CHAPTER 8

CONCLUSIONS

8.1 CONCLUSIONS

(a) This comprehensive study on the effect of hydrotropes on the solubility and mass transfer coefficient of a series of organic solutes under a wide range of hydrotrope concentrations at different temperatures gives rise to the following conclusions.

1. All hydrotropes used in this work enhance the solubility and mass transfer coefficient of the selected organic solutes significantly.

2. A Minimum Hydrotrope Concentration (MHC) in the aqueous phase is found to be essential for the initiation of the hydrotripic solubilization of the selected organic solutes.

3. On the same lines, a threshold value, which is nothing but MHC is found necessary to bring significant increase in the mass transfer coefficient of organic solutes.

4. MHC values of different hydrotropes used in this study range between 0.20 and 0.60 mol.L\(^{-1}\) with respect to a series of selected organic solutes. However such values of a particular hydrotrope are in the narrow range.
5. MHC values seem to depend on the hydrophilicity of a hydrotrope. However, for few solute-hydrotrope systems, the hydrophobicity of the solute also contributes to some extent in determining such values.

6. The maximum concentration of hydrotropes in most cases approaches the values between 2.20 and 2.60 mol.L⁻¹ and further increase in hydrotrope concentration does not bring any significant increase in the solubility of the organic solutes studied.

7. Any change in system temperature has negligible effect on MHC and $C_{\text{max}}$ values of the hydrotrope.

8. Even though the hydrotropic solubilization exists in a region between MHC and $C_{\text{max}}$, the effect of hydrotropes is found to be predominant at hydrotropic concentrations close to $C_{\text{max}}$ in most cases.

9. The knowledge of MHC and $C_{\text{max}}$ values of a particular hydrotrope towards each organic compound is necessary for the recovery of the dissolved solutes and hydrotrope solutions at any hydrotrope concentration between MHC and $C_{\text{max}}$.

10. The solubilization effect of hydrotrope increases with increase in hydrotrope concentration and also with system temperature.

11. Consequent to the increase in the solubility of the selected solutes, the mass transfer coefficient of the
same was also found to increase with increase in hydrotrope concentration.

12. As the system temperature increases, lesser hydrotrope concentration is found adequate in the aqueous phase to achieve the solubility of the selected organic solute to a certain value, which was obtained with higher hydrotrope concentration at the lower temperature.

13. The solubilization effected by hydrotropes is not a linear function of the hydrotrope concentration.

14. The order of increase in the solubility of the solutes studied is

Ethylbenzene > Amyl nitrite > n-Butyl chloride > Cyclohexene > L-Aspartic acid

15. The values of $K_s$, Setschenow constant, determined for each solute-hydrotrope at different temperatures can be considered as a measure of the effectiveness of a hydrotrope. The order of effectiveness of various hydrotropes based on such values is,

Sodium salicylate > Nicotinamide > Urea > Citric acid > Sodium benzoate > Resorcinol > Pyrogallol

16. The values of hydrotrope-hydrotrope association constant ($K_2$) and hydrotrope-solute association constant ($K_{hs}$) for all the organic solutes under study can be considered as a measure of the aggregation behavior of hydrotrope and the solubilization of solutes.
17. In all cases, association constants ($K_{hs}$, $K_2$) effected by the corresponding best hydrotrope is much higher for the organic solutes used in this work.

18. For each solute studied, the best one among the other hydrotropes has been selected for obtaining maximum solubilization. Such data can also be used for effective separation of the particular solute from any mixture.

19. Thermodynamic parameters like standard gibbs free energy ($\Delta G^\circ$), standard enthalpy ($\Delta H^\circ$) and standard entropy ($\Delta S^\circ$) obtained for various hydrotropes relevant to the solute studied influence hydrotropic phenomenon.

20. An artificial neural network model was developed to predict the solubility of organic solutes in aqueous hydrotrope solutions.


(b) The conclusions drawn from the study on the mechanism of hydrotropic phenomenon are:

1. The inaction of hydrotropes to effect solubilization of solutes below MHC may be due to the inability of hydrotropes to form aggregates with required number of hydrotrope molecules available in the aqueous phase.

2. The unprecedent increase in the solubilizing effect of hydrotropes above MHC may be due to the formation of
organized aggregates of hydrotrope molecules at this particular concentration.

3. The deviation from linearity of solution properties of hydrotropes at MHC can be taken as an indication of an aggregate formation. Such a trend may also be considered as a characteristic of the hydrotrope solubilization.

4. The difference in surface tension and other allied solution properties of hydrotrope aggregates with respect to aqueous solution acquired at MHC may be the factor responsible for solubilization of the solute into the aqueous phase at this particular concentration.

5. The increase in solubilizing effect of hydrotropes with increase in hydrotrope concentration may be due to the availability of more MHC aggregates for interaction with the solute molecules at the existing conditions of the aqueous phase.

6. The saturation of the solubilizing effect of hydrotropes beyond C_{max} may be due to the non-availability of water molecules to form further aggregates comprising of additional MHC agglomerates.

(c) The conclusions drawn from the study on the recovery of solute from hydrotrope solution:

1. The recovery of the dissolved solute from hydrotrope solution is ensured at any hydrotrope concentration between MHC and C_{max} by simple dilution with distilled
water, which alters the solution properties of hydrotrope aggregates instantaneously affecting the MHC agglomerates.

2. The order of increase in the percentage recovery of the dissolved organic solutes from hydrotrope solution is

Amyl nitrite > n-Butyl chloride > Ethylbenzene > Cyclohexene > L-Aspartic acid.

8.2 TECHNICAL AND ECONOMICAL FEASIBILITY OF THE PRESENT STUDY

The study on hydrotropic phenomenon has the following practical implications at the industrial levels.

1. The solubility of organic solutes having a wide range of industrial applications, which are practically insoluble in water has been increased significantly and hence their mass transfer coefficient. These characteristics would be much useful in increasing the rate of output of the desired product made from these solutes under study.

2. The separation of such organic solutes from any mixture which is found to be difficult, until now, can be carried out effectively.

3. This study provides the cheapest and most effective solubilization technique, since huge cost and energy normally involved in the separation of the solubilized material from its solution is totally eliminated.
8.3 SCOPE FOR FUTURE WORK

1. It would be worthwhile investigating the effect of hydrotropes towards other organic solutes such as alcohols, aldehydes, esters and ketones, whose solubility in water is negligible and which are useful in process industries.

2. The solubilization efficiency of hydrotropes can be exploited for extractive separations based on selective solubilization technique.

3. Enhancing the solubility of insoluble or sparingly soluble drugs in blood through hydrotropy.

4. FTIR analysis and Raman spectral analysis can be done for pure solute and solute-hydrotrope system, to further supplement discussion for aggregation phenomenon.

8.4 SUMMARY OF THE CHAPTERS

The thesis is divided into eight chapters. Chapter 1 deals with the introductory remarks on the need for undertaking hydrotrope study and the scope of the present investigation.

Chapter 2 is concerned with the absence of data on the study of hydrotropes on a series of organic solutes with a wide range of industrial applications. However a summary on the different types of hydrotropes used for the study of esters and other solutes was given. The literature review provides the background and guidance for the scope of the present work.

In chapter 3, the experimental procedures used for the determination of solubility and mass transfer coefficient of organic
compounds in solid and liquid phase, in different hydrotrope solutions were described. The experimental procedures used for the measurement of various properties such as viscosity, specific gravity, surface tension, specific conductance and refractive index of hydrotrope solution were also discussed.

Chapter 4 discusses aggregation association model used to represent the solubilization of solute in hydrotrope solutions. The model considers stepwise aggregation of the hydrotrope molecules and solubilization of the solute by organized aggregation of hydrotrope molecules. A study on thermodynamic parameters like free energy, standard enthalpy and standard entropy were discussed with the standard equations. Artificial Neural Network (ANN) model illustrating the percentage extraction of organic solutes in hydrotrope solutions. It explains about computation of descriptors for organic solutes using software, which is used as an input in ANN and procedure followed to predict the percentage extraction of organic solutes in hydrotrope solutions using ANN with minimum error.

Chapter 5 has two sections. In section one the minimum and maximum concentration range of hydrotropes used and its effect on temperature for various dissolved solutes from hydrotrope solutions were enumerated while section two gives the percentage recovery of dissolved solutes from hydrotrope solutions.

In chapter 6, the results of the experimental investigations carried out were discussed and presented in six sections. The effect of hydrotropes on the solubility and mass transfer coefficient of organic compounds were presented in section one and two. In section three, the effectiveness of hydrotropes based on Setschenow constant \( (K_s) \) values of each hydrotrope towards a series of organic compounds studied was given.
In section four association constants ($K_2$ and $K_{hs}$) determined from association model which are used to represent the solubilization of the selected solutes in hydrotrope solutions were presented.

Section five presents a study on thermodynamic parameters such as Gibb’s free energy ($\Delta G^\circ$), standard enthalpy ($\Delta H^\circ$) and standard entropy ($\Delta S^\circ$) pertaining to aggregation characteristics of hydrotropes.

Section six presents the result obtained using artificial neural network model. The predicted results were compared with experimental values and statistically discussed.

The influence of solution properties such as viscosity, specific gravity, surface tension, specific conductance and refractive index on the possible mechanism for the solubilizing effect of hydrotropes were discussed in chapter 7.

In chapter 8, the salient features drawn from the present study of hydrotropes on a series of the selected solutes were summarized and scope for future research is suggested.