Systematic screening methodology and energy efficient design of ionic liquid-based separation processes

A systematic methodology for the screening of ionic liquids (ILs) as entrainers and for the design of ILs-based separation processes in various homogeneous binary azeotropic mixtures has been developed. The methodology focuses on the homogeneous binary aqueous azeotropic systems (for example, water+alcohols). Additionally, a Hildebrand solubility parameter group contribution model for ILs, and ILs miscibility database have been developed to screen the miscibility of the ILs with the target solute component and these parameters are considered as the main criteria for the screening of ILs. ILs were further screened based on a combination of criteria such as stability, toxicity, and their environmental impacts. All best ILs were used as entrainers, and an extractive distillation column (EDC) and ionic liquid recovery column were designed and simulated with a process simulator to determine the overall energy consumption of the ILs-based separation processes. Among all candidates, the best IL was selected based on the minimum energy requirement obtained from the simulation. Finally, the modification of the separation process to obtain design flexibility for other azeotropic series with respect to the change in size of the target solute was investigated using the same separation process and IL entrainer to obtain the same product purity. The proposed methodology has been evaluated through a case study of binary alcoholic aqueous azeotropic separation: water+ethanol and water+isopropanol.