Optimal Design of Ionic Liquid Entrainers for Extractive Distillation of Azeotrope Systems

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Ionic liquids have shown great promise as alternative green solvents. The low vapor pressure exhibited by ionic liquids offers an environmental benefit over many traditional solvents used in industrial processes. However, the toxicity of ionic liquids can still be a concern and must be considered when selecting a solvent. Ionic liquids can also degrade due to thermal decomposition or hydrolysis. Such factors should be taken into account when designing or selecting an ionic liquid solvent. The cation, anion, and alkyl chain length on the cation can be altered to design an ionic liquid with desired properties. These tunable properties show the promise of designing ionic liquids as environmentally friendly entrainers for the separation of azeotropes. With an ionic liquid entrainer designed or selected for a specific azeotrope mixture, an extractive distillation process can be subsequently designed.

The design of ionic liquid entrainers for the separation of azeotropes has been investigated. The azeotropic systems considered were methanol-acetone, methanol-benzene, methanol-cyclohexane, water-ethanol, ethanol-benzene, and ethanol-cyclohexane. Several group contribution (GC) models were developed and used for the initial design and selection of candidate ionic liquids. Previously published experimental data was used in the development of the GC models. A solubility parameter model was used to optimally design cation, anion, and alkyl chain length combinations that were similar in value to the azeotrope mixture volume-fraction average solubility parameter value. Prediction intervals at 95% were used to represent the uncertainty in the predicted solubility parameter values and compare solutions to the design problem. Ionic liquid candidates were screened using a thermal decomposition temperature GC-model and several different GC-models for toxicity measures. Stable, non-toxic ionic liquids with optimal solubility parameter values were obtained.

A UNIFAC activity coefficient model for ionic liquids was developed using previously published experimental infinite dilution activity coefficient data. The UNIFAC model describes an ionic liquid as an anion group, a cation group, and alkyl groups for the chain on the cation. The UNIFAC model has been compared to several published experimental vapor-liquid equilibria (VLE) data sets and shows reasonable modeling of the VLE. The UNIFAC model was used to verify that a specified azeotrope was broken by the designed ionic liquid. The minimum amount of ionic liquid needed to break the azeotrope was determined for each system. The predicted VLE was tested for stability to determine if a liquid-liquid phase split occurred. After verification, an extractive distillation process was designed for each azeotrope mixture using the driving-force method. By designing the distillation column based upon the maximum driving force for separation, the energy input is minimized. For each azeotropic system considered, an optimal ionic liquid entrainer has been designed and an extractive distillation process has been designed using minimal energy inputs and ionic liquid concentrations.

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