EFFECT OF SOLVATION WITH SALTING EFFECT ON SOLUBILITIES OF VOLATILE ORGANIC COMPOUNDS

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Solubilities of volatile organic compounds (VOC) in a solution with electrolytes such as sodium hydroxide or ionic liquids can be understood by a solvation model in this work.

We are proposing a new dechlorination process for chlorinated fluorocarbons. Reaction rate is determined by the solubilities of fluorocarbons in an alcohol-NaOH solution. We found that the solubility decreased with NaOH concentration in a solution which was caused by the salting effect. In a previous paper, we correlated the Henry's constants of a fluorocarbon in an alcohol as a following function form, $C_i = C_i^0 \exp(-hC_k)$. Where C_i is the concentration of i (fluorocarbon or VOC) in a ternary-component solution composed of fluorocarbon-alcohol-NaOH. C_i^0 is the concentration of i (fluorocarbon or VOC) in a binary-component solution composed of fluorocarbon-alcohol, that is the solubility of fluorocarbon in alcohols without NaOH. C_k is the concentration of k (NaOH or electrolyte) in the solution. The coefficient of h is the Setchenov coefficient which is considered as salting effect parameter. The values of *h* for a system were found to be proper independent of temperature.

Assuming that alcohol solvates on electrolyte, i.e. NaOH in this work, we derived the following relation, $N_s = hC_j$. Where N_s, C_j is solvation number and concentration of solvent j (alcohol in this work), respectively. For four kinds of fluorocarbons, solvation number of methanol and ethanol were found about 8 and 4, respectively.

Fitting the solubility data, the Setchenov coefficients, h were correlated by the group contribution method. Contributions were divided into fluorocarbon part (i) and alcohol part (j). For four kinds of fluorocarbons in methanol or ethanol solvent, the values of h were reproduced within 5 %. Gelatinization occurred, however we carried out the solubility measurements in 1-propnol or higher alcohols. To use the group contribution method, the viscous term should be considered. According to the model, any fluorocarbon should not influence on h. But the group contribution method demands the contribution of fluorocarbons. It means that the segments of fluorocarbon solvates on NaOH, however we have no means to detect it.

Teja et.al reported the values of h for the solubility of alcohols, ketones etc. in water under the existence of Na_2SO_4, NaCl, TEAB (teraethylammonium bromide) or TMAB (teramethylammonium bromide). The group contribution method succeeded in correlation of solubility within 0.5% deviation for the system containing Na_2SO_4 and NaCl. For the salt-out systems containing TEAB and TMAB, the negative values for C-C segment lead success of reproduction, however the solvation model fails.