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Dada, Emmanuel A.; Mustaffa, Azizul Azri; Gani, Rafiqul

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Emmanuel A. Dada, ChemProcess Technologies (CPT), LLC, League City, TX, Azizul Azri Mustaffa, Department of Chemical and Biochemical Engineering (CAPEC), Technical University of Denmark, Kgs. Lyngby, Denmark and Rafiqul Gani, CAPEC, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark

Dialkyl **c**arbonates like dimethyl carbonate (DMC) and diphenyl carbonate (DPC) are environmentally benign and biodegradable products and have found wide applications in polycarbonates plastics and as important solvents in the emerging battery markets. In particular, DMC is the solvent of choice for lithium ion battery solutions. The synthesis of dialkyl carbonates are generally carried out by continuous reactive distillation that produce azeotropic mixtures of the dialkyl carbonates and linear alcohols followed by the recovery of the dialkyl carbonates. The recovery of a typical dialkyl carbonate from the azeotropic mixture is achieved by either using pressure swing distillation process where the pressure sensitive azeotropic mixture is separated or by using extractive distillation process where the azeotropic mixture is contacted with an entrainer like phenol, aniline and diethyl oxylate to produce high purity dialkyl carbonate. In all of these distillation processes (reactive, pressure-swing, and extractive distillations), accurate predictions of the binary VLE systems involving the carbonate group (-OCOO-) and other components especially the linear alcohols in the production of high purity dialkyl carbonates are very important. The UNIFAC group interaction parameters (GIPs) involving the carbonate group are very limited in the literature. We have used the UNIFAC-CI model where all the group interaction parameters (GIPs) are predicted and/or fine tuned using the GC^{Plus}/UNIFAC-CI method in the latest ICAS regressed atom interaction parameters (AIPs). Typical GIPs generated will be presented. With these parameters, we were able to accurately predict the VLE of the azeotropic mixtures. The results were used for the design of the reactive-extractive and reactive-pressure swing distillations to produce high purity dialky carbonates. The energy consumption of the extractive distillation is less than the pressure-swing distillation. Overall, a heat integrated reactive and extractive distillation system provides the best option for energy savings than those without the heat integration.

Extended Abstract: File Not Uploaded

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