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# INTERMOLECULAR INTERACTIONS IN PHENOL – SLS – WATER TERNARY SYSTEM

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## Abstract

The phenol – water binary system is known to have limited solubility within specific concentration and temperature range. The effect of adding the surfactant, sodium laurylsulphate, on the acoustic properties like internal pressure, free volume, adiabatic compressibility, etc., has been studied and the results are presented in this paper. The surfactant has been observed to strengthen the intermolecular interactions between phenol and water more effectively below the critical micelle concentration.

**Keywords:** phenol, water, sodium laurylsulphate, acoustic properties, internal pressure, molecular interaction.

## 1. Introduction

Surfactants are organic substances of amphipathic nature consisting of both nonpolar (hydrophobic) and polar (hydrophilic) groups. Due to this, surfactants are adsorbed mainly on the surface of the solutions creating a thin monolayer and are called surface active substances. Consequently, they significantly decrease the surface tension of water at relatively low concentrations. In solution, they begin to associate and organize themselves into more complex units, called micelles. The characteristic concentration where the association process begins, is called the critical micelle concentration (cmc). The cmc is one of the most useful physicochemical characteristics of many biologically active substances and drugs. The micelles are becoming more significant in different industries including pharmaceuticals, oil recovery industry, environmental and nano technological system. The effect of micellization confers many special characteristics for the surfactants as indicated, by the perceptible, abrupt change in the behavior of these substances around their cmc, (Anilkumar,1990), (Mehrotra, et al., 1988, 1997, 1990, 1995). In the present work an attempt has been made to study the effect of micelles on the phenol-water system. Sodium laurylsulphate (SLS), an anionic surfactant capable of forming micelles, has been chosen and its effect on the phenol-water system has been studied at 303 K.

## 2. Experimental

### 2.1 Materials:

Phenol (Merck India, >99.5% purity) was distilled before use. Sodium laurylsulphate, SLS (S.D.Fine chemicals, India, with purity > 99.5%) was used as such. Double distilled water has been used for preparing the SLS solution.

### 2.2 Methods:

The densities of the liquids and liquid mixtures were determined by using specific gravity bottle by relative measurement, with an excellent reproducibility (+/- 0.0001g/mL). An Ostwald's viscometer having capacity of about 10 mL and the capillary having a length of about 90 mm and 0.5 mm internal diameter has been used to measure the flow time of pure liquids and liquid mixtures and it was calibrated with benzene (density ≈ 0.8738 g $cm^{-3}$) and doubly distilled water (density ≈ 0.9970 g $cm^{3}$). The flow time of pure liquids and liquid mixtures were repeated, at least five times. The uncertainty in the viscosity values were ± 0.005 X 10 $^{-3}$ m Pas. The sound velocity was measured by using a variable path, single crystal interferometer, working at 2 MHz frequency(Mittal India, model F-81).The interferometer cell was filled with the test liquid, and water was circulated around the measuring cell from a thermostat to maintain temperature. The uncertainty in the measured velocity values were estimated to be 0.1ms$^{-1}$. The experiments have been carried out with known volumes of the components to determine the ultrasonic velocity, density and viscosity. From the experimental data the acoustical parameters such as internal pressure ($\pi^i$), free volume ($V_f$), free length ($L_f$), adiabatic compressibility (β) and acoustic impedance (Z) have been calculated using the established relations (Rachna Nagar, et al., 1995), (Tabhane, et al., 2000), (Anwar Ali, et al., 1996).

## 3. Results and Discussion

### 3.1 Physical parameters of binary mixtures:

The ultrasonic velocity, density and viscosity have been experimentally determined for the ternary mixture of phenol-SLS-water and the data are presented in table-1.

**Table – 1. The ultrasonic velocity (U), density (ρ) and viscosity (η) of mixture of phenol - SLS - water. [phenol] = 4.54 M**

| [SLS]M | U m/s | ρ kg m$^{-3}$ | η mPas |
|---|---|---|---|
| 0.0092 | 1491.3 | 1.0725 | 5.6985 |
| 0.0083 | 1490.3 | 1.0722 | 5.5563 |
| 0.0071 | 1489.2 | 1.0719 | 5.4954 |
| 0.0060 | 1435.3 | 1.0716 | 5.0056 |
| 0.0051 | 1397.6 | 1.0711 | 4.6324 |
| 0.0042 | 1350.5 | 1.0703 | 4.2321 |
| 0.0031 | 1382.3 | 1.0698 | 3.6259 |
| 0.0020 | 1322.6 | 1.0652 | 2.1456 |
| 0.0010 | 1301.2 | 1.0623 | 1.2123 |

It is obvious from the data in Table - 1 that with increase in concentration of sodium laurylsulphate sound velocity, density and viscosity increase. This suggests the number of molecules per unit volume is increasing and gets tightly packed on increasing [SLS]. Obviously, sodium laurylsulphate being a surfactant is capable of forming micelles at concentrations above its critical micelle concentration (cmc). On forming micelles, the physical characteristics of the solutions would be inflicted with a perceptible abrupt change. Consequently, the velocity (Fig.1) and the viscosity (Fig. 3) which exhibit a progressive rise with increase in [SLS] reach almost a saturation with little change in their values above 0.007 M of SLS. It should be noted that the cmc value for a surfactant depends on the method of determination and this value(0.007 M) is in good agreement with the range of cmc values for SLS reported, (Mohamed A. Bahria, et al, 2006). This value is in good agreement with the reported cmc of SLS. Though the density profile (Fig.2) also has similar trend the saturation break point is seen at about 0.003 M of SLS. Perhaps association of SLS molecules commenced at 0.003 M resulting in pre-micelle formation which culminates at 0.007 M in fully grown micelles. Obviously, below cmc, the molecular interactions between phenol and SLS would sharply increase the physical properties of the solution; but, above cmc, the interactions would be a simple adsorption of phenol molecules on to the SLS micelles which only feebly affect the properties.

### 3.2 Acoustic parameters of phenol-sodiumlauryl sulphate-water.

From the experimentally determined parameters, acoustic parameters such as the internal pressure, free volume, free length, adiabatic compressibility, acoustic impedance have been derived. The derived acoustical parameters are listed in the table - 2. The existence of molecular interaction in the mixture of phenol-sodium laurylsulphate-water has been indicated from the values in table-2, as the internal pressure increases steadily (Fig.4) with increase in concentration of sodium laurylsulphate. Increase in internal pressure is usually accompanied by increase in free volume. However, such a straight relation has not been observed (Fig.5). This may be explained on the basis of the fact that increasing the concentration of surfactant would result in formation of pre- micellar aggregates which ultimately results in increase in pressure but decrease in the volume. Obviously, with increase in internal pressure the liquid structure becomes more tightened and hence a decrease in adiabatic compressibility(fig.6). The decrease in free length (fig.7) and increase in acoustic impedence observed with increase in [SLS] also uphold the strong molecular interactions

 

**Table – 2. The acoustic parameters of ternary mixtures of phenol – SLS - water.**
**[Phenol] = 4.54 M**

| [SLS]M | $\pi^{i}$ x $10^{-3}$ Pa | $V_f$ x$10^{-2}$ $m^3$ $mol^{-1}$ | $L_f$ x$10^{-11}$ m | β x$10^{-11}$ $Pa^{-1}$ | Z x $10^{-6}$ Kg $m^{-2}s^{-1}$ |
|---|---|---|---|---|---|
| 0.0092 | 8.60 | 1.53 | 0.127 | 0.419 | 1.599 |
| 0.0083 | 7.79 | 1.78 | 0.127 | 0.420 | 1.598 |
| 0.0071 | 7.05 | 2.04 | 0.128 | 0.421 | 1.596 |
| 0.0060 | 6.19 | 2.53 | 0.132 | 0.453 | 1.538 |
| 0.0051 | 5.39 | 3.16 | 0.136 | 0.478 | 1.496 |
| 0.0042 | 4.62 | 4.03 | 0.141 | 0.512 | 1.445 |
| 0.0031 | 3.68 | 6.31 | 0.138 | 0.489 | 1.479 |
| 0.0020 | 2.46 | 15.91 | 0.144 | 0.537 | 1.409 |
| 0.0010 | 1.55 | 46.35 | 0.147 | 0.556 | 1.382 |

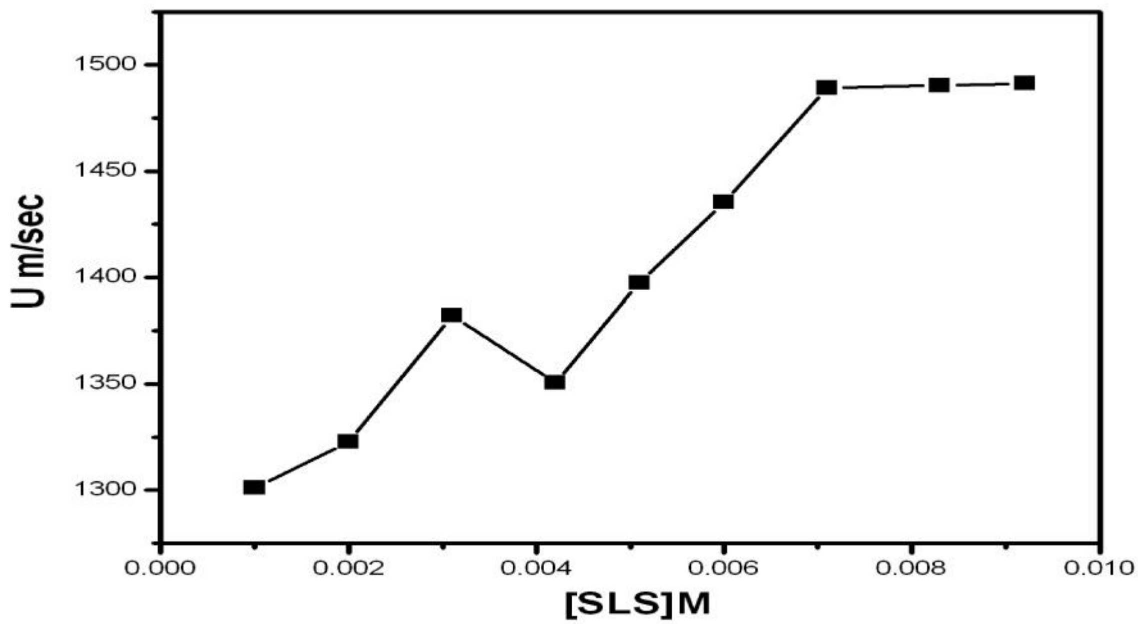


**Fig. 1 Variation of ultrasonic velocity with [SLS]**

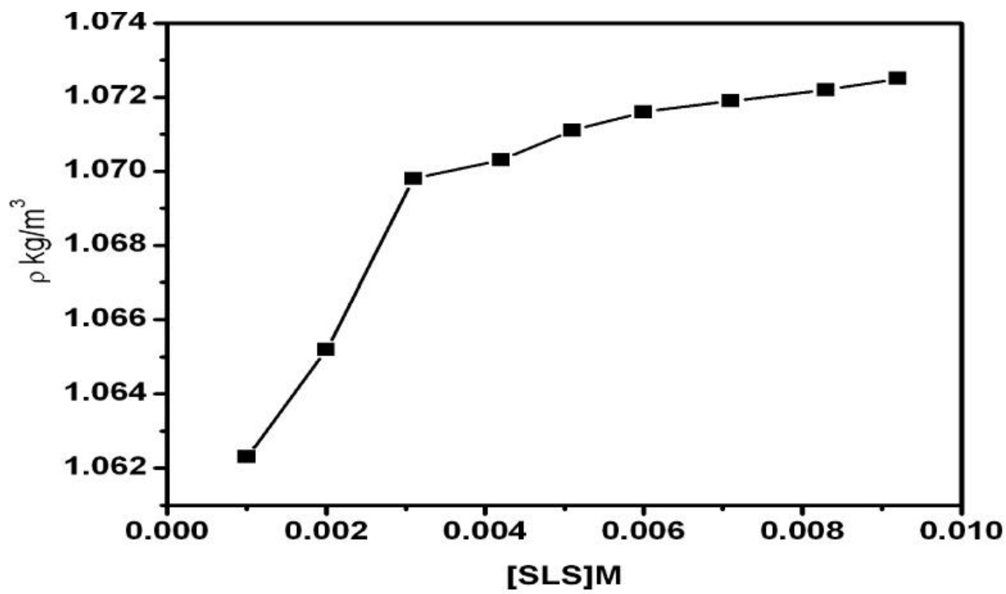


**Fig. 2. Variation of density with [SLS]**

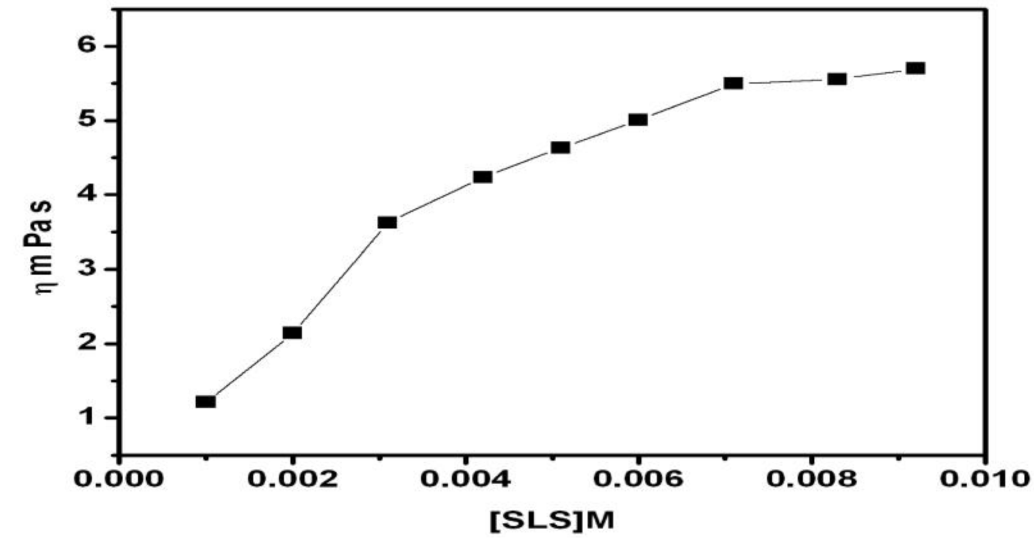


**Fig.3. Variation of viscosity with [SLS]**

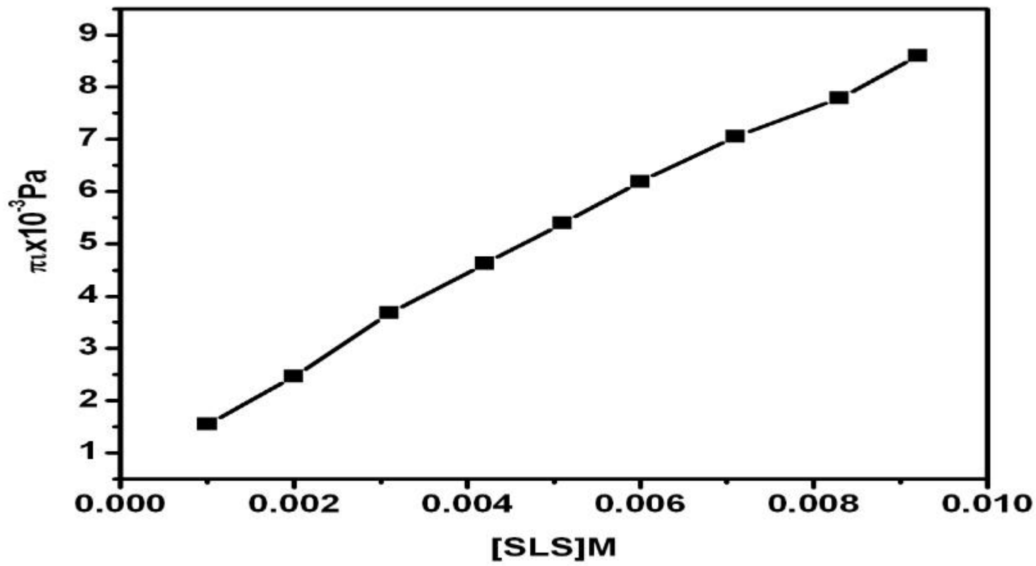


**Fig.4 Variation of internal pressure with [SLS]**

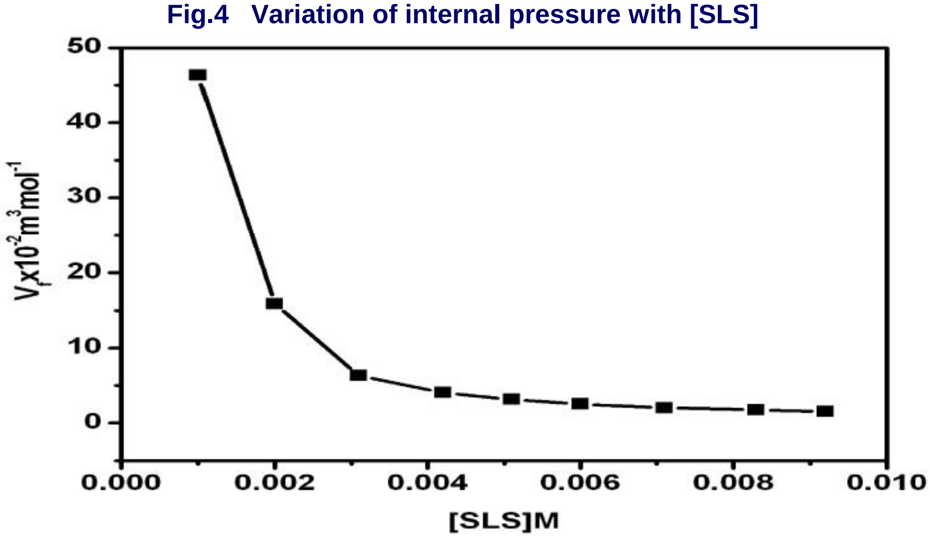


**Fig.5 Variation of free volume with [SLS]**

 

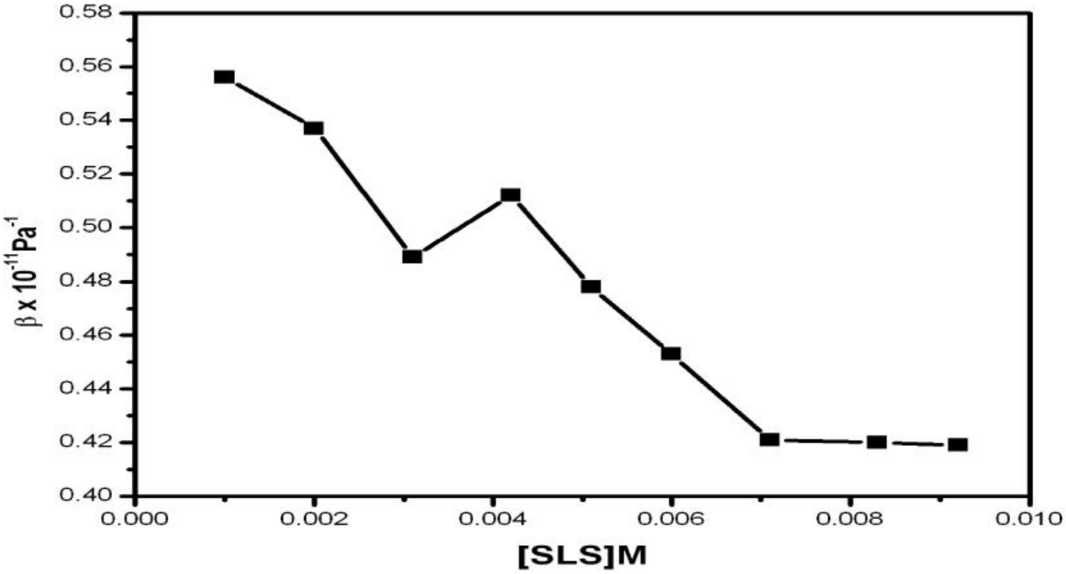


**Fig.6 Variation of adiabatic compressibility with [SLS]**

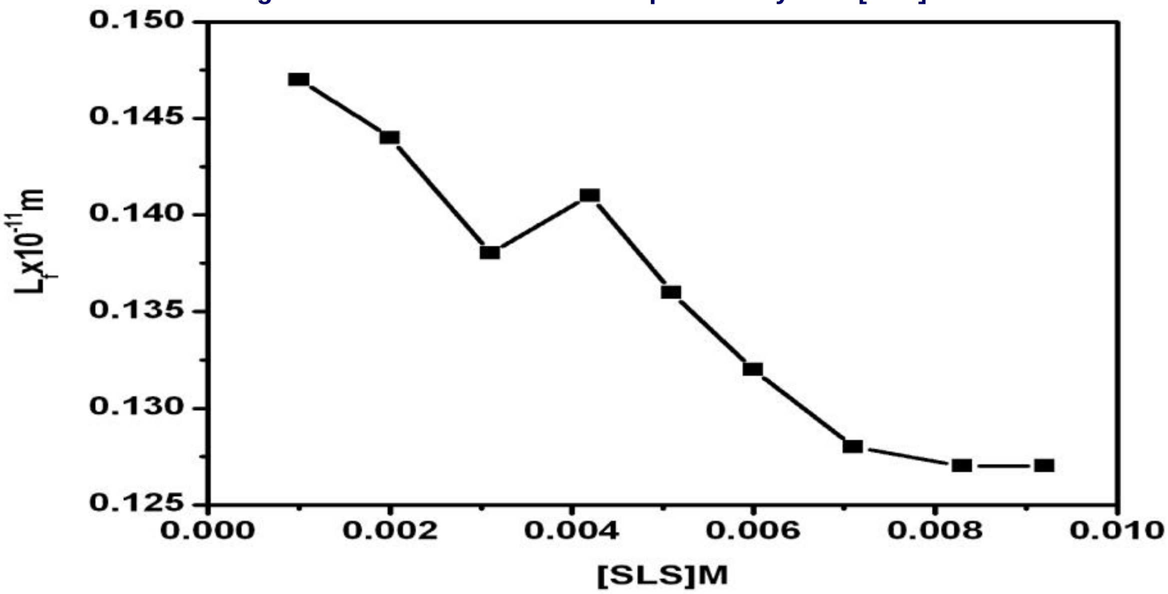


**Fig. 7. Variation of free length with [SLS]**

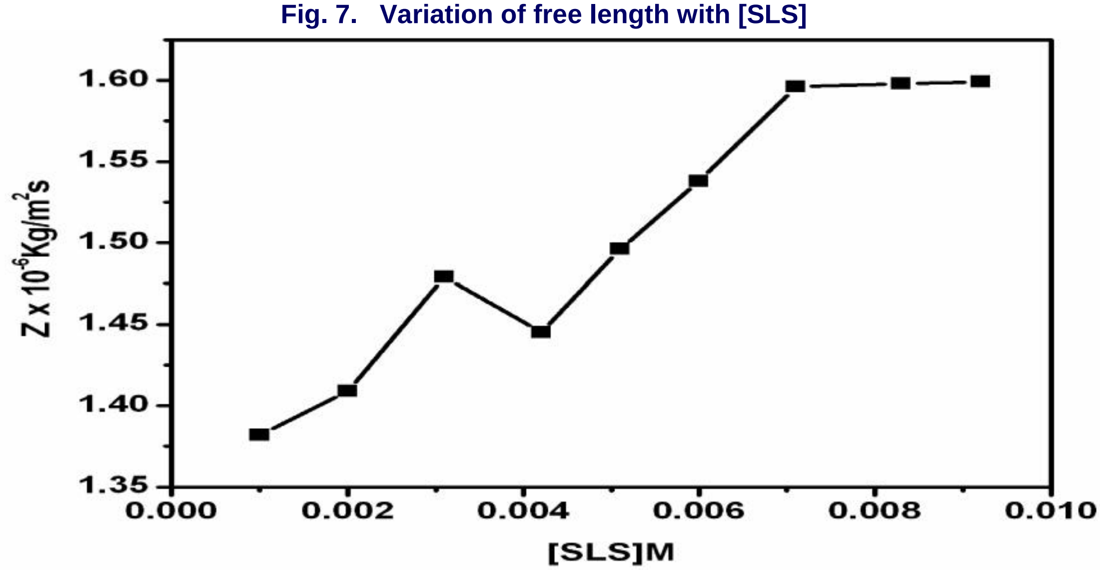


**Fig.8 Variation of acoustic impedance with [SLS]**

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