

Investigating the Performance of Ethanolamine and Benzylamine Blends as Promising Sorbents for Postcombustion CO₂ Capture through ¹³C NMR Speciation and Heat of CO₂ Absorption Analysis

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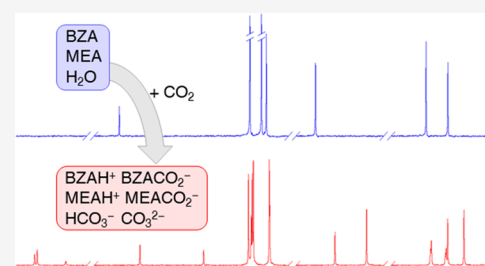


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ABSTRACT: Aiming at formulating efficient sorbents for carbon capture and separation (CCS) processes, in this work, we evaluated the CO₂ capture performance of aqueous blends of two primary amines, namely, ethanolamine (MEA), the benchmark for any capture process, combined with benzylamine (BZA), which has intriguing characteristics for industrial use, such as low corrosivity and good resistance to thermal and oxidative degradation. The CO₂ loading, the CO₂ absorption rate, and the CO₂ heat of absorption were determined at 313 K for three different formulations of aqueous BZA/MEA blends, all with the same overall amine concentration (6 M) but with different amine molar ratios (1/2, 1/1, 2/1) by treating a gas mixture containing 15% CO₂ (by volume) mimicking a fossil-derived flue gas. Furthermore, through an accurate ¹³C NMR study, the species present in solution during the CO₂ absorption process were identified and quantified to understand the capture mechanism and to evaluate the interactions of the two primary amines when present together in different molar ratios. As a result, the three tested blends show similar high CO₂ absorption rates, and their final loading values decrease in the order BZA/MEA 1/2 > BZA/MEA 1/1 > BZA/MEA 2/1, suggesting that a greater relative amount of MEA in the blend is advantageous to achieve a relatively higher CO₂ loading. The ¹³C NMR analysis confirmed that the greater alkalinity of MEA leads to a greater formation of bicarbonate in solution and consequently higher loading. Finally, the CO₂ absorption heat of all tested mixtures, measured using a high-precision microcalorimeter, was found to be comparable, if not even higher, to that of each individual amine.



INTRODUCTION

The incessant growth of the world population and the simultaneous improvement of society's standard of living has led in recent decades to a continuous increase in global energy needs. Fossil fuels as dominant energy resources have played, and will continue to play, an important role in the energy supply system around the world. Unfortunately, the combustion of fossil fuels leads to an inevitable increase in the concentration of carbon dioxide (CO₂) in the atmosphere, which is closely related to the so-called global warming, one of the most serious environmental challenges.^{1,2} As a result, the topic of carbon capture and storage (CCS) has recently attracted a lot of attention from the scientific community and from politicians in every government. According to the best technologies identified so far, postcombustion capture (PCC) has become a commonly accepted method for controlling CO₂ emission from energy-related sources.^{3,4} Among the various PCC technologies developed, the chemical absorption using amine-based liquid solutions is considered the most mature and functional method and has several advantages in terms of selectivity for CO₂, absorption rate, and loading capacity⁵ compared to other techniques, such as adsorption with solid sorbents⁶ or the use of a membrane contactor.⁷ It is well known that there are three kinds of amine that can be used to

capture CO₂ from a flue gas, namely, primary, secondary, and tertiary amines.^{8,9} In general, in an aqueous solution, primary and secondary amines can react directly (and rapidly) with CO₂ to form stable carbamates, ensuring efficient separation and a high CO₂ absorption rate but requiring high temperatures (and energy) to regenerate the sorbent. On the other hand, tertiary amines cannot react directly with CO₂ (because they do not have hydrogens on the amino functionality necessary for the formation of carbamate) and act as a base to promote the CO₂ hydration reaction and form bicarbonate and carbonate ions.^{10–12} As a result, the tertiary amines always demonstrate much lower reaction kinetics for CO₂ absorption than the primary/secondary amines but they can be regenerated with less energy consumption and can provide higher CO₂ loading capacities.³ Recently, the blending of different amines with different properties has attracted great interest, as it has been shown that it is possible to exploit the

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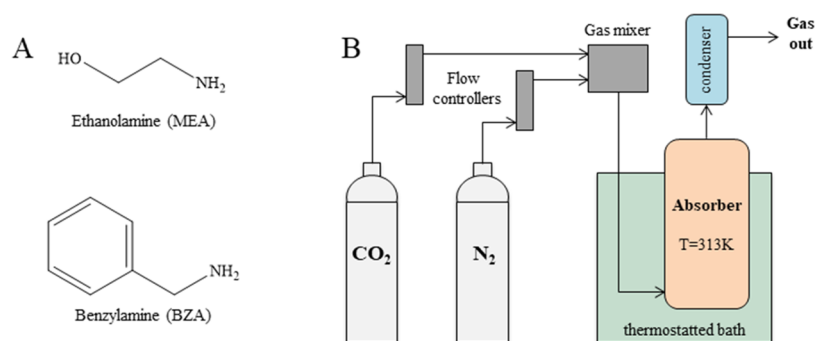


Figure 1. (A) Molecular structure of the used primary amines and (B) schematic diagram of the apparatus for the CO₂ loading measurement.

advantage of each individual amine solvent to formulate absorbents with superior CO₂ capture performance.^{13–21}

Ethanolamine (MEA) is certainly the most studied and used amine and is considered the benchmark for every sorbent-based CCS process.^{21–23} More recently, benzylamine (BZA), another primary amine, has also aroused the interest of numerous research groups to be used both individually and mixed with other amines.^{3,24–28} Many studies have shown that BZA and MEA have similar absorption capacity,²⁶ carbamate stability,²⁷ comparable vapor pressure, and boiling point.^{29,30} Compared to MEA, BZA exhibits higher cyclic capacity,²⁶ lower viscosity and lower heat capacity,²⁷ faster absorption rate, and a better ability to promote mass transfer in blends.²⁸ Furthermore, BZA is less subject to oxidative degradation than MEA and has a less corrosive behavior for the equipment.³¹ On the other hand, when used individually, BZA forms a poorly soluble carbamate, which precipitates easily and severely limits further CO₂ capture.³ To emphasize its strengths and limit its drawbacks, BZA can be conveniently mixed with other amines. Conway et al.²⁴ investigated the CO₂ capture performance of a series of BZA-based blend solvents under the same operating conditions: the results obtained showed that the blend of the two primary amines BZA and MEA has similar absorption capacity, relative higher cyclic capacity, and better mass transfer performance than blends of BZA with sterically hindered amines (2-amino-2-methyl-1-propanol, AMP) or with tertiary amines, such as *N,N*-dimethylethanolamine (DMEA), *N,N*-diethylethanolamine (DEEA), 2-dimethylamino-2-methyl-1-propanol (2DMA2MIP), and 3-quinuclidinol (3-QUIN). This work demonstrates that the dual-primary amine BZA/MEA system could be a competitive candidate sorbent for CO₂ capture, which is particularly attractive also due to the low commercial cost of BZA: it is, therefore, worth investigating its properties to identify the best formulation and the best operating conditions.

With the ambition to better understand the potential of sorbents obtained by mixing together the two primary amines benzylamine and ethanolamine, in this work, we thoroughly investigated the CO₂ capture performance of three of their blends, all with the same total amine concentration (6 M) but with a different BZA/MEA molar ratio, i.e., 1/2, 1/1, and 2/1. The CO₂ loading (ratio between the maximum amount of CO₂ captured and the total amount of amine in solution) and the CO₂ absorption rate of each formulated blend were evaluated in batch experiments of CO₂ capture from a gas mixture (CO₂, 15% in N₂) at 313 K. During the absorption process, several solution samples were subsequently collected, and they were

analyzed by ¹³C NMR to identify and quantify the different carbonated species present:^{32–34} an accurate speciation study as a function of the absorption time allows us to understand the CO₂ capture mechanism in the BZA–MEA–CO₂–H₂O system, as well as the relative role of the two different primary amines when present together. Furthermore, the exact knowledge of the products and their relative amounts allows us to better understand the different behaviors of the sorbent during the desorption processes, given that the formed bicarbonate and carbamates show opposite effects on the heat consumption in the sorbent regeneration process.^{13,35} Finally, the heat of CO₂ absorption, an important parameter to assess the heating cost for CO₂ release from rich solutions,³⁵ has been measured for the three blends with a high-precision microcalorimeter. In our opinion, the results obtained in this experimental study can help to better understand the functioning of this intriguing blend of primary amines, and, above all, they can help to formulate the most performing composition for CO₂ capture applications from the gaseous mixture.

MATERIALS AND METHODS

General Information. The two primary amines ethanolamine (MEA) and benzylamine (BZA) were of analytical grade (Sigma-Aldrich) and were used as received, without further purification. Their molecular structures are presented in Figure 1A. BZA and MEA were used to prepare three different aqueous blends, all with the same total amine concentration of 6 M (mol/dm³) but with different relative ratios between the amines, and in particular: BZA/MEA 1/2 (2 M BZA + 4 M MEA), BZA/MEA 1/1 (3 M BZA + 3 M MEA), and BZA/MEA 2/1 (4 M BZA + 2 M MEA). Pure CO₂ and N₂ (Rivoira) were mixed together to obtain a gas mixture with CO₂ = 15% v/v to mimic the typical composition of a flue gas coming from a fossil fuel-fired power plant. The gas flow rates were measured with gas mass flow meters (Aalborg) equipped with gas controllers (Cole Parmer).

CO₂ Absorption Experiments. All absorption experiments were performed at 313 K and ambient pressure. The absorber was a gas washing bottle, equipped with a sintered glass diffuser (16–40 μm pores), kept at the desired temperature by means of a thermostatted bath (Julabo model F33-MC bath, accuracy ± 0.1 K). A schematic representation of the apparatus used is shown in Figure 1B. The absorber was charged with 50 cm³ of the tested sorbent (0.3 total moles of amines) and was continuously fed with a gas mixture containing 15% (v/v) CO₂ in N₂, at a constant flow rate of 37.0 dm³/h (0.230 mol CO₂/h). A cold condenser, maintained at 268 K, was equipped to avoid the solvent loss during the CO₂ absorption process.

After 5, 10, 20, 40, and 60 min, the experiment was temporarily stopped, the absorber was weighed, and a small sample of the solution (about 0.5 cm³) was collected for ¹³C NMR analysis. The absorption was definitively stopped after 90 min. From the weight increase due to

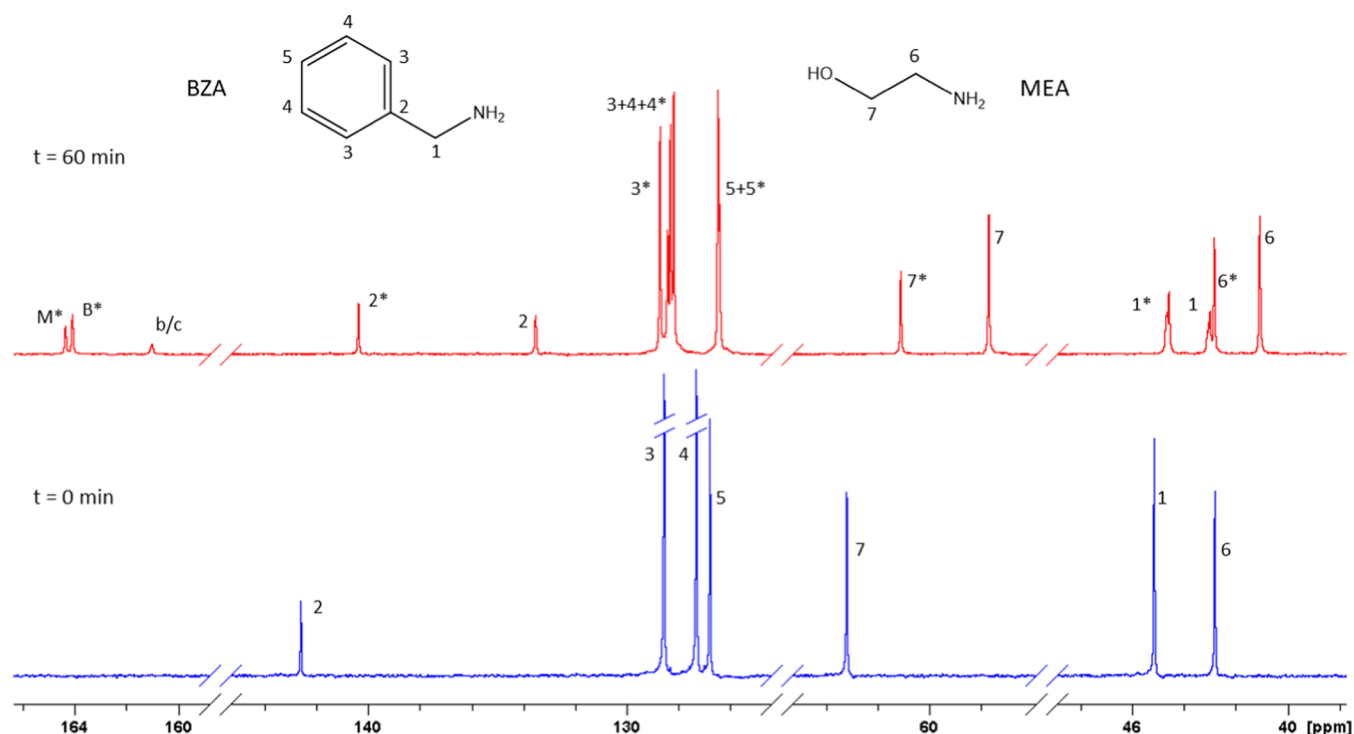


Figure 2. ^{13}C NMR spectra of aqueous BZA/MEA 1/1 at the beginning of the experiment ($t = 0$) and after 60 min of CO_2 absorption. The numbers indicate the carbon atom referred to both free and protonated amine fast exchanging in the NMR scale, assigned as reported in the relative amine structure. Asterisks refer to the carbon atoms of amine carbamate. M^* and B^* denote the carbonyl carbon atoms of MEA and BZA carbamate, respectively; b/c refers to the bicarbonate/carbonate ion.

the captured CO_2 , it is possible to calculate the CO_2 loading (mol CO_2 captured/mol total amine) at each absorption step.

^{13}C NMR Analysis. The solution samples collected for each BZA/MEA blend after 5, 10, 20, 40, 60, and 90 min of CO_2 capture were stored at a constant temperature of 40°C and were finally analyzed by ^{13}C NMR using a Bruker Avance III 400 spectrometer operating at 100.613 MHz, with a well-established procedure that allowed us to identify the carbonated species formed in solution during the absorption process and to evaluate their relative amounts.^{36,37} Tetramethylsilane was used as an external standard at 0.00 ppm, while CH_3CN was used as an internal reference (CH_3 , $\delta = 1.47$). A sealed glass capillary containing D_2O (Sigma-Aldrich) was introduced into the NMR tube with the amine solution sample to provide a good signal for deuterium lock. To obtain quantitative ^{13}C NMR spectra, a pulse sequence with proton decoupling and NOE suppression was used to acquire $^{13}\text{C}/^1\text{H}$ with the following acquisition parameters: pulse angle = 90.0° , acquisition time = 1.3632 s, delay time = 2–30 s, data points = 65 K, and the number of scans = 250–500. The data were processed by Bruker-Biospin Topspin software. The peak integration of the carbon atoms of the $-\text{CH}_2-$ and $-\text{CH}-$ backbone of each amine allowed us to evaluate the relative amounts of carbamate and the fast equilibrating (free amine)/(protonated amine).³⁸ The ^{13}C atoms of HCO_3^- , CO_3^{2-} , and R-CO_2^- (amine carbamate, R = BZA, MEA) have no attached hydrogens; they show a longer relaxation time compared to that of $-\text{CH}_2-$ and $-\text{CH}-$ groups, resulting in lower intensity resonances. Notwithstanding, a careful peak integration of the carbon resonances in the range 160–165 ppm could provide an estimation of the relative amounts of the species formed. The relative amount of carbonate and bicarbonate in solution has been evaluated with a procedure already described,³⁹ with a deviation from the average value lower than 5%. Further details on the ^{13}C NMR analysis procedure, along with the complete method for calculating all of the different species in the solution can be found in the [Supporting Information](#).

Measurement of CO_2 Absorption Heat. The CO_2 absorption heat for each solution was measured directly with a high-precision

microcalorimeter, a powerful tool that is being increasingly used and approved for this type of determination.^{40,41} The experimental setup and procedure followed were the same as those already described by Zheng and Liu in previous papers.^{42,43} Briefly, before the absorption process starts, an appropriate amount of the tested blend solution was placed in the sample cell and the reaction temperature was set to the desired value of 313 K. When both the sample temperature and the heat flow signal were stabilized, a gaseous mixture with a known amount of CO_2 (in these experiments, 15% v/v) was continuously injected into the reactor. The chemical absorption of CO_2 by the sorbent involves variations in the heat flow, continuously recorded by the microcalorimeter. When the reaction process is finished, there are no more changes in the heat flow and the experiment is considered finished. The CO_2 absorption heat can be calculated by the following equations

$$\Delta H_{\text{abs}} = \frac{E_{\text{abs}}}{n_{\text{abs}}} \quad (1)$$

$$Q_{\text{abs}} = \int_{t_1}^{t_2} q(t) dt \quad (2)$$

where E_{abs} (kJ) is the cumulative heat released during CO_2 absorption, n_{abs} (mol) is the total amount of CO_2 captured in the absorption process, and $q(t)$ is the transient heat flow changes, expressed in mW. The total amount of CO_2 captured in the absorption process (n_{abs}) was measured using a Chittick apparatus with a 1 M HCl solution.⁴⁴

RESULTS AND DISCUSSION

Identification of the Species Formed during the CO_2 Capture Process. The CO_2 absorption experiments for the three different aqueous blends of benzylamine (BZA) and ethanolamine (MEA) were performed as described in the [Materials and Methods](#) section. As evident from their molecular structures (Figure 1A), both BZA and MEA have

a primary amino group and can react directly with CO₂. According to the reaction mechanism between primary amine and CO₂ proposed by Caplow⁴⁵ and Danckwerts,⁴⁶ the possible species formed in aqueous BZA/MEA blends are protonated amines, BZA carbamate, MEA carbamate, bicarbonate, and carbonate ions. Obviously, CO₂ would exist in the CO₂-loaded amine solution as amine carbamates (C–N bond) and bicarbonate and carbonate ions (C–O bond).^{13,32,35} As an exemplification of the species formed in solution by the reaction between BZA, MEA, and CO₂, the ¹³C NMR spectra of 1/1 aqueous BZA/MEA at the beginning and after 60 min of CO₂ absorption (at *T* = 313 K) are shown in Figure 2.

The comparison between the spectra before (blue line) and after (red line) the CO₂ absorption process clearly highlights the chemical species produced. In the spectrum at *t* = 60 min, corresponding in this particular case to a loading of 0.524 (mol CO₂/mol amine), three new ¹³C signals can be detected at a low magnetic field, within the range 160–165 ppm: two of them correspond to the carbonylic carbon atoms of MEA carbamate and BZA carbamate (peaks M* and B*, respectively), while the peak “b/c” refers to the carbonylic carbon atom of bicarbonate and carbonate ions, which provide a single peak due to the fast proton transfer between them.^{47–49} The formation of the carbamates of the two primary amines is further confirmed at higher magnetic fields (lower ppm) by the new signals that appear (marked with an asterisk) related to the carbon atoms of the aliphatic and aromatic chains of the amines. Similarly to the bicarbonate/carbonate signal, the carbon atoms of free amine and protonated amine also provide a single signal due to fast proton transfer between them.^{33,50}

To better appreciate the variation of the reaction products at different CO₂ loadings, Figure 3 shows the spectra of the carbonyl atoms (in the range 160–165 ppm) of the aqueous BZA/MEA 1/1 solution, after 5, 10, 20, 40, 60, and 90 min of CO₂ absorption at 313 K.

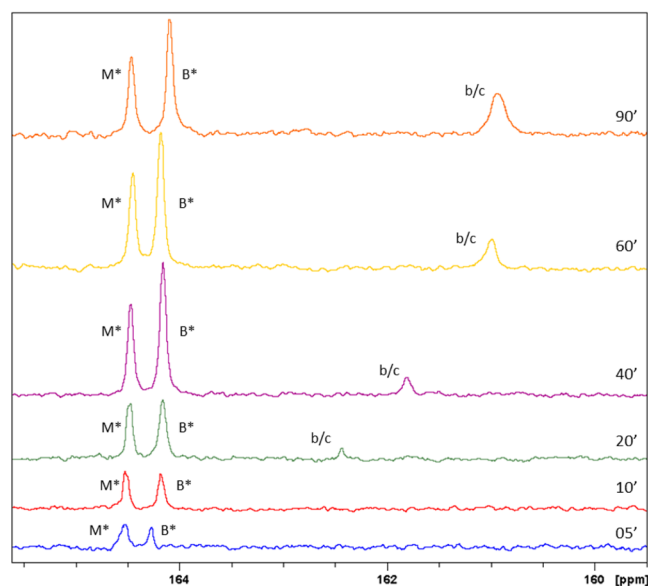
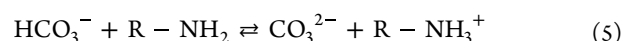
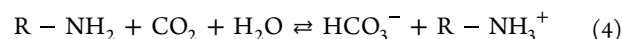


Figure 3. ¹³C NMR spectra of the carbonyl zone of aqueous BZA/MEA 1/1 at different steps of the CO₂ absorption experiment. M* and B* denote the carbonyl atoms of MEA and BZA carbamate, respectively; b/c refers to the bicarbonate/carbonate signal.

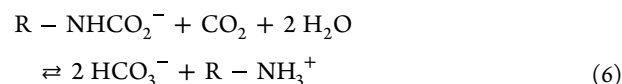
At the beginning of the experiment (5–10 min), CO₂ quickly reacted with the two primary amines, in great excess with respect to CO₂, to produce the relative amine carbamates, as described by reaction (3), where R–NH₂ refers to a generic primary amine.



Interestingly, it is possible to observe (from the peak intensities) that the formation of MEA carbamate (M*) was faster than BZA carbamate (B*). Conversely, after 20 min of absorption, the reaction between CO₂ and BZA became predominant and the amount of BZA carbamate increased more than that of MEA carbamate. Furthermore, after 20 min, the signal related to bicarbonate and carbonate ions (single peak, b/c), which are formed according to reactions (4) and (5), also appears.



As the absorption continued, with the progressive decrease of free amine in solution, CO₂ was further absorbed by the reaction with the carbamate ions in solution, according to reaction (6): as a consequence, the amount of bicarbonate increased.



As a confirmation, Figure 3 clearly shows that the peak of the fast exchanging bicarbonate/carbonate (b/c) increased in intensity over time (from 40 to 90 min) and moved to the high field to chemical shift values (ppm) corresponding to higher percentages of bicarbonate.³⁹ Moreover, Figure 3 and Table S2 (in Supporting Information) highlight the slight decrease in the intensity of the MEA and BZA carbamate signals from 60 to 90 min of absorption due to the reaction (6) and also favored by a relative increase of the acidity of the solution at high loading, which makes the carbamates less stable.³²

CO₂ Loading and Quantitative ¹³C NMR Speciation during the Absorption Process. The amount of CO₂ progressively captured by each tested blend during the absorption experiments was measured by weighing. The CO₂ loading (mol captured CO₂/mol amines) was calculated at several subsequent steps, and, in particular, after 5, 10, 20, 40, and 60 min of absorption. Finally, after 90 min, the experiment was stopped and the final loading value was calculated. All of the obtained loading values for each tested BZA/MEA blend during the capture process are reported in Table 1. It should be mentioned that at the end of the absorption experiment, the BZA/MEA 2/1 solution contained a white solid due to the precipitation of the poorly soluble BZA carbamate.³

The loading data reported in Table 1 show that in the first 40 min of capture, all of the tested blends rapidly react and absorb CO₂ from the gas stream, regardless of the relative amount of BZA and MEA present in the solution, and the loading values double as time doubled. Interestingly, in this first period, the loading values (at the same absorption time) are almost identical for all of the solutions. The excess of free amine with respect to CO₂ that passes through the solution, combined with the direct rapid reaction of carbamate formation due to the primary amino functionalities, determines this behavior. After 40 min, the sorbents have almost reached

Table 1. Loading Values (mol CO₂/mol Amines) Calculated at Different Absorption Steps^a

absorption time (min)	CO ₂ loading		
	BZA/MEA 1/2	BZA/MEA 1/1	BZA/MEA 2/1
5	0.061	0.062	0.061
10	0.127	0.126	0.127
20	0.254	0.255	0.255
40	0.481	0.473	0.478
60	0.540	0.524	0.517
90	0.561	0.540	0.533

^aSorbent volume = 50 cm³, sorbent total concentration = 6 M, *T* = 313 K, CO₂ flow rate = 0.230 mol/h.

the equilibrium state, and the measured values of CO₂ loading of the different blends start to differ increasingly from each other as the absorption proceeds. The loading values decrease in the order BZA/MEA 1/2 > BZA/MEA 1/1 > BZA/MEA 2/1, suggesting that a greater relative amount of MEA in the blend is advantageous to achieving a relatively higher CO₂ loading, in agreement with the fact that MEA has a higher CO₂ equilibrium solubility than BZA.⁵¹ A larger amount of BZA in solution does not seem useful to increase the CO₂ absorption capacity, probably also due to the easy precipitation of carbamate when the BZA concentration is higher than 3 M.²⁴

To better understand the reaction mechanisms of the two primary amines with CO₂ when mixed together, a quantitative speciation study was performed for each different BZA–MEA–CO₂–H₂O system at various CO₂ loadings. Sorbent

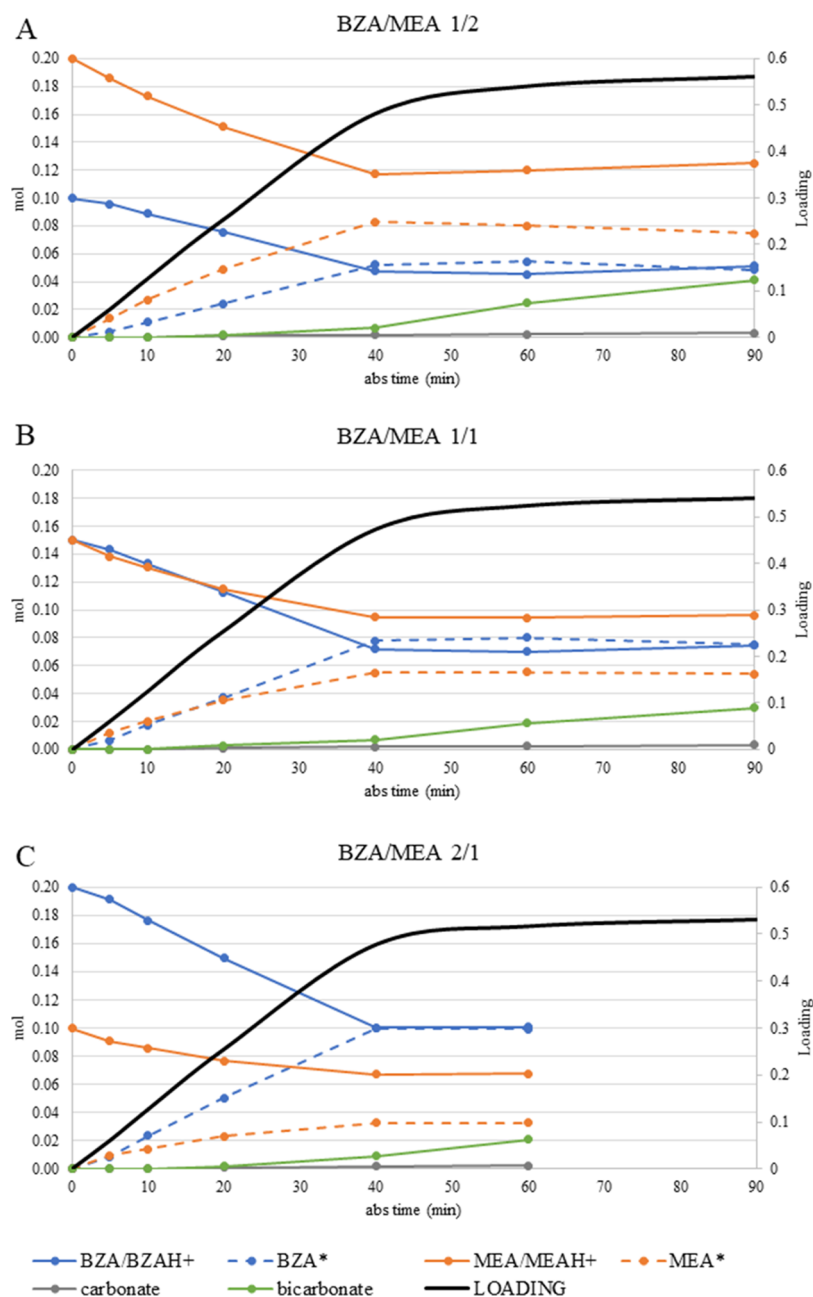


Figure 4. CO₂ loading and quantitative speciation (reported as mol of each species) as a function of the increasing absorption time (*T* = 313 K) for (A) BZA/MEA 1/2, (B) BZA/MEA 1/1, and (C) BZA/MEA 2/1.

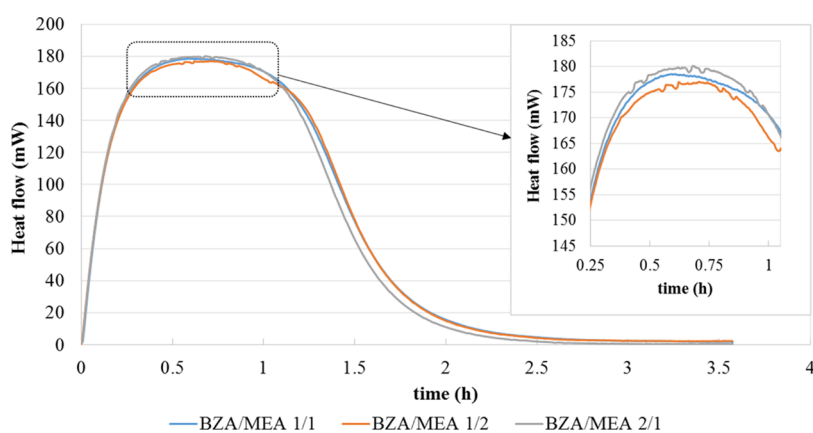


Figure 5. Heat flow curve recorded during the CO₂ absorption process.

samples were collected after 5, 10, 20, 40, 60, and 90 min of CO₂ absorption and were analyzed using ¹³C NMR: from the signal integrations of each obtained spectrum, the amount of each species in solution was calculated. Tables S1–S3 (in Supporting Information) show the calculated amount (mol) of carbamate of BZA and MEA (indicated as BZA* and MEA*, respectively) for each tested blend and at each absorption step and the summed amount of the fast equilibrating (free amine)/ (protonated amine) for both BZA and MEA (indicated as BZA/BZAH⁺ and MEA/MEA⁺, respectively) and bicarbonate and carbonate ions.

Due to the precipitation of the poorly soluble BZA carbamate, it was not possible to perform the ¹³C NMR spectrum of BZA/MEA 2/1 at 90 min, and therefore the relative data are not reported.

The variations in the amounts (mol) of each species in solution as a function of the absorption time for each tested blend are shown in Figure 4, together with their absorption rate, reported as the variation of CO₂ loading during the capture process.

The data reported in Tables S1–S3 and in Figure 4 underline the different behavior of the three blends and allow us to understand how the two different amines and their relative amount in solution influence the CO₂ capture process. At the beginning of the process, for each blend, a rapid increase in carbamates (BZA* and MEA*) in solution is observed, accompanied by a consequent decrease in amine (BZA/BZAH⁺ and MEA/MEA⁺), as described by reaction 3. Observing the variation of carbamates over time (Figure 4), it can be seen that the amount of BZA* constantly increases until it equals approximately the sum of BZA and BZAH⁺. At the same time, MEA* also increases, but more slowly, as clearly shown in Figure 4B,C. Furthermore, the maximum amount of MEA* that is formed is always significantly lower than the sum of MEA and MEAH⁺.

These two observations suggest that after a first step in which both amines react quickly to give directly the relative carbamates, when the amount of total amine in the solution decreases, MEA tends to act more as a base, given its higher alkalinity compared to BZA (pK_a MEA = 9.50; pK_a BZA = 9.34),⁵² and therefore to form the protonated species MEAH⁺ also as a counter ion for BZA*. This would also explain the fact that when in the starting blend MEA is equal to or greater than BZA, after a sufficient absorption time, BZA* is even greater than the sum of BZA and BZAH⁺ (Figure 4A,B). In the BZA/MEA 2/1 blend, the carbamate probably reaches its solubility

limit (about 0.1 mol in 50 cm³) and begins to precipitate in the form of a white solid.

When most of the free amine has been consumed (here after about 40 min), the bicarbonate formation reaction (reaction 4, amine/CO₂ stoichiometry = 1/1) prevails over the carbamate formation reaction (reaction 3, amine/CO₂ stoichiometry = 2/1): as a matter of fact, the amount of bicarbonate increases rapidly, more than any other species in solution. It is also interesting to note that in the last 20 min of absorption, the quantities of carbamates decrease slightly: this is due to the further formation of bicarbonate, according to reaction 6. The higher final quantity of bicarbonate in the BZA/MEA 1/2 blend compared to that 1/1 (Figure 4A,B) represents a further confirmation of the prevailing behavior of MEA as a base. The molar concentrations of BZA in blends 2/1 and 1/1 are 4 M and 3 M, respectively: as demonstrated by Conway et al.,²⁴ precipitation (caused by the BZA*) easily forms in the blend when the concentration of BZA is more than 3 M at a high CO₂ loading stage; as a result, the BZA* cannot further hydrolyze to form bicarbonate and BZAH⁺ at a relative acidity solution (high CO₂ loading stage). On the contrary, blend 1/2 contains more MEA, while the concentration of BZA is lower than 3 M: the formed MEA*, which does not precipitate, can further hydrolyze to form bicarbonate and MEAH⁺. This is why, BZA/MEA 1/2 produces more bicarbonate than the other two blends.

Evaluation of the CO₂ Absorption Heat. The heat required for the sorbent regeneration process consists of three main parts: (i) the desorption heat required to desorb CO₂ from the absorbent; (ii) the sensible heat required to increase the temperature of the CO₂-rich solution in the desorption tower; and (iii) the evaporation heat required for the water evaporation, necessary to strip CO₂ in the regeneration tower.^{53,54} Of these three parts, only the CO₂ desorption strictly depends on the intrinsic characteristics of the absorbent itself: in fact, the evaporation heat can be regulated by controlling the operating conditions, while the sensible heat is affected by the solution concentration, heat capacity of the diluent, quantity of ions in solution, and other physical factors. Therefore, the determination of the desorption heat is necessary to evaluate the performance of the sorbent in a CO₂ capture process. The desorption process is usually considered to be the reverse of the absorption process, and consequently, the desorption heat is numerically equal to the heat of absorption. The CO₂ absorption heat can be determined both indirectly from the Gibbs–Helmholtz

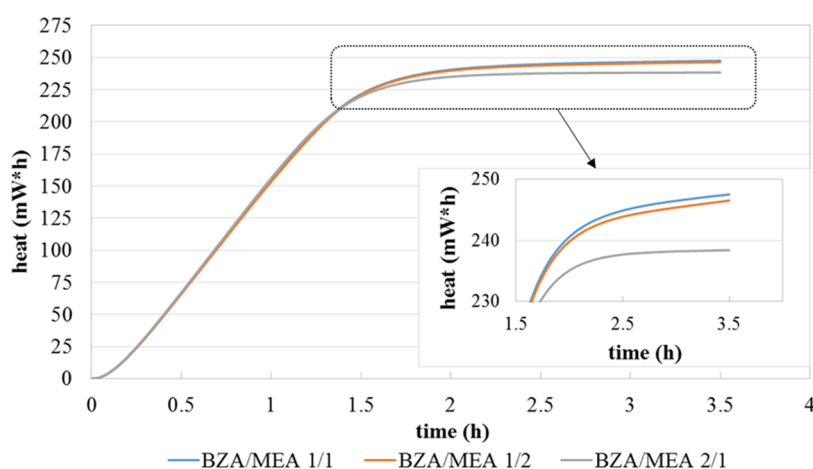


Figure 6. Heat flow curve of the CO₂ absorption process.

equation on the basis of VLE data, through a complex and long experimental procedure already used in previous publications,⁴⁴ and by direct measurement of the heat of reaction using a high-precision microcalorimeter, as done in this work.

The heat flow curve recorded during the CO₂ absorption reaction for all of the tested blends is shown in Figure 5.

The intensity of the heat released during the reaction can be reflected by the highest peak value of the heat flow. The higher the peak value of the heat flow, the greater the heat released at a given period, which was reflected in temperature fluctuations in the absorber in industrial applications. Since temperature fluctuations are detrimental to the stability of the absorption process, sorbents with small heat flow peaks are considered more suitable for industrial applications. From the results obtained, it can be seen that the order of magnitude of the peak heat flow is: BZA/MEA 1/2 > BZA/MEA 1/1 > BZA/MEA 2/1.

Figure 6 shows the increased total heat release as a function of absorption time, while the CO₂ absorption heat of each blend, calculated as in eqs 1 and 2, is reported in Table 2.

Table 2. Calculated Values of CO₂ Absorption Heat of BZA/MEA Blends with 15% CO₂ at 313 K

absorbent blend	CO ₂ absorption heat ΔH (kJ/mol CO ₂)
BZA/MEA 1/2	-89.69
BZA/MEA 1/1	-96.01
BZA/MEA 2/1	-89.02

From the results obtained, it is clear that BZA/MEA 1/1 has the greatest CO₂ absorption heat, which leads to higher energy consumption during the desorption process. The CO₂ absorption heat values of BZA/MEA 2/1 and BZA/MEA 1/2, on the other hand, are very close to each other, and both are significantly lower than BZA/MEA 1/1. It should be noted that the values measured for the blends 1/2 and 2/1 are very similar to the values reported in the literature for the individual amines in an aqueous solution,^{55,56} while the mixture 1/1 has a higher absolute value, corresponding to the need for more energy for desorption. In fact, the mixing of these two primary amines with each other does not bring appreciable advantages from the point of view of energy saving for the regeneration of the sorbent.

For comparison, Table S4 in the Supporting Information shows the heat of CO₂ absorption of some aqueous sorbents

with three amines. From these data, it can be inferred that introducing a tertiary amine (or even a sterically hindered primary amine) into the sorbent system may be advantageous to have lower ΔH_{abs} values. Therefore, in future works, it will be interesting to investigate the CO₂ capture performance, including energy cost, of trio-amine BZA/MEA/tertiary amine systems.

CONCLUSIONS

This work investigated the CO₂ absorption performance of three different aqueous blends of two primary amines, namely, benzylamine (BZA) and ethanolamine (MEA). Their 6 M solutions, with different amine ratios (BZA/MEA 2/1, BZA/MEA 1/1, and BZA/MEA 1/2) were tested for the CO₂ capture from a gas stream containing 15% v/v of CO₂ at 313 K, and for each solution, the CO₂ loading, the absorption rate, and the heat of CO₂ absorption were determined. Furthermore, to understand the mechanisms of CO₂ capture and how the two amines interact in the process, an accurate ¹³C NMR speciation study was conducted on samples taken during the absorption experiments, and the species present in solution were identified and quantified. The obtained results indicate that the three tested blends have similar high CO₂ absorption rates and their final loading values decrease in the order BZA/MEA 1/2 > BZA/MEA 1/1 > BZA/MEA 2/1, suggesting that a greater relative amount of MEA in the blend is advantageous to achieve a relatively higher CO₂ loading. As a confirmation, the ¹³C NMR speciation analysis highlighted that the greater alkalinity of MEA leads to a greater formation of bicarbonate in solution and consequently higher loading, compared to blends where a greater amount of BZA is present. Moreover, consistently with what has already been reported in other publications, it is confirmed that the concentration of BZA in the starting solution should not exceed 3 M to avoid the formation of a white precipitate that hinders further absorption of CO₂ and, in industrial use, makes the transfer of the loaded solution from the absorber to the desorber more complicated. Finally, the CO₂ heat of absorption values measured with a high-precision microcalorimeter were found similar to those of each individual amine, if not significantly higher as in the case of BZA/MEA 1/1: this suggests that the mixing of two primary amines can be advantageous in regard to the CO₂ absorption rate, but it does not substantially decrease the heat necessary for the sorbent regeneration. However, due

to its low corrosive behavior, low commercial cost, and environmental friendly effect compared to MEA, BZA could be used as an additive in MEA to replace the single use of MEA for capturing CO₂, with the potential advantage of reducing the operating and capital costs. In addition, the results obtained in this work confirm that BZA could be a positive candidate to replace MEA as a promoter of the absorption rate when formulating new absorbent mixtures for CO₂ capture.

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.energyfuels.2c01930>.

¹³C NMR analysis method, detailed ¹³C NMR speciation analysis of the three different tested amine blends during the CO₂ absorption process, and heat of CO₂ absorption of some aqueous sorbents with three amines (PDF)

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Notes

The authors declare no competing financial interest.

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