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Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

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Monday, October 29, 2012

Hall B (Convention Center)

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A methodology and tool set for the simultaneous design of ionic liquids and separation processes is presented. By manipulating the structure of the cation and anion, the properties of an ionic liquid can be adjusted for specific applications, such as azeotropic separation or CO_2 recovery. To estimate key properties, several group contribution models available in the literature have been used, along with newly developed group contribution models. For a given set of operational constraints, an ionic liquid is designed using a computer-aided molecular design (CAMD) method and the UNIFAC-IL model is used to screen design candidates or known ionic liquids.

The developed tool set allows users to select target objectives and input and output constraints while optimally designing both the ionic liquid and the separation process. Alternatively, the software package can simultaneously select from a database of ionic liquids with experimentally verified properties while optimizing the separation process. New group contribution models have been developed to predict ionic liquid viscosity and CO_2 solubility. Viscosity prediction allows computation of pumping costs, providing more accurate estimation of energy requirements for a given process. As an example, an absorption system for CO_2 capture is designed, involving both the design of the IL solvent itself as well as the separation scheme to remove the CO_2 from the ionic liquid. Simulations were used to determine the overall energy usage for the entire process, such that the optimal solvent structure and process design is determined.

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