ABSTRACT

In the present work a comprehensive study on the effect of hydrotropes such as citric acid, pyrogallol, resorcinol, sodium benzoate, sodium salicylate, nicotinamide and urea on the solubility and mass transfer coefficient for a series of organic solutes such as amyl nitrite, cyclohexene, ethylbenzene, n-butyl chloride and L-aspartic acid has been carried out. The influence of a wide range of hydrotrope concentrations (0 - 3.0 mol.L\(^{-1}\)) and different system temperatures (303 - 333 K) on the solubility of organic solutes has been studied. The influence of different hydrotrope concentrations on the mass transfer coefficient of organic solutes has been ascertained.

The solubility determinations were made by measuring the concentration of the dissolved organic solute in aqueous hydrotrope solutions using standard procedures. A plot of \(-\log [1-C_b/C^*]\) vs \(t\) is drawn, where ‘\(C_b\)’ is the concentration of the solute at any given time ‘\(t\)’ and \(C^*\) is the equilibrium solubility. From the slope of the graph, the mass transfer coefficient, \(k_{L,a}\) was determined.

Data on various aspects of hydrotropic study on the solubility and mass transfer coefficient for a series of organic solutes having a wide range of industrial and commercial applications have been provided for the first time.
The experimental solubility data for various solutes at different temperatures have been analyzed using the modified Setschenow equation,

$$\log [S/S_m] = K_s [C_s-C_m]$$

where $S$ and $S_m$ are the solubilities of the organic solute at any hydrotrope concentration $C_s$ and minimum hydrotrope concentration $C_m$ respectively. Setschenow constant, $K_s$, a measure of the effectiveness of the hydrotrope has been determined and reported for each case.

To ascertain the aggregation characteristics of hydrotropes at different temperatures, thermodynamic parameters such as Gibb’s free energy, enthalpy, and entropy were determined using standard equations. The calculations were based on MHC values.

To characterize the aggregation of hydrotrope molecules, the association constants between hydrotrope-hydrotrope ($K_2$) and hydrotrope-solute ($K_{hs}$) were determined by fitting the experimental solubility data in an Association model.

The solubility of the organic solutes increases with increase in hydrotrope concentration and also with system temperature. A Minimum Hydrotrope Concentration (MHC) in the aqueous phase is required to show significant increase in the solubilities of organic solutes used.

To propose a possible mechanism of hydrotropic phenomenon, a study on solution properties of hydrotropes such as viscosity, specific gravity, surface tension, specific conductance and refractive index have been
determined for a range of hydrotrope concentrations (0 - 2.0 mol.L$^{-1}$). Scanning Electron Microscope (SEM) images of pure L-aspartic acid i.e., the only solute in solid phase and solubilized L-aspartic acid in the presence of corresponding best hydrotrope have been presented and discussed in detail.

Consequent to the increase in the solubility of the organic solute, the mass transfer coefficient was also found to increase with increase in hydrotrope concentration. On the same lines, a threshold value which is nothing but MHC is to be maintained to have appreciable enhancement in mass transfer coefficient.

The percentage recovery of organic solutes from hydrotrope solution was determined by simple dilution with distilled water at any concentration between MHC and Maximum Hydrotrope Concentration ($C_{\text{max}}$).

To predict the solubility of organic solutes in different hydrotrope solutions, Artificial Neural Network (ANN) model has been developed. Mean Squared Error (MSE) was calculated to evaluate the accuracy of proposed ANN model by using a validating data in order to establish the network applicability.

All hydrotropes used in this work showed an enhancement in the solubility and mass transfer coefficient to different degrees. The maximum enhancement factor, which is the ratio of the value in presence and absence of a hydrotrope, has been determined for both the cases.

The implications of the study have been fully discussed and the scope for future research has been suggested.