Simultaneous design of ionic liquid entrainers and energy efficient azeotropic separation processes - DTU Orbit (16/05/2019)

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A methodology and tool set for the simultaneous design of ionic liquid entrainers and azeotropic separation processes is presented. By adjusting the cation, anion, and alkyl chain length on the cation, the properties of the ionic liquid can be adjusted to design an entrainer for a given azeotropic mixture. Several group contribution property models available in literature have been used along with a newly developed group contribution solubility parameter model and UNIFAC model for ionic liquids (UNIFAC-IL). For a given azeotropic mixture, an ionic liquid is designed using a computer-aided molecular design (CAMD) method and the UNIFAC-IL model is used to screen design candidates based on minimum ionic liquid concentration needed to break the azeotrope. Once the ionic liquid has been designed, the extractive distillation column for the azeotropic mixture is designed using the driving force method with a new proposed feed stage scaling to minimize energy inputs. Along with the distillation column, an ionic liquid recovery stage is designed and simulations are used to determine the overall heat duty for the entire process for the best ionic liquid candidates. Use of a designed ionic liquid reduces material and energy requirements when compared to an ionic liquid known to experimentally break a given azeotrope but not designed using CAMD methods. The acetone–methanol and ethanol–water azeotropes are provided as examples.

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