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Thermo physical properties of organic compound and its impact on environment

K. Sathya[1], R. Baskaran[2] and T.R. Kubendran[3]

[1]Department of Biotechnology, Rajalakshmi Engineering College, Chennai-602 105, India
[2]Department of Chemical Engineering, St. Joseph's College of Engineering, Chennai-600 119, India
[3]Department of Chemical Engineering, A.C. College of Technology, Anna University, Chennai-600 025, India
*Corresponding Author E-mail: sathyak80@gmail.com

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Abstract

Liquid mixtures have attracted considerable attention due to their unusual behaviour.In pharmaceutical, chemical and biochemical industries, organic compounds are used as an intermediate and are normally handled in fluid form and as a consequence, the physical, chemical, and thermo physical properties of fluids assume importance due to their environmental impact. The emission of volatile or partially volatile compounds must be reduced to appropriate levels before exposing industrial streams to atmosphere. One of the most widespread technologies used to achieve that reduction is activated carbon fixed bed adsorption. These processes are operated at different temperatures. Design of such operations require quantitative estimates of thermo physical properties of fluid mixtures and equilibrium constant. In the present study, densities, viscosities and ultrasonic velocitiesof paraanisaldehyde-ethylacetate organic mixture was measured over the entire mole fractions at 308.15, 318.15 and 328.15K.Studies on determination of different thermo physical properties of liquid mixtures within wide range of composition and temperature are valuable sources of information that might be used to examine relation between the internal structure of the system and its physical properties. Excess Gibbs free energy was obtained at different temperature from the measured properties and the spontaneity of the process was discussed.The impact of organic compound, based on Gibbs free energy values were also discussed. The positive Gibbs free energy revealed that the adsorption is not favourable (non-spontaneity) and hence the impact on the environment of the binary liquid mixtures is high at 308.15, 318.15 and 328.15K.

Key words

Density, Excess gibbs free energy, Viscosity

Introduction

Organic compounds like paraanisaldehyde - ethyl acetate mixtures are widely used as intermediates in pharmaceuticals and agrochemicals industries. the paraanisaldehyde along with acid and ethanol is frequently used to stain thin layer chromatography plates (Saravana kumar *et al.,* 2012). The unused organic compounds are discharged as waste in effluent water. The removal of these organic compounds from waste water is essential before the stream are let out or recycled back. Adsorption process is recognized as one of the effective and low cost technique for removal of organic pollutants from the waste water, and produces high quality treated effluent (Rasheed, 2013). The present work discusses about the feasibility of the treatment of the above waste water at various temperatures, based on the excess Gibbs free energy of compounds. For the successful design and operation of adsorption process, the data of thermo physical properties like density, viscosity and ultrasonic sound of the organic liquid mixture is important to establish. The feasibility studies of the adsorption process for organic liquid mixtures are essential before the adsorption process which involves the excess Gibbs energy calculation. since no data is reported in the literature. The present study aimed is to find out the feasibility of the process by estimating excess Gibbs free energy in terms of thermo physical properties like density, viscosity and ultrasonic velocity at various temperatures to conclude the impact on environment.

Properties of Organic Compound

I. Paraanisaldehyde

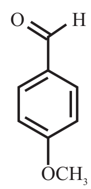

Fig . 1 : Molecular structure of Paraanisaldehyde

Paraanisaldehyde is an organic compound that is a clear to slightly yellow oily liquidwithstrong aroma. Its molecular formula is $C_8H_8O_2$. It occurs naturally in the fennel and anise plants. It is a high volume chemical with production over 1 million pounds annually.The compound consists of a benzene ring with an aldehyde and a methoxy group. It is a clear liquid with a strong aroma(Fahlbush 2003).

Formula : $C_8H_8O_2$

Density : 1.12 g cm^{-3}

Molar mass: 136.15 g mol^{-1}

Melting point: 0 °C

Boiling point: 248 °C

ii. Ethyl acetate

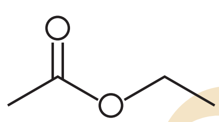

Fig . 2 : Molecular structure of Ethyl acetate

Ethyl acetate is the organic compound with the molecular formula CHƒ -COO-CH, -CHƒ , simplified to C,, Hˆ O, . This colourless liquid has a characteristic sweet smell and is used in glues, nail polish removers, decaffeinating tea and coffee, and cigarettes(Fahlbush 2003).

Formula: $C_4H_8O_2$

Density: 0.897g cm^{-3}

Molar mass: 88.11 g mol^{-1}

Melting point: -83.6 °C

Boiling point: 77.1 °C

Impact on Environment

General : Volatile organic compounds (VOCs) are gases or vapours emitted by various solids and liquids, many of which have short- and long-term adverse effects on human health and the environment. VOCs from petroleum are toxic and foul the air, extremely toxic, carcinogenic and cause DNA damage (Rasheed 2013).

Major sources of man-made VOCs are coatings, especially paints and protective coatings. Solvents are required to spread a protective or decorative film. Approximately 12 billion litres of paints are produced annually. Typical solvents are aliphatic hydrocarbons, ethyl acetate, glycol ethers, and acetone (Luo *et al.*, 2013).

Respiratory, allergic, or immune effects in infants are associated with man-made VOCs and other indoor or outdoor air pollutants. Health effects include eye, nose, and throat irritation; headaches, loss of coordination, nausea; and damage to the liver, kidney, and central nervous system. Some organics can cause cancer in animals; some are suspected or known to cause cancer in humans. Key signs or symptoms associated with exposure to VOCs include conjunctival irritation, nose and throat discomfort, headache, allergic skin reaction, dyspnea, declines in serum cholinesterase levels, nausea, vomiting, nose bleeding, fatigue, dizziness.

Many organic compounds are known to cause cancer in animals; some are suspected of causing, or are known to cause, cancer in humans (Huiping *et al.*, 2014).

Selected compound : Short-term exposure to high levels of ethyl acetate results first in irritation of the eyes, nose and throat, followed by headache, nausea, vomiting, sleepiness, and unconsciousness. Very high concentrations may cause a stupor. Prolonged exposures may cause clouding of the eye, damage to the lung, heart, kidney and liver problems (Peder *et al.*, 2007).

Paraanisaldehyde is a suspected neurotoxicant according to the Registry of Toxic Effects of Chemical Substances

Ethyl Acetate enters the environment through evaporation and is a volatile organic chemical (VOC) (Wolkoff *et al.*, 2006).

Materials and Methods

All the chemicals (paraanisaldehyde-ethyl acetate) used in this study were of analytical grade and obtained from

Lobo Chemicals, India. The claimed mass fraction purity of the chemicals was $p \geq 0.998$. These chemicals were dried over molecular sieves and partially degassed prior to use (Perrin *et al.,*1998; Saravana kumar *et al.*, 2012). The purity of these experimental chemicals was checked by comparing the observed densities, viscosities with those reported in the literature.

Binary mixtures were prepared by mixing appropriate volume of the liquid components in the specially designed glass bottles with air tight Teflon coated caps and the mass was measured on a Shimadzu Corporation Japan type BL 2205 electronic balance, with a precision of ± 0.01 mg. The required properties were measured on the same day immediately after preparing each composition. The uncertainty of mole fraction were ± 0.001. For all the measurements, temperatures were controlled by circulating the water through a thermostat (Technico, Madras. made in India) keeping temperature fluctuations within ±0.03K.

Density : Densities were determined by using a 25 cm^3 bicapillary pycnometer and calibrated with deionized double distilled water with a density of 996.0 kg. m^{-3} at a temperature of 308.15 K. The pycnometer was thermostatted in a transparent walled water bath (maintained constant to ± 0.01 K) for 15 min to attain thermal equilibrium, and the level of liquid in the two arms was obtained with a travelling microscope which could read upto 0.01 mm. The precision of the density measurements was estimated to be ± 0.003 g $\cdot cm^{-3}$(Saravanakumar *et al.*, 2012).

Viscosity : Viscosities were measured with Ostwald viscometer previously calibrated using water. The time was measured with a precision of 0.01s, and the uncertainty in the viscosity was estimated to be less than 0.003 mPa·s. The kinematic viscosity was obtained from the working equation

$$\upsilon = at + b/t \quad (1)$$

where, the two constants a and b were obtained by measuring the flow time t of benzene (Saravanakumar *et al.*, 2012).

Sound speed: Speed of sound was measured by using a variable path, single crystal interferometer. (Mittal Enterprises, New Delhi) at a frequency of 2 MHz. The interferometer was calibrated using toluene. The interferometer cell was filled with test liquid, and temperature of the solution was maintained constant within ± 0.01 K by circulation of water from a thermostatically regulated water bath through water jacketed cell. The uncertainty was estimated to be 2 ms^{-1}(Saravanakumar *et al.,* 2012).

Excess Gibbs free energy of binary mixture was obtained from the following equation

$$\Delta G^E = RT\,[\ln(\eta V) - (X_1 \ln(\eta_1 V_1) + X_2 \ln(\eta_2 V_2))] \quad (2)$$

where, R is the universal constant of gases; T is the absolute temperature, V_1 and V_2 are the molar volumes of component 1 and 2; x_1 and x_2 represents the mole fraction of component 1 and 2. $V_m$was obtained from equation 4 below. η_1, η_2 and η_m are the viscosity of component 1 and 2 and mixture, respectively.

$$V_m = x_1 m_1 + x_2 m_2 / \rho_m \quad (3)$$

Where,ρ_m is the density of mixture (Mardones *et al.*, 2014).

Results and Discussion

Measured values of densities, viscosities and ultrasonic velocities of paraanisaldehyde-ethyl acetate binary liquid mixture at different temperature is shown in Fig. 3, 4 and 5. The present of data revealed decrease in density, viscosity and ultrasonic velocity with temperature. It was due to more molecular interaction between the binary liquid mixture (Saravanakumar *et al.*, 2012; Saravanakumar *et al.,* 2011). Effect of temperature on density, viscosity and ultrasonic velocity is considered important, because excess Gibbs free energy is mainly depends on these properties and is calculated from the measured experimental data.

Excess Gibbs free energy provides information about the molecular interactions and macroscopic behaviour of fluid mixtures which can be used to test and improve thermodynamic models for calculating and predicting fluid phase equilibrium(Mchaweh *et al.,* 2004). The magnitude of excess Gibbs free energy represents the strength of interaction between unlike molecules (Riddick 1986; Perrin 1988; Gales and Mendes 2000).

The Gibbs free energy change indicates the degree of spontaneity of an adsorption process. The negative and positive value reflects favourable, as well as unfavourable adsorption. The Gibbs free energy has been also used to find equilibrium constant in the adsorption studies of organic compound. (Gales and Mendes 2000; Mardones *et al.,* 2014; Setiyanto *et al.*, 2013; Liu 2009).

The effect of temperature on Excess Gibbs free energy for paraanisaldehyde- ethyl acetate binary system is shown in Fig. 6, 7 and 8.Excess Gibbs free energy was found to be positive for all temperatures. The positive value of excess Gibbs free energy of binary mixture indicate the presence of specific and strong interactions in the systems (Ezekiel *et al.*, 2012; Kondaiah and Krishna Rao 2013). Positive Gibbs free energy indicates the non-spontaneous nature of the process. A positive value of Gibbs free energy revealed that there was an energy barrier. When the ions enter from the solution into the particle surface, some of the water

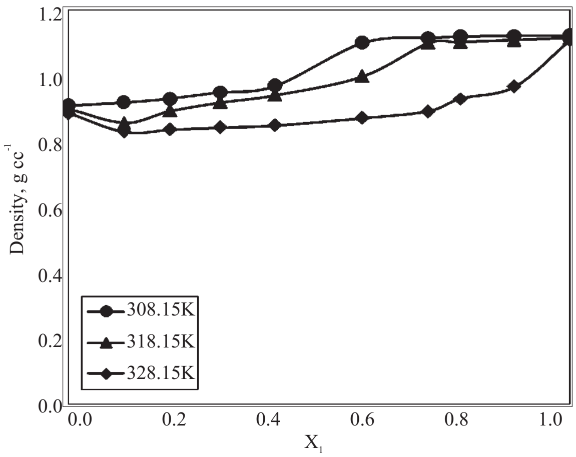

Fig. 3 : Effect of temperature on density on binary mixture of p-anisaldehyde and + ethyl acetate]

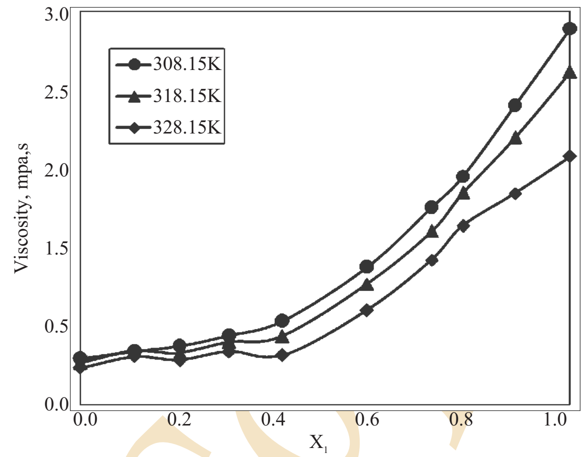

Fig. 4 : Effect of temperature on viscosity of binary mixture of p-anisaldehyde and + ethyl acetate]

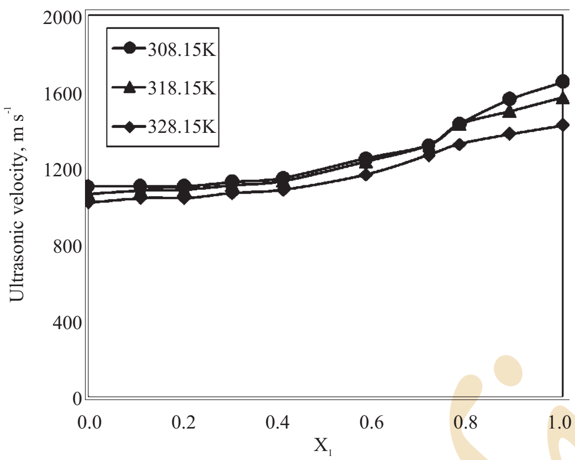

Fig. 5 : Effect of temperature on Ultrasonic velocity p-anisaldehyde (1) + ethyl acetate (2)

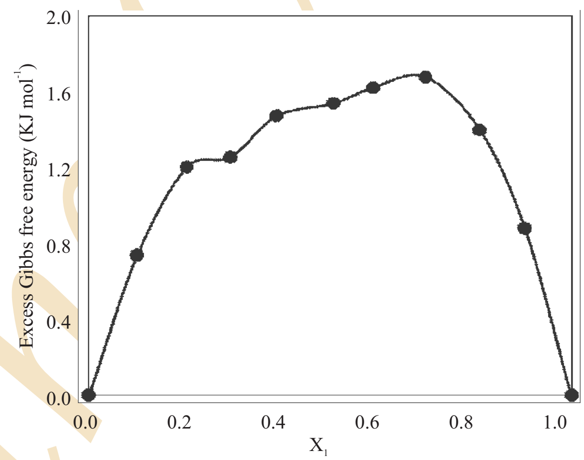

Fig. 6 : Effect of temperature on Excess Gibbs free energy at 308.15K for [p-anisaldehyde (1) + ethyl acetate (2)]

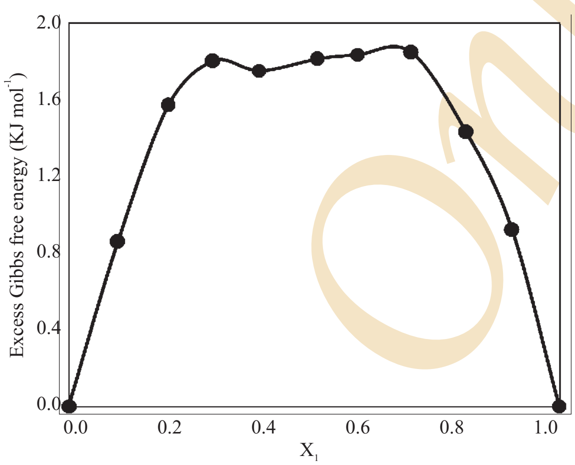

Fig. 7 : Effect of temperature on Excess Gibbs free energy at 318.15K for [p-anisaldehyde (1) + ethyl acetate (2)]

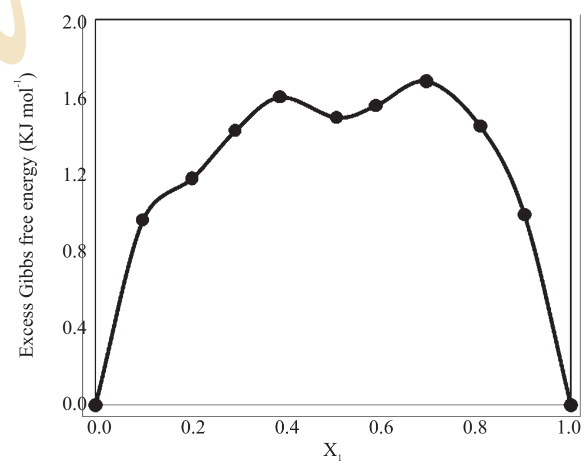

Fig. 8 : Effect of temperature on Excess Gibbs free energy at 328.15K for [p-anisaldehyde (1) + ethyl acetate (2)]

molecules forming hydration shell of ions gets stripped off and simultaneously the degree of freedom of ions is decreased. so the feasibility of the process is reduced. Hence, the adsorption did not occur or adsorption will be endothermic in nature (Ayar *et al.,* 2008). So treatment of these types of organic mixtures is not feasible at 308.15, 318.15 and 328.15 K. The impact of these compounds on environment can not be reduced easily due to non spontaneity nature or less feasibility.

Hence, densities, viscosities and ultrasonic velocities for organic binary mixtures are measured experimentally at different temperature over wide concentration range. The effects of temperature on densities, viscosities, ultrasonic velocities and excess Gibbs free energies on mixture were reported in Fig. 3, 4, 5, 6,7 and 8. Positive Gibbs free energy indicates the non-spontaneous nature of the adsorption process involves in the treatment of effluent waste water. It revealed that the impact of paraanisaldehyde- ethyl acetate binary system on environment would be high at 308.15, 318.15 and 328.15 K.

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