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Thermodynamic and transport properties of sodium dodecylbenzenesulphonate (SDBS) in aqueous medium over the temperature range 298.15 K to 333.15 K

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ABSTRACT

Measurements of density and dynamic viscosity of binary mixtures of water + sodium dodecylbenzenesulphonate (SDBS) solutions have been carried out over the entire concentration regime in the temperature range (298.15 K to 333.15 K) at 5 K intervals. The densities were measured by using a Mettler Toledo, DE45 delta range density meter, based on electromagnetically induced oscillations of a U-shaped glass tube. An automated Anton Paar microviscometer was used for the measurement of dynamic viscosities. Both the instruments have an automatic temperature control system maintained by Peltier effect. Temperature dependent densities were satisfactorily correlated with a second order quadratic polynomial equation and dynamic viscosities were correlated with Arrhenius equation. Various useful thermodynamic parameters viz. thermal expansion coefficient and apparent molar volume have been calculated from density data. The results are critically discussed in terms of interactions. The work mainly focuses on environmental consideration and significance of thermodynamic and transport properties data of ubiquitous environmental pollutant (SDBS) and their utilisation in the improvement of design and calculation methods for its treatment and separation processes to minimize its toxicity and environmental hazards.

1. Introduction

The anionic surfactants, among which are the alkylbenzene sulphonates, major constituents of synthetic detergents, are widely used in various industrial processes, such as in paper industries, electroplating, cosmetics, food processing, laundry, and vehicle washing [1]. These surfactants and especially the products of their degradation (sulphophenyl carboxylate) may remain for long periods of time and may be responsible for foams in rivers and surface waters, thereby reducing the oxygen penetration in water and causing environmental risks for aquatic organisms [2]. Strong detergents representing alkylbenzene sulphonates with branched alkyl chains were the first class of compounds showing problems of recalcitrant harmful waste in the environment [3]. Detergent induced foaming in aerotanks reduces their efficiency and settling ability of sludge; this is particularly the case with the treatment of industrial wastewater, which may contain up to 300 mg/L surfactants [4]. Reliable thermodynamic and transport property data of environmental contaminants are highly significant from both practical and theoretical points of view. Environmental and chemical engineers explore these data for transfer modelling of these pollutants in the aquatic environment, solve the remediation of contaminated soils, sediments and surface waters, minimize the presence of hazardous pollutants in aqueous effluents, contribute new strategies for economical and effective cleaning procedures and then, adequate decisions and remediation policies [5,6].

In the present work, we have measured the density, dynamic viscosity, of the aqueous solutions of aforesaid surfactant. Thermal expansivity and apparent molar volume were calculated from density data. Temperature and concentration dependent density and viscosity data of aqueous solutions containing surfactants have great application in designing various theoretical models related to fluid flow, heat and mass transfer, oil recovery [7] and also in improving the separation, desalination, oxidation, and other remediation methods for the effective removal of toxic contaminants from water [8,9]. Several workers successfully employed density and viscosity data in computation and modelling of other useful thermodynamic parameters of great relevance [10–15]. Pandey et al. [16–18] successfully explored the temperature dependent density and viscosity data and empirically calculated many thermodynamic properties of industrial and environmental concerns of multicomponent liquid systems of hazardous polyaromatic hydrocarbons and many other organic and inorganic pollutants. The aim of this study is to thermophysically characterize the toxic organic surfactant sodium dodecylbenzenesulphonate, its fate and thermodynamic behaviour in aqueous media in order to develop cost effective remediation plans.

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2. Materials and methods

2.1. Chemicals

Sodium dodecylbenzenesulphonate (SDBS) has been purchased from M/S Loba Chemie, SD fine chemicals. Molecular structure of the surfactant has been given in Fig. 1. Doubly-distilled deionised water was used for preparing solutions and obtained from Millipore, Milli-Q Academic water purification system. The molarities of the solutions were prepared with an accuracy of ± 0.0001 mM.

2.2. Density measurement

The (water + SDBS) containing different millimolar concentrations of SDBS were prepared by mass using Adventurer Ohaus AR2130 balance having a precision of ± 0.1 mg. Densities of the solutions (water + SDBS) were measured using a Mettler Toledo, DE45 delta range density meter. The U-tube of the density meter was washed with water and acetone and dried with air before measurement. The density meter was calibrated by dry air and ultra pure water. The measurements were performed at 5 K intervals over the temperature range (298.15 to 333.15) K. The uncertainty associated with temperature was measured to within ± 0.1 K. The standard deviations associated with the density measurement are $\leq 5 \times 10^{-3}$ g/cm^3. The density measurement of the above mentioned density is based on electromagnetically-induced oscillations of a U-shaped glass tube.

2.3. Viscosity measurement

The dynamic viscosities were measured with a Peltier-based automated Anton Paar microviscometer having calibrated glass capillaries of different diameters (1.6 mm, 1.8 mm, 3.0 mm, and 4.0 mm). The instrument has an automatic temperature control system maintained by Peltier effect with a resolution of 0.001 °C. The uncertainty associated with viscosity was measured to within 3.5×10^{-3} mPa. This instrument is based on the rolling ball principle where the steel ball rolls down the inside of inclined, sample filled calibrated glass capillaries.

3. Theoretical calculation

3.1. Estimation of thermal expansion coefficients (α)

Density data have been employed for the determination of thermal expansion coefficient, using the equation.

$$\alpha = \frac{1}{V}\left(\frac{\delta V}{\delta T}\right) = \rho\left(\frac{\delta \rho^{-1}}{\delta T}\right)_p \quad (1)$$

where subscript p indicates constant pressure. Values of α were obtained graphically using the above equation.

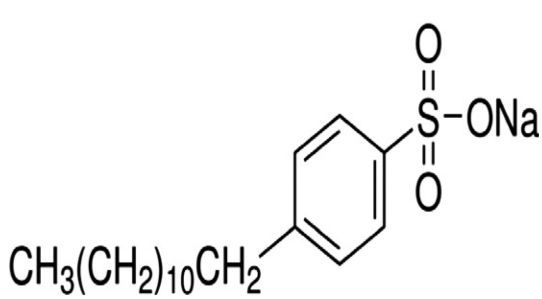

Fig. 1. Molecular structure of SDBS.

3.2. Calculation of apparent molar volume (ϕ_V)

Density data were again applied for the calculation of apparent molar volume (ϕ_V) using the following relationship.

$$\phi_v = \frac{1000\left(\rho^0 - \rho\right)}{c\rho^0} + \frac{M}{\rho^0} \quad (2)$$

where ρ and ρ^0 are the densities of solution and solvent respectively, c is molar concentration of solute in the solvent and M is the molecular weight of the solute.

4. Results and discussion

The density and viscosity measurements of four (40, 75, 150 and 300) mol ml^{-1} binary aqueous SDBS solutions have been performed in the temperature range from 298.15 to 333.15 K. All experimental density and dynamic viscosity data were obtained as a function of temperature and concentration. Experimental densities were utilized for the computation of α and ϕ_V. Table 1 depicts all the measured and

Table 1
Experimental densities (ρ), viscosities (η), thermal expansivities (α) and apparent molar volumes (ϕ_V) of system (water + SDBS) from 298.15 K to 333.15 K and different concentration range.

[SDBS] mM	ρ (g cm^{-3})	η(mPa)	$\alpha \times 10^3$ (K^{-1})	ϕ_V (cm^3 mol^{-1})
298.15 K				
40	0.9990	0.9901	3.771	348.68
75	1.0009	1.0273	3.818	348.01
150	1.0045	1.0779	3.968	346.75
300	1.0115	1.3784	4.211	344.36
303.15 K				
40	0.9975	0.9076	3.765	349.24
75	0.9993	0.9456	3.812	348.57
150	1.0029	0.9796	3.962	347.34
300	1.0097	1.2129	4.203	344.98
308.15 K				
40	0.9958	0.8232	3.759	349.80
75	0.9977	0.8823	3.805	349.15
150	1.0011	0.9188	3.955	347.95
300	1.0079	1.0843	4.196	345.62
313.15 K				
40	0.9940	0.7644	3.753	350.44
75	0.9958	0.8233	3.798	349.81
150	0.9992	0.8577	3.947	348.63
300	1.0058	0.9817	4.187	346.34
318.15 K				
40	0.9920	0.7003	3.745	351.15
75	0.9940	0.7601	3.791	350.45
150	0.9972	0.7902	3.939	349.33
300	1.0034	0.8961	4.177	347.16
323.15 K				
40	0.9898	0.6311	3.737	351.91
75	0.9916	0.6722	3.782	351.28
150	0.9952	0.7154	3.931	350.03
300	1.0012	0.8237	4.168	347.93
328.15 K				
40	0.9875	0.5899	3.728	352.76
75	0.9893	0.6167	3.773	352.12
150	0.9909	0.6441	3.921	350.91
300	0.9989	0.7616	4.158	348.75
333.15 K				
40	0.9857	0.5622	3.721	353.37
75	0.9873	0.5822	3.766	352.79
150	0.9910	0.6199	3.915	349.50
300	0.9964	0.7079	4.147	349.63