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Measurement of high-pressure properties for aqueous solutions of amines: Densities and isobaric heat capacities of 3-(methylamino)propylamine and 1-methylpiperazine binary mixtures

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ABSTRACT

The density and isobaric heat capacity of 3-(methylamino)propylamine (MAPA) + H₂O and 1-methylpiperazine (1-MPZ) + H₂O mixtures were measured using a vibrating tube densimeter and a flow calorimeter, respectively. Density measurements were carried out with a relative expanded uncertainty of 0.1 % (k = 2) over a wide range of temperatures (from 293.15 K to 393.15 K), pressure up to 100 MPa, and amine mass fractions of 0.1, 0.2, 0.3, and 0.4. Isobaric heat capacity experimental data was acquired with a relative expanded uncertainty better than 1 % (k = 2). These measurements reached pressures up to 25 MPa and temperatures from 293.15 K to 353.15 K, in the same amine mass fractions compositions. A modified Tammann-Tait empirical equation was used to develop density correlation as a function of temperature, pressure, and molality. Additionally, an empirical function of temperature and amine mass fraction was used to fit the isobaric heat capacity data. Both correlations showed good agreement with the experimental data of the aqueous amine solutions under study, within 0.1 % for density correlation and 1 % for isobaric heat capacity correlation. Compared to the limited experimental data found in literature, the deviations observed were smaller than the reported uncertainties.

1. Introduction

Carbon Capture, Storage and Utilization (CCS) is an emerging technology that has proven to be effective in mitigating the accelerating increase of CO_2 emissions into the atmosphere. The burning of fossil fuels from industrial activities such as power generation is one of the main sources of CO_2 emissions [1,2]. Therefore, the gas sweetening process, which allows CO_2 separate from flue gas, has been widely used for more than eight decades. In this process, CO_2 is chemically absorbed using aqueous amine solutions at high pressures, typically close to 7 MPa [3–5]. Although this technology has been on the market since 1930 [6], there are still some aspects that need to be optimized. For instance, the high energy consumption in the regeneration step of the aqueous amine solution, the high thermal and oxidative degradation to which the aqueous amine solution is exposed, and the CO_2 cycle capacity [7,8]. In addition, fast reactions with CO_2 and good thermophysical properties such as low density and low viscosity are also needed [9,10]. In the search for new solvents to improve the above aspects, diamines and cyclic amines have been identified as good candidates.

The performance of diamines such as 3-(methylamino)propylamine (MAPA) and cyclic amines like 1-methylpiperazine (1-MPZ) in CO_2 capture has been studied previously by [11–14]. MAPA is a diamine with a primary and a secondary group. According to Monteiro et al. [11], at 298.15 K, a 1 M MAPA aqueous solution reacts with CO_2 roughly twice as fast as piperazine (PZ) and fifteen times faster than monoethanolamine (MEA), resulting in an increase of 15 % in the CO_2 absorption rates [14]. On the other hand, 1-MPZ solutions present reaction rates like primary or secondary amines but lower than PZ solutions [13] but in this context, pure 1-MPZ has the advantage of being liquid at atmospheric temperature and its solubility in water is higher than PZ [12]. In addition, 1-MPZ aqueous solutions offer a lower enthalpy of absorption (from $-55 \text{ kJ} \cdot \text{mol}^{-1}$ to $-67 \text{ kJ} \cdot \text{mol}^{-1}$) than primary and secondary amines (from $-75 \text{ kJ} \cdot \text{mol}^{-1}$ to $-86 \text{ kJ} \cdot \text{mol}^{-1}$), considering 30 % amine mass composition at 313.15 K [12,15]. Finally, both

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aqueous solutions mixtures studied presented lower densities at same temperature, pressure and amine mass fraction than MEA solutions and PZ solutions [16,17], with a maximum reduction of 6 % in the case of MAPA + H_2O at 0.4 mass fraction and 393.15 K.

Regarding thermophysical properties such as density and isobaric heat capacity for aqueous solutions of MAPA or 1-MPZ, limited references in the literature report experimental measurements [11,18–22]. The measured ranges of these properties do not reach conditions of high temperature and pressures other than atmospheric. However, design and optimisation of CO2 capture processes using new amines require thermodynamic models calibrated and validated on those missing data conditions. Thermophysical properties such as density and isobaric heat capacity are essential to operating pumps, heat exchangers, and designing gas-liquid contactors [23]. Density is also useful in determining liquid diffusivity and reaction rate constants, especially in kinetic studies involving wetted-wall columns. Furthermore, density play a key role in mass transfer rate modelling for absorbers and regenerators because it affects the liquid film coefficient. Accurate isobaric heat capacity experimental data for amine solutions is paramount in every energy balance, particularly essential for designing efficient heat exchangers in CO_2 capture facilities [7,8,23].

The primary purpose of the present study is to measure the density and isobaric heat capacity of MAPA + H_2O and 1-MPZ + H_2O at amine mass fractions ranging from 0.1 to 0.4, throughout a wide pressure and temperature range. Therefore, this study focused on the impact of amine mass fraction, temperature and pressure on the density and isobaric heat capacity of aqueous MAPA or 1-MPZ solutions. The present research additionally proposed empirical correlations for these properties.

2. Experimental

2.1. Materials

Table 1 lists the samples that were used in this experiment. No further purifying procedures were performed; the purity listed in Table 1 is reported as provided by the supplier Sigma-Aldrich. Two binary mixtures 3-(methylamino)propylamine (MAPA) + H₂O and 1-methylpiperazine (1-MPZ) + H₂O were analysed. The aqueous amine solutions were prepared by weighing the samples using an analytical balance (Radwag scale model PS750/C/2) with a resolution of 1 mg. At 95.5 % confidence level, the amine mass fraction's estimated expanded uncertainty is 0.0004. Immediately following preparation, amine aqueous solutions were degassed using a Branson 3210 water-filled ultrasonic bath. To ensure their stability and prevent the CO₂ absorption from the air, mixtures were stored in sealed glass bottles with a lid and sealing film, avoiding light exposure.

2.2. Apparatus and procedure

2.2.1. Density measurements

For density ρ measurements, an Anton Paar DMA HPM vibrating tube densimeter was used. The description of this fully automated equipment was given earlier by [24,25]. Measurements were carried out at six different temperatures between 293.15 K and 393.15 K, and pressures up to 100 MPa. The calibration was made using water and vacuum

Table 1

Material description.

Samples	CAS Number	Source	Mass Fraction Purity ^a
MAPA ^b	6291–84-5	Sigma-Aldrich	$\label{eq:conductivity} \begin{split} &\geq 0.995 \\ &\geq 0.98 \\ & \text{Conductivity} \leq 2{\cdot}10^{-6}~\Omega^{-1}{\cdot}\text{cm}^{-1} \end{split}$
1-MPZ ^c	109–01-3	Sigma-Aldrich	
Water	7732–18-5	Sigma-Aldrich	

^a As stated by the supplier by gas chromatography.

^b MAPA = 3-(methylamino)propylamine.

 c 1-MPZ = 1-methylpiperazine.

following the Lagourette method [26]. A Pt100 temperature sensor calibrated with an expanded uncertainty of 0.02 K (95.5 % confidence level) was used to measure the temperature within the densimeter. The temperature was controlled using an external thermostatic bath (Julabo F25-HE). The measuring fluid was pressurised by a HiP Model 68–5.75–15 pressure generator coupled with a stepper motor ACP&D type 6530-R211 with a reducer gearbox to control the piston within the generator. The expanded uncertainty of pressure was 0.02 MPa, using a pressure indicator Druck DPI 104.

The uncertainty calculation was carried out following the procedure described by Segovia et al. [24] and according to the document JCGM 100:2008 ("Evaluation of measurement data – Guide to the expression of uncertainty in measurement") [27]. Uncertainty analysis showed an expanded relative uncertainty better than 0.1 % for a 95.5 % level of confidence, as illustrated in Table 2.

2.2.2. Isobaric heat capacity measurement

Isobaric heat capacity c_p was measured using a quasi-isothermal flow calorimeter. The completed description and the working principle of this apparatus were detailed earlier by [25,28]. An Agilent 1100 Series HPLC isocratic pump was used to maintain a constant flow rate through the calorimetric cell. The calorimetric cell is immersed in a thermostatic bath (Hart Scientific 7041), which maintains the inlet temperature of the fluid. This temperature is measured using a long-stem Platinium Resistance Thermometer 25 Ω (25 Ω PRT) connected to a resistance bridge (Multifunction Reference Thermometer Readout Additel 286) with an uncertainty better than 5 mK. The expanded uncertainty (k = 2) in the temperature set-point is better than 20 mK. A Peltier cooler device is used to remove heat at constat rate, and a control-heater compensates for this energy loss to maintain the desired temperature difference 500 mK between inlet and outlet temperatures. The latter was measured by a 10 k Ω NTC thermistor located in the upper part of the cell, which was calibrated against the 25 Ω PRT immersed in the thermostatic bath prior to each isotherm. The pressure was measured with a pressure indicator Druck DPI 104 with an expanded relative uncertainty (k = 2) of 0.05 %. A Mity-Mite model S91XW back pressure regulator valve, installed at the outlet of the calorimetric cell, maintains a pressure in the circuit higher than the pressure in the sample container. This pressure is established by the action of a variable volume piston HiP Model 87-6-5 controlled by a stepper motor ACP&D type 6530-24-4-0.4. The back pressure regulator valve isolates the measurement flow circuit and the hydraulic pressure control circuit. A thermal calibration experiment was conducted using water as the calibration fluid due to its well-characterized isobaric heat capacity; more details can be found in [28]. The isobaric heat capacity was measured at four different temperatures from 293.15 K to 353.15 K

Uncertainty	' budget	for the	density	using	JCGM	[27]
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	Units	Estimate	Divisor	$u(x)/kg \cdot m^{-3}$	$u(x)^2$
Repeatability $u(\tau)$	μs	$5 \cdot 10^{-4}$	1	$7.5 \cdot 10^{-3}$	5.63
Resolution $u(\tau)$		1.10^{-3}	$2\sqrt{3}$		10^{-5}
Reference Material u (ρ_{ref})	kg·m ^{−3}	0.01	$\sqrt{3}$	$6 \cdot 10^{-3}$	$3.60 \cdot 10^{-5}$
u(A(T))	kg∙m ⁻³ ∙µ s ⁻²	$7 \cdot 10^{-8}$	2	0.25	$6.25 \cdot 10^{-2}$
u(B(T,p))	$kg \cdot m^{-3}$	0.5	2	0.25	$6.25 \cdot 10^{-2}$
Calibration $u(T)$	К	0.02	2	$1.4 \cdot 10^{-2}$	1.96
Resolution $u(T)$		0.01	$2\sqrt{3}$		10^{-4}
Repeatability $u(T)$		$5 \cdot 10^{-3}$	1		
Calibration $u(p)$	MPa	0.02	2	$7.5 \cdot 10^{-3}$	5.63
Resolution $u(p)$		0.01	$2\sqrt{3}$		10^{-5}
Repeatability u(p)		0.01	1		
$u(\rho)$	kg∙m ⁻³				0.35
			$U(\rho)$	(k = 2)	0.7
			(ho = 897.	4 kg·m ^{−3})	0.1~%

and pressures up to 25 MPa.

The uncertainty calculation was carried out following the procedure described by Segovia et al. [28] and according to the document JCGM 100:2008 [27]. Uncertainty analysis showed an expanded relative uncertainty better than 1 % for a 95.5 % level of confidence, as detailed in Table 3.

Friction along the tube causes a pressure loss and therefore the process is not isobaric. Furthermore, viscous dissipation implies heat that should be accounted for. Dynamic viscosity is a necessary input to the friction correction term, as explained in [25]. Experimental viscosity data for MAPA + H₂O and 1-MPZ + H₂O is scarce in the literature; however, we found three references, one for MAPA + H₂O [11] and two for 1-MPZ + H₂O [19,20], that cover the temperature and amine mass fraction conditions considered in this study but at ambient pressure. High-pressure viscosity estimation was considered unnecessary due to the negligible error introduced by using ambient-pressure viscosity. This error introduced to the isobaric heat capacity is only 0.03 % for the largest viscosity correction at the highest flow rate. This value is nearly an order of magnitude lower than the reported uncertainty.

3. Results and discussion

3.1. Density measurement

Experimental density data for binary mixtures MAPA + H_2O and 1-MPZ + H_2O are reported in Tables S1 and S2, respectively reported in supplementary data. Measurement was conducted at six temperatures from 293.15 K to 393.15 K, pressure up to 100 MPa, and amine mass fraction of 0.1, 0.2, 0.3 and 0.4. The amine molality is reported in terms of mol of amine per kg of H_2O .

Tables S1 and S2 and Figs. 1 and 2 show that experimental densities of the 1-MPZ aqueous solutions are higher than MAPA + H_2O values under the same conditions of pressure, temperature, and amine mass fraction. This difference increases with amine mass fraction, temperature and pressure, reaching a maximum of 3 %. The density of these mixtures increases with pressure while maintaining very similar trends for all systems, as can be seen in Figs. 1 and 2. As expected, a rise in temperature leads to a decrease in density and increasing pressure, density rises. This trend resembles a non-linear behaviour for the two aqueous mixtures studied.

Two types of behaviour are observed regarding the tendency of density with respect to amine mass fraction. In the first case, according to Table S1, it is observed that as the amine mass fraction increases, the density decreases for MAPA aqueous solutions for all the experimental conditions. In the second type of behaviour, as can be seen in Table S2 and Fig. 2, there is a change in the slope of the curve that describes the

Table 3

Uncertainty budge	t for the isobaric hea	t capacity using	JCGM [27].
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: 0		1		= =	
	Units	Estimate	Divisor	u(x)	$u(x)^2$
Repeatability $u(c_p)$	kJ·	0.010	1	0.0102	$1.1 \cdot 10^{-4}$
	kg ⁻¹ ·K ⁻¹	6	_	E	0
Resolution $u(Q)$	W	4.10-0	$2\sqrt{3}$	$8.5 \cdot 10^{-3}$	7.2.10-9
Repeatability $u(\dot{Q})$	W	$2.0 \cdot 10^{-7}$	1	$1.5 \cdot 10^{-5}$	$2.1 \cdot 10^{-10}$
Non-linearity $u(\dot{Q})$	W	$1.0 \cdot 10^{-5}$	1	$7.35 \cdot 10^{-4}$	$5.4 \cdot 10^{-7}$
Accuracy u(V)	$ml \cdot s^{-1}$	$2.5 \cdot 10^{-5}$	2	$1.76 \cdot 10^{-3}$	$3.1 \cdot 10^{-6}$
Resolution $u(\dot{V})$	$ml \cdot s^{-1}$	$1.7 \cdot 10^{-5}$	$2\sqrt{3}$	$6.8 \cdot 10^{-4}$	$4.5 \cdot 10^{-7}$
Resolution $u(\Delta T)$	K	$1 \cdot 10^{-3}$	$2\sqrt{3}$	$2.27 \cdot 10^{-3}$	$5.2 \cdot 10^{-6}$
Stability (inlet) u (ΔT)	K	$1 \cdot 10^{-3}$	$\sqrt{3}$	$4.55 \cdot 10^{-3}$	$2.0 \cdot 10^{-5}$
Stability (outlet) u (ΔT)	К	$1 \cdot 10^{-3}$	$\sqrt{3}$	$4.55 \cdot 10^{-3}$	$2.0 \cdot 10^{-5}$
$u(c_p)$	kJ∙				0.012
•	$kg^{-1} \cdot K^{-1}$				
			$U(c_p)$	(k = 2)	0.025
			$(c_p = 3.73)$	3 kJ∙	1 %
			$kg^{-1} \cdot K^{-1}$)	



Fig. 1. Experimental density ρ , of the system MAPA(1) + H₂O(2) as a function of temperature *T*, at pressure p = 1 MPa. Amine mass fractions: (-) $w_1 = 0$, (\circ) $w_1 = 0.1$, (()) $w_1 = 0.2$, (\diamond) $w_1 = 0.3$, and (Δ) $w_1 = 0.4$. Solid lines represent Tammann-Tait fitting correlation using parameters from Table 5 and 6. Data of pure water ($w_1 = 0$) from Equation of State integrated in NIST REFPROP database [29].



Fig. 2. Experimental density ρ , of the system 1-MPZ(1) + H₂O(2) as a function of temperature *T*, at pressure p = 1 MPa. Amine mass fractions: (-) $w_1 = 0$, (\circ) $w_1 = 0.1$, (()) $w_1 = 0.2$, (\diamond) $w_1 = 0.3$, and (Δ) $w_1 = 0.4$. Solid lines represent Tammann-Tait fitting correlation using parameters from Table 5 and 6. Calculated for pure water ($w_1 = 0$) from Equation of State integrated in NIST REFPROP database [29].

trend of density as a function of temperature when the amine mass fraction varies from 0 to 0.4 for 1-MPZ aqueous solutions. At temperatures approximately lower than 325 K the density increases with the amine mass fraction; however, at temperatures above approximately 325 K density decreases with the amine mass fraction. The justification for this behaviour was given earlier by Rayer et al. [19], who studied the experimental density of 1-MPZ aqueous solutions across the entire range of molar compositions proposing that the self-association of pure 1-MPZ decreases when mixed with water. This is due to the hydrogen bonding interactions between 1-MPZ and water, as well as the ability of 1-MPZ molecules to fill the cavities within the loose structure of water. The magnitude of the contributions of these different types of interactions will vary with the amine, the composition of the mixture, and the temperature.

The experimental values were correlated using a semiempirical Tammann–Tait (Eq. (1) for each composition as function of pressure and temperature:

$$\rho(T,p) = \frac{A_0 + A_1 T + A_2 T^2}{1 - C \ln \left(\frac{B_0 + B_1 T + B_2 T^2 + p}{B_0 + B_1 T + B_2 T^2 + p_{ref}}\right)} \tag{1}$$

where ρ (*T*, *p*) represents the correlated density as function of pressure (*p*) and temperature (*T*), *p_{ref}* is the reference pressure (fixed in 1 MPa for all cases). Numerator shows the temperature dependent correlated density at *p_{ref}* with the fitting parameters *A_i*. Denominator represents the temperature and pressure correction using the fitting parameters *B_i* and *C*.

A statistical analysis was executed using both experimental and calculated data to evaluate the performance of the models: AAD (Average Absolute Deviation (Eq. (2))); MAD (Maximum Absolute Deviation (Eq. (3))); and (σ) standard deviation (Eq. (4)).

AAD,
$$X = \frac{1}{N} \sum_{i=1}^{N} \frac{|X_{\exp,i} - X_{cal,i}|}{X_{\exp,i}}$$
 (2)

MAD,
$$X = \max\left(\frac{|X_{\exp,i} - X_{cal,i}|}{X_{\exp,i}}\right)$$
 (3)

$$\sigma = \sqrt{\left[\frac{1}{N-m}\right] \sum_{i=1}^{N} \left(X_{\exp,i} - X_{cal,i}\right)^2}$$
(4)

where $X_{exp,i}$ is the *i*th experimental value of a defined property X, $X_{cal,i}$ is the *i*th calculated value using the correlation at the same condition, N is the total number of experimental points, and m is the number of fitting parameters.

The fitting results are shown in Table 4, which contains the adjustable parameters, the standard deviation of the adjustment (σ) absolute average deviation (AAD) and maximum average deviation (MAD) defined by Eqs. (2) to (4) respectively.

A modified Tammann-Tait equation was used to correlate the experimental density ρ , data with temperature *T*, pressure *p*, and amine molality b_1 . Al Ghafri et al. [30,31] originally modified the equation, as presented in Eqs. (5) to (8). Our previous work [25] explained in detail the resolution method for this model, effectively correlating

Table 4

Fitting parameters of Eq. (1), standard deviations σ , absolute average deviation (AAD) and maximum average deviation (MAD) for Tammann-Tait correlation.

MAPA (1) + H_2O	$w_1 =$	$w_1 =$	$w_1 =$	$w_1 =$
(2)	0.1000 ^a	0.2000 ^a	0.3000 ^a	0.4007 ^a
$A_0/\text{kg}\cdot\text{m}^{-3}$	864.15	928.89	1025.25	1108.39
$A_1/\text{kg}\cdot\text{m}^{-3}\cdot\text{K}^{-1}$	1.2005	0.84644	0.32702	-0.12629
$A_2/\text{kg}\cdot\text{m}^{-3}\cdot\text{K}^{-2}$	-0.00261	-0.0022	-0.00158	-0.00104
<i>B</i> ₀ /MPa	-275.04	279.31	698.87	801.66
$B_1/MPa\cdot K^{-1}$	3.9795	0.96246	-1.4053	-2.1257
$B_2/MPa\cdot K^{-2}$	-0.00682	-0.00289	0.00026	0.00128
С	0.12690	0.11707	0.10812	0.101
p _{ref} /MPa	1	1	1	1
$\sigma/\text{kg}\cdot\text{m}^{-3}$	0.19	0.14	0.07	0.05
AAD/%	0.02	0.01	0.01	0.004
MAD/%	0.5	0.4	0.3	0.2
$1-MPZ(1) + H_2O$	$w_1 =$	$w_1 =$	$w_1 =$	$w_1 =$
(2)	0.1000 ^a	0.2000 ^a	0.3002 ^a	0.4003 ^a
$A_0/\text{kg}\cdot\text{m}^{-3}$	860.30	920.10	1015.94	1116.49
$A_1/\text{kg}\cdot\text{m}^{-3}\cdot\text{K}^{-1}$	1.2597	0.97692	0.51078	0.02105
$A_2/\text{kg}\cdot\text{m}^{-3}\cdot\text{K}^{-2}$	-0.00269	-0.00238	-0.00184	-0.00128
<i>B</i> ₀ /MPa	-328.21	178.06	663.85	840.62
$B_1/MPa\cdot K^{-1}$	4.2356	1.4972	-1.1956	-2.2654
$B_2/\text{MPa}\cdot\text{K}^{-2}$	-0.00714	-0.00361	-0.00004	0.00140
С	0.12493	0.11480	0.10691	0.10091
p _{ref} /MPa	1	1	1	1
$\sigma/\text{kg}\cdot\text{m}^{-3}$	0.21	0.16	0.08	0.06
AAD/%	0.02	0.01	0.01	0.004
MAD/%	0.5	0.4	0.3	0.2

^a w_i : mass fraction of component i.

experimental density data for aqueous amine solutions. The statistical parameters: absolute average relative deviation (AAD), the maximum absolute relative deviation (MAD) and the standard deviation (σ), defined by Eqs. (2) to (4) respectively, were calculated to assess the goodness-of-fit. As a result, an excellent representation of the data was achieved, as it is represented in Figs. 3 and 4, for MAPA solutions and 1-MPZ solutions, respectively. Tables 5 and 6 list the resulting parameters for Eqs. (5) to (8) and statistical parameters, applicable to both systems under study.

$$\rho(T, p, b_1) = \frac{\rho_{ref}(T, b_1)}{1 - C(b_1) \ln\left(\frac{B(T, b_1) + p}{B(T, b_1) + p_{ref}(T)}\right)}$$
(5)

$$[\rho_{ref}(T,b_1) - \rho_0(T)] / (\text{kg} \cdot \text{m}^{-3}) = \sum_{i=1}^{i=3} \sum_{j=1}^{j=3} \alpha_{ij} [b_1 / (\text{mol} \cdot \text{kg}^{-1})]^{(i+1)/2} (T/T_c)^{(j+1)/2}$$
(6)

$$B(T,b_1)/\text{MPa} = \sum_{i=0}^{i=1} \sum_{j=0}^{j=3} \beta_{ij} [b_1/(\text{mol}\cdot\text{kg}^{-1})]^i (T/T_c)^j$$
(7)

$$C(b_1) = \gamma_0 + \gamma_2 \left[b_1 / (\text{mol·kg}^{-1}) \right]^2$$
(8)

where, ρ_{ref} is the reference density, which is calculated using Eq. (6), $\rho_o(T)$ is the saturated liquid density at $b_1 = 0 \text{ mol-kg}^{-1}$ (pure water) and at the vapor pressure of pure water at the given temperature. Data for pure water was obtained from NIST REFPROP database [29]. The critical temperature T_c in Eqs. (6) and (7) was the value for water (647.10 K).

Comparison from literature data have been carried out using the modified Tammann-Tait equation (Eqs. (5) - (8), with the parameters reported in Table 5 and 6), correcting our experimental density measurements to the temperature, pressure and composition reported by the authors. As shown in Table 7 and Fig. 5a for the comparison of experimental densities of MAPA + H₂O, three authors report measurements of this system at atmospheric pressure. Monteiro et al. [11] reported a total of 24 comparable data points, Wang et al. [18] show 40 related data and Pinto et al. [22] reports an additional 6 comparable points showing an absolute average deviation of 0.08 %, 0.11 % and 0.03 % respetively. In the case of 1-MPZ + H₂O mixture, two authors report experimental measurements at 0.1 MPa (Fig. 5b). Rayer et al. [19] detailed 18 comparable experimental points and Vamja et al. [20] dispatch and additional 40 experimental points, showing and absolute average deviation



Fig. 3. Relative deviations (%) for MAPA(1) + H₂O(2) mixture of experimental density measurements, ρ_{exp} , in comparison with calculated density, ρ_{cab} , using Eqs. (5) to (8). Dashed lines represent the relative expanded uncertainty of our density measurements.



Fig. 4. Relative deviations (%) for 1-MPZ(1) + H₂O(2) mixture of experimental density measurements, ρ_{exp} , in comparison with calculated density, ρ_{cal} , using Eqs. (5) to (8). Dashed lines represent the relative expanded uncertainty of our density measurements.

Table 5

Parameters β_{0i} , and γ_0 for pure water ($b_1 = 0 \text{ mol·kg}^{-1}$) in Eqs. (7) and (8).

β_{00}	β_{01}	β_{02}	β_{03}	γο
-2894.13	16489.61	-27612.67	14807.00	0.13265

Table 6

Coefficients α_{ij} , β_{ij} , and γ_i in Eqs. (6) to (8), and statistical parameters AAD, MAD and σ in Eqs. (2) to (4).

Parameters	Binary Mixtures		
	$MAPA + H_2O$	$1-MPZ + H_2O$	
α_{11}	-77.609	-50.658	
α_{12}	75.431	56.125	
α_{13}	0	0	
α_{21}	353.117	360.574	
α_{22}	-849.461	-858.122	
a23	515.958	511.884	
a_{31}	-76.123	-76.420	
α_{32}	186.356	182.500	
α_{33}	-114.524	-109.301	
β_{10}	403.237	395.671	
β_{11}	-1331.896	-1270.312	
β_{12}	1107.78	1029.274	
β_{13}	0	0	
γ2	$3.768 \cdot 10^{-4}$	$5.0526 \cdot 10^{-4}$	
AAD/%	0.02	0.02	
MAD/%	0.1	0.1	
$\sigma/(\text{kg}\cdot\text{m}^{-3})$	0.3	0.3	

of 0.04 % and 0.09 % respectively from our experimental data. It should be noted that all data display a negative deviation from the literature data. That behaviour cannot be explained considering only the uncertainty from the fitting equation or the different uncertainties provided by the authors. The exact details of the experimental conditions of the measurements carried out by all the authors can be found in Table 7.

3.2. Isobaric heat capacity measurement

The experimental data for isobaric heat capacity measurements were obtained at four different temperatures from 293.15 K to 353.15 K. Tables S3 and S4, from Supplementary information, presents the experimental data for MAPA + H_2O system and for 1-MPZ + H_2O respectively. The measured pressure varied from 0.1 MPa to 25 MPa. The amine mass fraction was studied from 0.1 to 0.4.

To analyze the influence of temperature, pressure, and amine mass

Table 7

Measurement conditions of literature data used to compare the experimental density or heat capacity of MAPA + H_2O and 1-MPZ + H_2O mixtures measured in this work.

Reference	System	Comparison Conditions	Number of Points	U_r^{a}
Monteiro et al. [11]	MAPA(1) + H ₂ O(2)	$w_1 = 0.0891 - 0.3676$ T = (293.15 - 343.15) K p = 0.1 MPa	24	0.006
Wang et al. [18]		$w_1 = 0.0908 - 0.3524$ T = (293.15 - 363.15) K p = 0.1 MPa	40	0.0006
Pinto et al. [22]		$w_1 = 0.352$ T = (298.15 - 353.15) K p = 0.1 MPa	6	0.04
Rayer et al. [19]	1-MPZ(1) + H ₂ O(2)	$w_1 = 0.2341 - 0.3920$ T = (298.15 - 343.15) K p = 0.1 MPa	18	NA ^b
Vamja et al. [20]		$w_1 = 0.1 - 0.4$ T = (298.15 - 348.15) K p = 0.1 MPa	40	0.07
Poozesh et al. [21]		$x_1 = 0.02 - 0.107$ T = (298.15 - 353.15) K p = 0.1 MPa	3	1

^a Relative expanded uncertainty (k = 2), %.

^b NA: Not Available.

fraction on isobaric heat capacities, the experimental data of the studied systems were plotted as a function of temperature at fixed pressure with different amine mass fractions (Figs. 6 and 8), and as a function of pressure at fixed temperature T = 313.15 K with different amine mass fractions (Figs. 7 and 9).

Regarding MAPA aqueous solutions (Fig. 6), the change with temperature was noticeable for all mass fractions, with increases from 2 % to 6 % when w_{MAPA} changed from 0.1 to 0.4. For the 1-MPZ + H₂O binary solution, as can be seen in Fig. 8, an increase in temperature resulted in increases in c_p of 3 %, 4 %, and 7 % for $w_{1-MPZ} = 0.2, 0.3$, and 0.4, respectively. This behaviour agrees with the fact that temperature has a slight influence on the isobaric heat capacity of pure amines [21,32]. For $w_{1-MPZ} = 0.1$, the change in c_p as a function of temperature is less than the measurement uncertainty. The effect of pressure on c_p , for MAPA + $\rm H_2O$ mixture, a decrease of 2 % was observed for $w_{\rm MAPA} = 0.3$ at 293.15 K, and an increase of 2 % for $w_{\rm MAPA}$ = 0.4 at 353.15 K. The 1-MPZ aqueous solution at $w_{1-MPZ} = 0.1$ experienced a 2 % decrease in c_p at a temperature of 293.15 K. For the rest of the amine mass fractions and temperature conditions, the change in c_p with pressure is within the measurement uncertainty. As the amine mass fraction increases from 0.1 to 0.4, the c_p decreases. In these terms, c_p decreases by an average of 3 % for MAPA + H₂O and 7 % for 1-MPZ + H₂O mixtures. A maximum in c_p was observed when $w_{\text{amine}} = 0.1$ for aqueous solutions of MAPA, or 1-MPZ.

Regarding the comparison of the isobaric heat capacity of the two studied systems with those reported in the literature, the largest differences were observed with the aqueous solution of the primary amine MEA [33], as shown in Fig. 10. These differences reach 8 % for the MAPA solution and 4 % for the 1-MPZ solution; in both cases, MEA exhibits the lowest isobaric heat capacity. As detailed in Fig. 10, the comparison with two other aqueous systems, DEAE (tertiary amine) and EAE (secondary amine) [25], revealed notable differences of up to 3 % with the 1-MPZ solution. Conversely, values were mostly within the expanded relative uncertainty (1 %) range when compared to the MAPA



Fig. 5. Relative deviations (%) of calculated density measurements (ρ_{cal}) using modified Tamman-Tait equation with the parameters provided in Table 5 and 6, in comparison with literature values (ρ_{lit}). a) Literature for MAPA + H₂O: (\circ) Monteiro et al. [11] and (\Box) Wang et al. [18], (\blacktriangle) Pinto et al. [22]. b) Literature for 1-MPZ + H₂O: (\diamond) Rayer et al. [19] and (+) Vamja et al. [20].



Fig. 6. Experimental isobaric heat capacity c_p , for MAPA(1) + H₂O(2) mixture as a function of temperature *T*, at pressure p = 0.1 MPa. Amine mass fraction: (*) $w_1 = 0$, (\diamondsuit) $w_1 = 0.1$, (\square) $w_1 = 0.2$, (\triangle) $w_1 = 0.3$, and (\circ) $w_1 = 0.4$. Isobaric heat capacity data of pure water ($w_1 = 0$) from NIST REFPROP database [29].



Fig. 7. Experimental isobaric heat capacity c_p , for MAPA(1) + H₂O(2) mixture as a function of pressure p, at temperature T = 313.15 K. Amine mass fraction: (\Diamond) $w_1 = 0.1$, (\Box) $w_1 = 0.2$, (Δ) $w_1 = 0.3$, and (\circ) $w_1 = 0.4$.



Fig. 8. Experimental isobaric heat capacity c_p , for 1-MPZ(1) + H₂O(2) mixture as a function of temperature *T*, at pressure p = 0.1 MPa. Amine mass fraction: (\Diamond) $w_1 = 0.1$, (\Box) $w_1 = 0.2$, (Δ) $w_1 = 0.3$, and (\circ) $w_1 = 0.4$.

solution. For all mentioned systems, the amine mass fraction was fixed at 0.4, and the pressure was maintained at atmospheric level.

As presented in [25] the experimental isobaric heat capacities were correlated with temperature T, and amine mass fraction w_1 at atmospheric pressure, using the empirical model proposed by Al-Ghawas et al. [34] and showed in Eqs. (9) and (10).

$$c_p = K_1 + K_2 T \tag{9}$$

$$K_i = k_{i,1} + k_{i,2}w_1 + k_{i,3}w_1^2 \tag{10}$$

where K_1 and K_2 are two parameters calculated by Eq. (10) using $k_{i,1}$, $k_{i,2}$ and $k_{i,3}$ values; *T* is the temperature in Kelvin and, w_1 is the amine mass fraction. Parameters k_{11} and k_{21} correspond to the fitting of the heat capacity of pure water and are fixed for both systems.

The correlation model parameters, determined by Eqs. (9) and (10), are presented in Table 8 for both amine solution systems. Fig. 11 compares the experimental isobaric heat capacities ($c_{p,exp}$) and calculated values ($c_{p,cal}$), showing that relative deviations are within the measurement uncertainty in most cases, except for three points belonging to



Fig. 9. Experimental isobaric heat capacity c_p , for 1-MPZ(1) + H₂O(2) mixture as a function of pressure p, at temperature T = 313.15 K. Amine mass fraction: (\Diamond) $w_1 = 0.1$, (\Box) $w_1 = 0.2$, (Δ) $w_1 = 0.3$, and (\circ) $w_1 = 0.4$.



Fig. 10. Experimental isobaric heat capacity c_p as a function of temperature *T*, at amine mass fraction w = 0.4 and pressure p = 0.1 MPa. Mixtures: (\Diamond) MAPA + H₂O, (\Box) 1-MPZ + H₂O, (\circ) MEA + H₂O [36], (*) EAE + H₂O [25], and (Δ) DEAE + H₂O [25].

Table 8

Fitted coefficients K_1 y K_2 in Eqs. (9) and (10) at pressure 0.1 MPa, and statistical metrics AAD, MAD, and σ in Eqs. (2) to (4).

Parameters	Binary Mixtures			
	$MAPA + H_2O$	$1-MPZ + H_2O$		
<i>k</i> ₁₁	4.1158	4.1158		
k ₁₂	-2.7279	-3.7294		
k ₂₁	$2.1821 \cdot 10^{-4}$	$2.1821 \cdot 10^{-4}$		
k ₂₂	$1.1062 \cdot 10^{-2}$	$1.1306 \cdot 10^{-2}$		
k ₂₃	$-9.6511 \cdot 10^{-3}$	$-4.8749 \cdot 10^{-3}$		
AAD/%	0.3	0.5		
MAD/%	0.9	1		
$\sigma/(kJ\cdot kg^{-1}\cdot K^{-1})$	0.02	0.03		

the 1-MPZ + H_2O mixture that drift slightly above 1 %. No systematic deviations were observed with respect to the isobaric heat capacity or the amine mass fraction. The statistical metrics: average absolute relative deviations (AAD) Eq. (2), the maximum absolute relative deviation



Fig. 11. Relative deviations between experimental isobaric heat capacity $c_{p,exp}$, and calculated isobaric heat capacity $c_{p,cab}$, using Eqs. (9) and (10) vs w_{amine} . Mixtures: (\Diamond) MAPA + H₂O, and (\square) 1-MPZ + H₂O. Dashed lines represent the relative expanded uncertainty of our measurements.

(MAD) Eq. (3) and the standard deviation (σ) Eq. (4) are satisfactory within the experimental uncertainty of our flow calorimeter. F-Test have been conducted [35] in order to find the best number of parameters for that correlation.

For the 1-MPZ + H₂O binary mixture, we found only one reference in the literature carried out by Poozesh et al. [21] reporting molar isobaric heat capacities in a range of amine mole fractions from $x_{amine} = (0.099$ to 1.000) mol/mol, temperatures from T = (298.15 to 353.15) K, and at atmospheric pressure p = 0.1 MPa. The expanded relative uncertainty (k = 2) in c_{pm} reported by Poozesh et al. [21] was 1 %. From this work three comparable data points have been found in terms of measurement conditions with respect to our work, as shown in Fig. 12. Relative deviations of less than 1 % have been obtained in the comparison, which is in good agreement with the reported uncertainty for the measurement. We found no isobaric heat capacity experimental data available in the literature for aqueous solutions of amines MAPA, therefore comparison could not be possible.



Fig. 12. Relative deviations (%) of molar isobaric heat capacity measurements $c_{pm,exp}$, in comparison with literature values $c_{pm,lit}$. Literature for 1-MPZ + H₂O: (__) Poozesh et al. [21].

4. Conclusions

In this work, experimental data for densities and isobaric heat capacities in a wide range of pressure and temperatures are presented. The mixtures under study were aqueous solutions of MAPA or 1-MPZ at an amine mass fraction between 0.1 and 0.4. Both solutions are good candidates for amine-based CO_2 capture, as indicated by studies available in literature related to their performance. However, experimental data for thermophysical properties such as density and isobaric heat capacity are almost missing in the literature, especially at high pressures. As an effort to cover this gap, the measurements were carried out over a wide range of temperatures, pressures, and amine mass fractions used for industrial CO_2 capture. For density, we studied temperatures between 293.15 K and 393.15 K and pressures up to 100 MPa. In the case of isobaric heat capacity, we reached temperatures up to 353.15 K and pressures up to 25 MPa.

For MAPA aqueous solutions, the density decreases as the concentration of amine increases. For 1-MPZ aqueous solutions, the relationship between density and amine concentration is more complex. At temperatures approximately below 325 K, the density increases as the amine concentration increases. However, at temperatures approximately above 325 K, the density decreases as the amine concentration increases. Density decreases with increasing temperature, whereas the opposite effect was observed when pressure increased. For both MAPA and 1-MPZ aqueous solutions, the isobaric heat capacity decreases as the amine concentration increases from 0.1 to 0.4. An increase in temperature causes an increase in isobaric heat capacity, which is particularly noticeable at the higher amine mass fractions considered in this work. Pressure had no significant effect on isobaric heat capacity. In addition, all mixtures exhibited high negative excess volume behaviour using the pure amine density from the literature. Experimental data follow the excess volume form literature with small deviations.

A modified Tammann-Tait equation [30,31] correctly represents the experimental data over the entire measurement conditions, achieving an absolute average relative deviation of 0.02 % between the experimental density values and the calculated densities. An exhaustive study of the fitting parameters has been conducted to determine the optimal number of parameters. Also, this correlation has been applied for comparison when literature data were not at the same experimental conditions (temperature or composition). For isobaric heat capacity, the calculated values from the empirical correlation proposed by Al-Ghawas [34] are in good agreement with the experimental data with an absolute average relative deviation of 0.4 %. The comparison with the scarce experimental data found in literature agreed with our measurements.

CRediT authorship contribution statement

Yisel Pérez-Milian: Writing – review & editing, Writing – original draft, Investigation, Data curation. David Vega-Maza: Writing – review & editing, Supervision, Methodology, Funding acquisition, Conceptualization. Juan D. Arroyave: Formal analysis, Data curation. Fredy Vélez: Writing – review & editing, Visualization, Validation, Methodology, Formal analysis. Xavier Paredes: Validation, Resources, Methodology, Formal analysis. Alejandro Moreau: Writing – review & editing, Validation, Supervision, Methodology, Investigation, Formal analysis, Data curation, Conceptualization.

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.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.molliq.2025.127685.

Data availability

Data will be made available on request.

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