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Thermophysical property characterization of ternary system containing {glycol (DEG/TEG/T_4EG) + 2-amino-2-hydroxymethyl-1,3-propanediol + water}

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ABSTRACT

As part of our systematic study on physicochemical characterization of (glycol + amine) systems, thermophysical properties, including refractive index, density, and electrolytic conductivity measurements were carried out on aqueous systems containing glycol and 2-amino-2-hydroxymethyl-1,3-propanediol (TRIS). The glycols studied are diethylene glycol (DEG), triethylene glycol (TEG), and tetraethylene glycol (T_4EG). The measurements were done over a temperature range of (298.15 to 343.15) K at normal atmospheric pressure. Different concentrations (4 to 16)% by weight TRIS or (56 to 44)% water, in a fixed amount 40% glycol were used. The influences of temperature and compositions on the measured properties are discussed and then correlated based on the equation proposed for aqueous (glycol + salt) systems. Calculated results show that the applied model is satisfactory in representing the measured properties in the aqueous systems containing the glycols and TRIS.

1. Introduction

The high absorption capacity and fast rate of absorption of alkanolamines have made this class of compounds a suitable choice as absorbent for absorption process such as acid–gas (CO_2 and H_2S) capture [1–11]. 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 (glycol + amine) systems for acid–gas absorption has become promising. The use of a (glycol + amine) system has the advantage of simultaneous purification and dehydration and lower steam consumption when compared to aqueous blended-amine systems. Furthermore, (glycol + amine) solutions can be stripped almost completely of CO_2, resulting in the capability of producing extremely high-purity gas [12]. However, the (glycol + amine) system has also a number of drawbacks which have seriously limited its usefulness such as high vaporization loss of the amine component [12]. Thus, the choice of amine in this solvent system seems to bear the more concern. Here, the amine used is not the conventional amine used in the industry but its biological counterpart, 2-amino-2-hydroxymethyl-1,3-propanediol (TRIS). It is an amine buffer that was first introduced for the clinical treatment of acid base disorders. Its low cost and biological applicability make it a suitable candidate as alternative to those highly volatile conventional amines.

To fully utilize such favorable properties of this solvent system for used in absorption process, complete knowledge of thermophysical properties (such as refractive index, density, viscosity, heat capacity, and electrical conductivity) is very necessary. However, to our knowledge very few have done a thorough thermophysical characterization, 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 refractive index, density, and electrolytic conductivity of aqueous solution containing glycol and TRIS for temperatures up to 343.15 K at normal atmospheric pressure. The concentration of glycol was fixed to 40% (w/w) and the TRIS (4 to 16)% and water (56 to 44)% were varied. The glycols considered glycols diethylene glycol (DEG), triethylene glycol (TEG), and tetraethylene glycol (T_4EG). 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 [13].

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 M · cm; total organics $15 \cdot 10^{-9}$) which was purified

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TABLE 1
Provenance and purity of the major chemicals used.

Chemical name	Mass fraction purity	$M/(g \cdot mol^{-1})$	Supplier
Diethylene glycol	>0.9990	106.12	TEDIA Co., Inc.
Triethylene glycol	>0.9996	150.17	TEDIA Co., Inc.
Tetraethylene glycol	>0.9950	194.23	ACROS Organics
2-Amino-2-hydroxymethyl-1,3 propanediol	>0.9995	121.14	MP Biomedicals

using a compact ultrapure water system (Barnsted Thermodyne Easy Pure LF). A digital balance (Mettler-Toledo AL204) (accuracy = $1 \cdot 10^{-4}$ g) was used to weigh out the chemical components of the solutions during preparation. The estimated uncertainty of the mole fraction of the aqueous solutions is $1.5 \cdot 10^{-4}$. 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 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 refractive index, density and viscosity, 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:

2.2.1. Refractive index (n_D)

The refractive index of each solution was measured in triplicate using an Abbemat WR-MW digital refractometer having an uncertainty of $\pm 4 \cdot 10^{-5}$. It consisted of an internal solid state Peltier thermostat and two internal Pt-100 Platinum resistance temperature sensors for exact temperature measurement. Through these features, exact temperature measurements were assured. For each trial, 1 cm^3 of the sample was used in the experiment. A total of 3 cm^3 per sample was used in the experiment. The refractometer finds the critical angle of an incident beam of monochromatic light. Here the sample to be measured is placed on the polished surface of a prism made of synthetic YAG, a hard scratchproof and corrosion resistant material. A cone-shaped yellow light beam of 589.3 nm sodium D wavelength illuminates the sample from its bottom side under different angle of reflection. Then a microprocessor calculates the refractive index of the sample from the results obtained. The estimated uncertainties for temperature and refractive index were ±0.03 K and $5 \cdot 10^{-5}$, respectively.

2.2.2. Specific density (ρ)

The density of the solutions was measured in triplicate by means of the SVM 3000 Stabinger density measuring cell having an uncertainty of $\pm 4 \cdot 10^{-4}\ g \cdot cm^{-3}$. The density meter used the principle of oscillating U-tube. The sample is introduced into a U-shaped tube that is electronically excited to oscillate at its characteristic frequency. The characteristic frequency changes depending on the density of the sample. Through precise determination of the characteristic frequency and an appropriate adjustment, the density of the sample is determined. But, due to the high temperature dependency of the density, the measuring cell has to be accurately thermostatted. For each concentration, 5 cm^3 was placed in a syringe, and 1.5 cm^3 of it was used per trial. The repeatability of the density measurement was $\pm 0.0002\ g \cdot cm^{-3}$ and the estimated uncertainty for temperature was ±0.002 K. The uncertainty of the reported ρ data was estimated to be $5 \cdot 10^{-4}\ g \cdot cm^{-3}$.

2.2.3. Electrolytic conductivity (κ)

The electrolytic conductivities of the investigated solutions were measured using SC-170 conductivity meter manufactured by Suntex, which operates with ac current of 60 Hz frequency. The temperature was monitored by a digital thermometer (model 3002, CROPICO), with an uncertainty of 0.01 K. The uncertainty of the reported κ data was estimated to be 1%.

2.3. Validation of the measurements

The measurement methodologies applied for the properties investigated were validated first before the measurement of the system considered as mentioned previously. The validation of the measurements using the calibration systems are presented in table 2. The measurements in this work are in good agreement with the available data (for similar systems) in the literature, as seen in this table. Such good agreement was quantitatively evaluated via the average percentage deviation (APD). The APD for the

TABLE 2
Comparison of thermophysical properties (n_D, ρ, κ) of the systems used for calibration.

T/K	$n_{D\ Water}$/dimensionless		$\rho_{Water}/(g \cdot cm^{-3})$		$\kappa_{KCl\ soln}/(\mu S \cdot cm^{-1})$	
	Schiebener and Straub [14]	This work	Wagner and Pruss [15]	This work	Merck	This work
298.15	1.33336	1.333506	0.99705	0.9971	1273	1267
303.15		1.332980	0.99565	0.9957	1324	1314
308.15	1.33230	1.329062	0.99403	0.9941	1378	1357
313.15		1.331767	0.99222	0.9924	1404	1391
318.15	1.33095	1.331040	0.99021	0.9904	1434	1443
323.15		1.330254	0.98804	0.9882	1491	1493
328.15	1.32937	1.329417	0.98569	0.9859	1547	1551
333.15		1.328512	0.98320	0.9835	1685	1688
338.15	1.32757	1.327550	0.98055	0.9809	1836	1835
343.15		1.326536	0.97776	0.9781	1981	1881
348.15	1.33336	1.333506	0.99705	0.9971	1273	1267
APD[a]	0.051		0.019		0.998	

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