Abstract

This research work investigates the separation of two azeotropic systems methanol/dimethyl carbonate and methyl acetate/methanol by means of extractive distillation through addition of a mass separating agent (MSA) with an intent to change the relative volatilitiy of the [constituent](https://www.google.com.tw/search?safe=off&rlz=1C1MSNA_enTW680TW680&q=constituent&spell=1&sa=X&ved=0ahUKEwjJltGMxP3RAhUBppQKHSybDbYQvwUIFygA) species. Physicochemical properties such as dielectric constant, Hanson solubility parameters and solute-solvent interaction factors have been looked into in an attempt to establish the relevance between those of a solvent and its suitability as an MSA. A composite index incorporating both selectivity and solubility factors has been proposed and correlated with separation cost .

As it is hard to achieve high selectivity and high solubility simultaneously with a single solvent, feasibility of using mixed solvents and their screening method have been explored.Take the methanol/ dimethyl carbonate system as an example, UNIFAC, UNIFAC-DMD and COSMO-SAC models have been employed, on the basis of selectivities at infinite distillation, to match MSA’s with great potential. The results showed that the mixed solvent of ethyl benzoate/methyl isobutyl ketone (EB/MIBK) exhibited synergy effect with the three models. Similar effect was also found by the mixed dimethyl sulfoxide/dimethylformamide (DMSO/DMF) solvent for the methyl acetate/methanol separation system.

Vapor-liquid equilibrium experiments were carried out for the mixed solvents with the synergy effect and the data obtained were regressed by the NRTL model and used in the simulation and optimization of the extractive distillation processes. The results revealed that the optimal blending ratio of the mixed EB/MIBK solvent in the methanol/dimethyl carbonate extractive distillation system is 0.78:0.22 (EB/MIBK). On the other hand, the mixed solvent of DMSO/DMF at the blending ratio of 0.77:0.23 (DMSO/DMF) was also shown to outperform all single solvents. In addition, the synergy effect of both mixed solvents was validated in batch distillation experiments, with the addition of 30% mixed solvent (EB/MIBK=0.75:0.25, DMSO/DMF=0.75:0.25).