Full Length Research Paper

Introducing mole fraction in the density calculations of liquid-liquid solutions

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Accepted 15 December, 2012

The densities of an ideal and a non-ideal liquid-liquid solution were determined experimentally. The experimental results were then compared to calculated values using two mathematical expressions for density, employing partial densities in one and mole fraction in the other. Results were presented in form of tables and graphs, indicating the validity of applying mole fractions in the estimation of liquid-liquid solutions.

Key words: Density, ideal solution, non-ideal solution, mole fraction.

INTRODUCTION

Density is a variable of state for a thermodynamic system meaning that, it depends on its values at the initial and final pressure and temperature state (Lago and Gluliano, 2011). The mass density or density, ρ , of a material is defined as its mass per unit volume, or, also, weight per unit volume. It is an intensive property indicating how tight the particles are packed inside the substance and it can be expressed as:

$$\rho = m/V \quad (1)$$

Where,

ρ = Density (kg/m³ or g/cm³)

m = Mass (kg or g)

V = Volume (m³ or cm³)

The most used units for density are the SI units (kg/m³) and the cgs units (g/cm³), and it is a dimensionless quantity when expressed as specific gravity (SG) or relative density (RD). Densities of materials differ and it is an important concept regarding buoyancy, purity, and packaging. It could be used to identify the material or calculate its volume mass and can also be used in analyzing how materials interact in fluid mechanics,

weather, geology, material sciences, engineering, and other fields of Physics.

Density concept is also thought of, as a spatial concept that is used as a tool in predicting and controlling land use (Boyko and Cooper, 2011). It is used as a metric by decision makers from many different disciplines and professions (Churchman, 1999). In that sense, it may be defined as a number of units in a given area, for example, number of people per hectare or number of dwellings in km² (Boyko and Cooper, 2011).

Experimental determination of density occupies a central place for several reasons. In one hand, measurements of density as a function of pressure and temperature allow to obtain two derived properties, the isobaric thermal expansivity and the isothermal compressibility (Rowlinson and Swinton, 1982). An experimental methodology for precise determination of density of room temperature ionic liquids as a function of temperature and pressure using vibrating tube densimeter was proposed by Sammamed et al. (2010). In fact, recently, there has been an increasing interest in the thermodynamics of room temperature ionic liquids (Marsh et al., 2004; Heintz, 2005), which are classified as potential "green" substitutes for the volatile organic compounds commonly used in industry (Holbrey and Seddon, 1999).

The determination of liquids density is usually carried out by weighing the mass of a measured volume of liquid using a digital balance. Most of the workers deal with experimental measurements of thermophysical

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Table 1. Density values of liquids used.

Material	Density g/cm ³
Water	1.0
96% ethanol	0.79
Benzene	0.88
Carbon tetrachloride	1.59

Table 2. Experimental and calculated density data for ethanol – water solutions.

Exp. no.	Volume (%)		ρ partial (calc.)		$\rho_{T \text{ exp.}}$	ρ calc.	
	H ₂ O	C ₂ H ₅ OH	H ₂ O	C ₂ H ₅ OH		$\Sigma \rho_i V_i / V_t$	$\Sigma x_i \rho_i$
1	100	0.00	1.0	0.00	0.988	1.0	1.0
2	83.3	16.70	0.833	0.131	0.959	0.965	0.988
3	62.5	37.50	0.615	0.296	0.916	0.921	0.968
4	50.0	50.00	0.50	0.395	0.892	0.895	0.95
5	41.66	58.34	0.416	0.460	0.873	0.877	0.936
6	35.7	64.30	0.357	0.507	0.860	0.865	0.924
7	31.25	68.75	0.312	0.543	0.853	0.855	0.914

properties at atmospheric pressure. Since the effect of pressure and temperature on the densities of liquids is small, determinations of liquids density are done at ambient temperature and pressure.

On the other hand, the density of a solution is the sum of mass concentrations of the components of that solution. Mass concentration of a given component p_i in a solution can be called partial density of that component:

$$P = \Sigma p_i \quad (2)$$

Expressed as a function of the densities of pure components of the mixture and their volume participation, it reads:

$$\rho = \Sigma p_i V_i / V_t \quad (3)$$

EXPERIMENTAL

Materials and apparatus

Distilled water, 96% ethanol (PANREAC QUIMICA SA), benzene (PANREAC QUIMICA SA), and carbon tetrachloride (E.MERK D-6100, Darmstadi, F.R. Germany) are used.

Instruments and apparatus

A four decimal digital balance, four burettes, two 25 ml beakers, and glass wares commonly found in laboratories were used

Instructions

The non-ideal solutions were prepared from distilled water and 96% ethanol. 5.0 ml of water was added from burette and its weight was

recorded. From another burette containing 96% ethanol, different portions of known volumes were added and the weights were recorded after each addition. The weight of 5.0 ml of ethanol was determined separately. While, the ideal solutions were prepared from benzene and carbon tetrachloride and the weights were determined similarly. A minimum of six readings were taken. The experimental density values were then compared to the calculated ones using the mathematical expressions in Equations 3 and 4:

$$\rho = \Sigma x_i \rho_i \quad (4)$$

Where,

ρ_i is the literature density values (Table 1), (Furniss et al., 1989), V_i and V_t are the component and total volumes, respectively, and x_i is the mole fraction of component.

RESULTS AND DISCUSSION

The results were presented in Tables 2 to 4 and Figures 1 to 4. Tables 2 and 3 lists the volume percent of solutions components, the partial density of each component in the different solutions, the experimental total densities of solutions and the calculated densities using Equations 3 and 4. The data are presented graphically by Figures 1, 2, and 3. Table 4 lists the mole fractions, partial densities of components and the total densities of the as prepared different ideal solutions. The data are graphically presented in Figure 4.

It is evident that Equation 4 is valid for non-ideal solutions, while both Equations 3 and 4 could be used to estimate the densities of ideal solutions. It was observed that there is a close analogy between the behavior of density and vapour pressure variations of ideal and non-ideal solutions.

Table 3. Experimental and calculated density data for benzene – carbon tetrachloride solutions.

Exp. no.	Volume (%)		ρ partial (calc.)		$\rho_{t \text{ exp.}}$	ρ calc.	
	C_6H_6	CCl_4	C_6H_6	CCl_4		$\Sigma \rho_i V_i / V_t$	$\Sigma x_i \rho_i$
1	100	0.0	0.878	0.00	0.891	0.877	0.878
2	00.0	100	0.00	1.59	1.587	1.59	1.59
3	83.3	16.7	0.731	0.265	0.993	0.995	0.988
4	62.5	37.5	0.548	0.596	1.143	1.144	1.134
5	50.0	50.0	0.439	0.795	1.233	1.233	1.233
6	41.66	58.34	0.365	0.927	1.294	1.292	1.279
7	33.33	66.67	0.292	1.06	1.354	1.352	1.339
8	29.41	70.59	0.258	1.122	1.381	1.380	1.368
9	25.00	75.0	0.219	1.192	1.413	1.411	1.401
10	20.00	80.0	0.175	1.272	1.449	1.447	1.438
11	16.66	83.34	0.146	1.325	1.472	1.471	1.463

Table 4. Mole fractions and partial densities of C_6H_6 and CCl_4 and total densities.

Exp. no.	C_6H_6		CCl_4		ρ_T
	X	ρ	X	ρ	
1	0	0	1	1.59	1.59
2	1	0.878	0	0	0.878
3	0.845	0.742	0.155	0.246	0.988
4	0.646	0.567	0.356	0.567	1.134
5	0.521	0.458	0.479	0.775	1.233
6	0.437	0.384	0.563	0.895	1.279
7	0.352	0.309	0.648	1.03	1.339
8	0.312	0.274	0.688	1.094	1.368
9	0.266	0.234	0.734	1.167	1.401
10	0.214	0.188	0.786	1.25	1.438
11	0.179	0.157	0.821	1.306	1.463

Figure 1. H_2O volume (%) versus partial and total densities of water-ethanol solutions ($\square$ ρ_T exp.; Δ ρ_T partial density of ethanol; $\bullet$ ρ_T partial density of H_2O).

Figure 2. H₂O volume (%) versus total densities (ρ_T) of water-ethanol solutions. [$\square$; ρ_T exp.; $\blacktriangle$ ρ_T calc.; (eq. 4); $\bullet$ ρ_T calc. Equation 5].

Figure 3. C₆H₆ volume (%) versus total density (ρ_T). $\square$ ρ_T exp.; $\blacktriangle$ ρ_T calc. (eq. 4); $\bullet$ ρ_T calc. (eq. 5).

Conclusion

In conclusion, one could estimate the density of liquid – liquid solutions employing the mole fraction of solution component. The results obtained are in good agreement with the experimental values. This will help much students and research workers where a densometer or even a digital balance is unavailable.

ACKNOWLEDGEMENTS

This project was supported by King Saud University, Deanship of Scientific Research, College of Science Research Center.

Figure 4. C₆H₆ mole fraction, χ , versus. total ($\square$ ρ_T) and partial densities of C₆H₆ ($\bullet$) and CCl₄ (Δ).

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