach, 2004, pp. 65–70, https://doi.org/10.1002/ceat.200401852.
[53] W. Conway, D. Fernandes, Y. Beyad, R. Burns, G. Lawrance, G. Puxty, M. Maeder, Reactions of CO2 with aqueous piperazine solutions: formation and decomposition of mono- and dicarbamic acids/carbamates of piperazine at 25.0 °C, J. Phys. Chem. A. 117 (2013) 806–813, https://doi.org/10.1021/jp310560b.
[54] J.T. Cullinane, G.T. Rochelle, Kinetics of carbon dioxide absorption into aqueous potassium carbonate and piperazine, Ind. Eng. Chem. Res. 45 (2006) 2531–2545, https://doi.org/10.1021/ie050230s.
[55] J.T. Cullinane, G.T. Rochelle, Thermodynamics of aqueous potassium carbonate, piperazine, and carbon dioxide, Fluid Phase Equilib 227 (2005) 197–213, https://doi.org/10.1016/j.fluid.2004.11.011.
[56] F. Khalili, A. Henni, A.L.L. East, PKa values of some Piperazines at (298, 303, 313, and 323) K, J. Chem. Eng. Data. 54 (2009) 2914–2917, https://doi.org/10.1021/je900005c.
[57] H. Mehdizadeh, M. Gupta, E.F. Da Silva, H.F. Svendsen, Representation of piperazine-CO2-H2O system using extended-UNIQUAC and computational chemistry, Energy Procedia 37 (2013) 1871–1880, https://doi.org/10.1016/j.egypro.2013.06.067.
[58] A.T. Inc, Rate-Based Model of the CO2 Capture Process by MEA Using Aspen Plus, 2012.
[59] R. Notz, H.P. Mangalapally, H. Hasse, Post combustion CO2 capture by reactive absorption: pilot plant description and results of systematic studies with MEA, Int. J. Greenh. Gas Control. 6 (2012) 84–112, https://doi.org/10.1016/j.ijggc.2011.11.004.
[60] H.P. Mangalapally, H. Hasse, Pilot plant experiments for post combustion carbon dioxide capture by reactive absorption with novel solvents, Energy Procedia 4 (2011) 1–8, https://doi.org/10.1016/j.egypro.2011.01.015.
[61] Y. Artanto, G. Puxty, Y. Elias, K. Hungerbuhler, L.L. Simon, Rate based modeling and validation of a carbon-dioxide pilot plant absorbtion column operating on monoethanolamine, Chem. Eng. Res. Des. 89 (2010) 1684–1692, https://doi.org/10.1016/j.cherd.2010.10.024.
[62] G. Manzolini, E. Sanchez Fernandez, S. Rezvani, E. Macchi, E.L.V. Goetheer, T.J. H. Vlugt, Economic assessment of novel amine based CO2 capture technologies integrated in power plants based on European Benchmarking Task Force methodology, Appl. Energy. 138 (2015) 546–558, https://doi.org/10.1016/j.apenergy.2014.04.066.
[63] E. Sanchez Fernandez, E.L.V. Goetheer, G. Manzolini, E. Macchi, S. Rezvani, T.J. H. Vlugt, Thermodynamic assessment of amine based CO2 capture technologies in power plants based on European Benchmarking Task Force methodology, Fuel 129 (2014) 318–329, https://doi.org/10.1016/j.fuel.2014.03.042.