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Thermophysical characterization of aqueous ternary system containing n-tris-[hydroxymethyl]methyl-3-amino propanesulfonic acid and glycol (PG or DPG or TPG)

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ABSTRACT

In this present work, a thermophysical property characterization of aqueous ternary system containing n-tris-[hydroxymethyl]methyl-3-aminopropanesulfonic acid (TAPS) and glycol was done. Thermophysical properties, including refractive index, density, and electrolytic conductivity, measurements were considered. The glycols considered are propylene glycol (PG), dipropylene glycol (DPG), and tripropylene glycol (TPG). The measurements were done over a temperature range of 298.15 K to 343.15 K and at normal atmospheric pressure. Different concentrations (4% to 16% by weight TAPS or 56% to 44% water, in a fixed amount of glycol – 40%) were used. The effects of temperature and compositions on the measured properties were discussed and then correlated based on the equation proposed for aqueous salt–glycol systems. Calculation results show that the applied model was satisfactory in representing the measured properties in the aqueous ternary systems containing TAPS and considered glycols.

1. Introduction

Considerable interest to enhance the rate of absorption of CO_2 in carbonate solution leads to investigation of various amino acids. Some amino acids have been used to enhance the rate of absorption of CO_2 in carbonate solution [1]. Several research groups have investigated the absorption of CO_2 in amino acid derivatives, such as amino acid salts and aqueous amino acid salts; the studies have reported encouraging observations [2–5]. The N-[tris(hydroxymethyl)methyl-3-amino] propanesulfonic acid (TAPS) is a derivative of taurine, an amino acid and biological buffer. On the basis of the predicted interaction between a weak acid (*i.e.*, HCOOH) and a zwitterion in one report [6], it is also predicted that CO_2, which usually forms the weak acid H_2CO_3 in aqueous environment, may be capable of association with the zwitterionic species of TAPS via strong OH–O hydrogen bonding interaction despite the weak acid not being capable of deprotonating the zwitterionic species.

Glycols on the other hand are known gas-dehydrating agents; some have been demonstrated to absorb acid gases, such as CO_2 and H_2S [1,7]. When mixed with an aqueous solution of TAPS, a possible candidate solvent for CO_2 absorption, a glycol is expected to lower the vapour pressure of the resulting mixture. Low solvent vapour pressure makes the separation of the absorbed gas during solvent recovery easier, resulting in recovery of high-purity gas [1]. However, other criteria in selecting the appropriate absorbent have sprung over issues like energy requirement, solvent regeneration and solvent corrosive property. In this regard, the use of amine-glycol systems for acid-gas absorption has become promising.

To fully utilize such favourable properties of this solvent system for used in absorption process, complete knowledge of thermophysical properties (such as density, refractive index, viscosity, heat capacity, electrical conductivity, *etc.*) is very necessary. However, to our knowledge very few have done a thorough thermophysical characterization [8–11], especially of a ternary solvent system. Therefore, in the light of the importance of this solvent system in absorption process as potential absorbent, this study measured and presented new data of density, refractive index, and electrolytic conductivity of aqueous solution containing TAPS and glycol for temperatures up to 343.15 K at normal atmospheric pressure. The concentration of glycol was fixed at 40% (w/w) and the TAPS (4% to 16%) and water (56% to 44%) were varied. The glycols considered are propylene glycol (PG), dipropylene glycol (DPG), and tripropylene glycol (TPG). The temperature and compositional dependency of the considered properties are presented and satisfactorily correlated using a modified form of the equation proposed by Söhnel and Novotný [12].

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TABLE 1
Details of the major chemicals used.

Chemical name	Mass fraction purity	M/(g·mol^{-1})	Supplier
Propylene Glycol	>0.99	76.09	ECHO Chemical
Dipropylene Glycol	>0.99	134.17	Alfa Aesar
Tripropylene Glycol	>0.99	192.26	Alfa Aesar
N-Tris-[hydroxymethyl]methyl-3-amino propanesulfonic acid	>0.99	243.27	ACROS Organics

2. Experimental

2.1. Chemicals

The purities (in mass fraction) of the chemicals as reported by their corresponding suppliers are presented in table 1. These chemical samples were used as received. The water used to prepare the aqueous solutions was Type 1 reagent grade (resistivity = 18.3 MΩ·cm; total organics 15×10^{-9}) which was purified using a compact ultrapure water system (Barnsted Thermodyne Easy Pure LF). A digital balance (Mettler-Toledo AL204) (accuracy = ±1 × 10^{-4} g) was used to weigh out the chemicals components of the solutions during preparation. The estimated uncertainty of the mole fraction of the aqueous solutions is 1.5×10^{-4}. The aqueous solutions were degassed using ultrasonic cleaner (Branson, Model 3510) before their properties were measured.

2.2. Property measurements

Prior to the measurements of the studied systems, substances having available literature data of the considered properties were measured first. This was done to ensure that the applied procedures and the apparatus for each property measurements could give acceptably accurate results. These solutions were referred to as calibration systems. For the measurement of density and refractive index, the deionised water mentioned before was used as calibration system, whereas for electrolytic conductivity measurements, the standard KCl solution (0.1 N) from Merck was used.

All measurements were carried out in three to five replicate runs and the average values were reported. The thermophysical property measurements for the considered ternary solutions were measured as follows:

TABLE 3
Densities (ρ) of the ternary (TAPS + Glycol + water) solutions investigated.

	ρ[a]/g·cm^{-3}		
	TAPS (1) + PG (2) + water (3): x_1/x_2[b]		
T/K	0.0045/0.1440	0.0109/0.1549	0.0217/0.1733
298.15	1.0724	1.0929	1.1226
303.15	1.0697	1.0900	1.1198
308.15	1.0669	1.0872	1.1167
313.15	1.0640	1.0842	1.1137
318.15	1.0610	1.0812	1.1106
323.15	1.0579	1.0780	1.1074
328.15	1.0548	1.0748	1.1042
333.15	1.0515	1.0716	1.1009
338.15	1.0482	1.0682	1.0975
343.15	1.0447	1.0648	1.0941
	TAPS (1) + DPG (2) + water (3): x_1/x_2		
T/K	0.0048/0.0786	0.0118/0.0850	0.0237/0.0960
298.15	1.0449	1.0635	1.0914
303.15	1.0417	1.0602	1.0881
308.15	1.0384	1.0569	1.0847
313.15	1.0351	1.0535	1.0813
318.15	1.0317	1.0501	1.0778
323.15	1.0282	1.0466	1.0742
328.15	1.0246	1.0430	1.0706
333.15	1.0209	1.0393	1.0669
338.15	1.0172	1.0356	1.0631
343.15	1.0133	1.0316	1.0593
	TAPS (1) + TPG (2) + water (3): x_1/x_2		
T/K	0.0049/0.0618	0.0120/0.0670	0.0242/0.0759
298.15	1.0451	1.0642	1.0924
303.15	1.0418	1.0608	1.0889
308.15	1.0384	1.0574	1.0855
313.15	1.0349	1.0538	1.0819
318.15	1.0314	1.0502	1.0782
323.15	1.0278	1.0466	1.0745
328.15	1.0241	1.0429	1.0708
333.15	1.0203	1.0390	1.0670
338.15	1.0165	1.0352	1.0630
343.15	1.0126	1.0313	1.0590

[a] $u(\rho) = \pm 5 \times 10^{-4}$ g·cm^{-3}.
[b] The compositions in mole fractions are based on the original weight percentages.

2.3. Specific density (ρ)

The densities of the solutions considered were measured using an integrated density measuring cell, which used the principle of oscillating U-tube and is supplied by Anton Paar Stabinger (model SVM 3000). The repeatability of the density measurement was

TABLE 2
Comparison of thermophysical properties (density, ρ; refractive index, n_D; electrolytic conductivity, κ) of the systems used for calibration.

T/K	ρ_{Water}/g·cm^{-3}		$n_{D\ Water}$/dimensionless		$\kappa_{KCl\ soln}$/mS·cm^{-1}	
	Wagner and Pruss [13]	This work	Leron *et al.* [14]	This work	Merck	This work
293.15					1.273	1.266
295.15					1.324	1.323
297.15					1.378	1.376
298.15	0.99705	0.9968	1.33246	1.332458	1.408	1.400
299.15					1.434	1.432
301.15					1.491	1.486
303.15	0.99565	0.9955	1.33189	1.331866	1.547	1.545
308.15	0.99403	0.9940	1.33126	1.331224	1.685	1.688
313.15	0.99222	0.9923	1.33052	1.330510	1.836	1.839
318.15	0.99021	0.9904	1.32973	1.329743	1.981	1.979
323.15	0.98804	0.9883	1.32888	1.328905	2.137	2.110
328.15	0.98569	0.9860	1.32797	1.327991		
333.15	0.98320	0.9836	1.32687	1.327051		
338.15	0.98055	0.9809		1.326048		
343.15	0.97776	0.9782		1.325045		
APD[a]	0.023		0.003		0.007	

[a] $APD/\% = \frac{100}{n} \times \sum_{i=1}^{n} |(\mathrm{Ref} - \mathrm{Expt})/\mathrm{Ref}|_i$, where n is the number of data points.