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Micellisation and Interaction Parameters of a non-ionic surfactant in aqueous and mixed solvents

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ABSTRACT

In the present study CMC values of a non-ionic surfactant, Triton X-100, were taken inwater, water + propan-2-ol and water + fructose systems at different concentrations. From CMC values micellisationconstant (K_M),Setchenov constant, (K_S^N) and interaction parameters 'P' and 'q' were calculated. $K_M$values are positive for propan-2-ol+water system and negative for fructose +water system.K_S^Nvalue in propan-2-ol system are more as compared to fructose system. It suggests that nature of polar group of additive plays major role in solubilisation process. The high 'P' and 'q' values in presence of propan-2-ol suggest that propan-2-ol penetrates in the interior of micelle.

Keywords: Micellisation constant, Setchenov constant, Ideal partition coefficient, Real partition coefficient.

INTRODUCTION

Surfactants play an important role in the field of agriculture and food technology, energy, environment, biology, pharmaceuticals, textiles and metallurgy[1-3].The physicochemical properties of surfactants are affected by presence of co-solutes/co-solvents and these provide a potential tool to investigate structural changes in these solutions [4]. In the present studies micellisation and interaction parameters of the systems; Triton X-100 + water +propan-2-ol, andTriton X-100 + water +fructose have been measured at different concentrations. These values helped to investigate the effect of added co-solute/co-solvents on the structure of the studied systems.

MATERIALS AND METHODS

Triton X-100, a purified product from Koch-light laboratories was used as such. Propan-2-ol was from Ranbaxy laboratories and fructose from Sysco research laboratories. These were used as supplied. Double distilled water having specific conductance of the order of 10^{-6} S cm^{-1} at 298 K was used for preparing solutions. The specific conductance values of solutions (within +5×10^{-6}S cm^{-1}) were measured using a digital conductivity meter (Naina NDC-732) and temperature around the solutions was maintained within +0.01K.

RESULTS AND DISCUSSION

Critical micelle concentration (CMC) values determined conductometrically are presented in Table-1.

Table-1: CMC values of Triton X-100 in Triton X-100 +water, Triton X-100 +water + propan-2-ol and Triton X-100 +water +fructose systems at 298.15K.

System	Mole fraction of propan-2-ol /fructose	CMC×10^3 (mol dm^{-3})
Triton X-100 +water	-	2.80
Triton X-100 +water + propan-2-ol	0.0936 0.1906	2.08 1.59
Triton X-100 +water +fructose	0.01 0.02	3.92 4.53

The decrease in CMC of Triton X-100 in propan-2-ol +water may be attributed to the ability of propan-2-ol to penetrate into the micellar interior i.e. palisade layer [5-6]. An increment in the CMC value of Triton X-100 in presence of fructose might be due to more hydrogen bonding capability of fructose in comparison to water. The classical Setchenov equation which relates variation of the solubility of solute in a given solvent to the molality of third component is applicable, to a good approximation to the surfactant solutions in presence of additives [7].

$$K_M.\mathrm{m} = \ln\left[\frac{\mathrm{CMC}_W}{\mathrm{CMC}_{\mathrm{w+A}}}\right]$$

Where 'm' is the molality of the additive, CMC_W and $\mathrm{CMC}_{\mathrm{w+A}}$ are critical micelle concentrations of surfactant in water and mixed solvent respectively. K_M is known as micellisation constant, which may be expressed by the equation.

$$K_M = \frac{1}{2}\left[K_S^N + \frac{qM1}{2.303x\ 1000}\right]$$

Where M_1 is molecular weight of the solvent, 'q' is ideal partition coefficient. K_S^N is the Setchenov constant and may be calculated by this empirical relation.

$$K_S^N = 0.637 - 0.014n(CH_2) - 0.1464\sigma$$

Where $n(CH_2)$ is the number of methylene groups in the linear hydrocarbon chain and σ is the hard sphere diameter of the solute which can be calculated from van der Waal'svolumes using Deligny's relation [8].

$$1/6\ \pi N\sigma^3 = -10+1.13V_W$$

Where 'N' is Avogadro's number and V_W is Bondi'svanderWaal's volumes [9].

The real partition coefficient (P) was calculated using the relation.

$$P = q\times F$$

Where q is ideal partition coefficient of co-solute in surfactant bulk solution and the micellar phase. F is a constant, named as activity coefficient which includes all non-ideal interactions between solutes and micelles. F is taken equal to 0.64 [10].

Table-2: Micellisation constant (K_M) for TritonX-100 in propan-2-ol+water and fructose+water systems.

System	Mole fraction of propan-2-ol/fructose	K_M (kg mol^{-1} at 298.15K)
Propan-2-ol+water	0.0936 0.1906	0.053 0.043
Fructose+water	0.01 0.02	– 0.599 – 0.361

K_M values are positive for propan-2-ol +water system and negativefor fructose +water system. Positive K_M values correspond to a decrease of CMC upon addition of solute, while negative K_M values correspond to a increase of CMC.

Setchenov constant (K_S^N) is proportional to a pair wise interaction coefficient between surfactant monomers and the additive molecule. Value of K_S^N for TritonX-100 in presence of propan-2-ol and fructose are calculated equal to – 0.0569 and – 0.0698 respectively. K_S^Nvalue in propan-2-ol system is more as compared to fructose system. It suggests that nature of polar group of additive plays major role in solubilisation process [7].

The ideal partition coefficient (q) and real partition coefficient (P) gives an indication of penetrating nature of additive molecules. The 'P' and 'q' values for the studied systems are listed in Table-3.

Table-3: The ideal partition coefficient (q) and real partition coefficient (P) ofpropan-2-oland fructose in TritonX-100 at 298.15K.

System	Mole fraction of propan-2-ol/fructose	'q' value	'P' value
Propan-2-ol +water	0.0936	71.19	45.86
	0.1906	26.94	17.24
Fructose+water	0.01	– 58.80	– 37.63
	0.02	– 2.51	– 1.60

The high 'P' and 'q' values in presence of propan-2-ol suggest that propan-2-ol penetrates in the interior of micelle [11]. The negative values in case of fructose indicate that fructose is highly hydrophobic and non penetrating additive.

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