

RECOVERY AND PURIFICATION OF INTERMEDIATE PRODUCTS OF DICARBOXYLIC ACID ESTERIFICATION

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Abstract

Carboxylic acids are present in a wide range of industrial processes, including the production of nylon, biodegradable plastics, soaps and detergents, and pharmaceuticals. In particular, dicarboxylic acids are versatile compounds and important ingredients in the manufacture of various commodity and specialty chemicals. Moreover, the increased interest in sustainable chemical products enhances the role of dicarboxylic acids derived from biomass, such as succinic, itaconic or adipic, as key building blocks for the chemical industry of the future.¹ In this context, the design and optimization of separation and purification units involved in their processing is needed, which in turn also require predictive thermodynamic models.

The esterification of dicarboxylic acids with *n*-alcohols is a reversible reaction, and therefore, the product is a mixture comprising unreacted diacid, monoester and diester products. Depending on the starting carboxylic acid and the alkyl chain length of the alcohols a wide variety of chemical products can be synthesized. The aim of this work is to assess the fractionation of mixtures comprising the products of dicarboxylic acid esterification with alcohols of different alkyl chain length. In particular, we investigate the process operating window, as well as the feasibility of using different solvents, classical and condensed fluids, in order to compare yields and select the best solvent. For this purpose, a group contribution approach not only allows predicting the phase behavior of systems for which experimental information is scarce or not available, but also is a convenient approach to describe different systems comprising many similar compounds. For this purpose, we extend the GCA-EOS² to model the phase equilibria in mixtures containing monocarboxylic and dicarboxylic acids with various organic compounds and water.

Keywords: Dicarboxylic acids, GCA-EOS, Chemical platforms.

References

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