Minimum reflux and bow tie region in a simple heterogeneous reactive distillation column for esterification reactions

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The basic design of the reactive distillation (RD) columns consists in: 1) establishing the feasibility of the separation, 2) calculating the minimum reflux (minimum energy condition) and 3) calculating the number of theoretical stages and the feed tray for a given reflux higher than minimum. The use of Doherty's transformed compositions allows formulating an analogy with the geometrical methods applied in the heterogeneous azeotropic distillation (HAD) to simplify the solution of the three basic design problems for RD columns in overall equilibrium (simultaneous chemical and phase equilibria). Particularly the minimum reflux problem (MRP) of the sharp reactive separations has the same geometry as the nonreactive case of the HAD when the analysis is performed in transformed molar fractions (Avami et al., 2012).

The solution of the MRP and the localization of the product composition region (bow tie region) for non hybrid columns in overall equilibrium can be made based on the analysis of the reactive pinch points trajectories (RPPT) associated with the distillation products. In relation with these two aspects it is underlined, that there are no numerical details on the calculation of the RPPT known by the authors. With this motivation, this work presents a robust numerical continuation method for the tracking the RPPT and demonstrates its utility solving the minimum reflux problem and locating de bow tie region for two study cases dealing with the synthesis by RD of isoamyl acetate and n-amyl acetate.

In a general perspective, the main contribution consists in adapting the geometrical methods used in the design of the HAD columns with ternary mixtures (Urdaneta et al., 2002; Kraemer et al., 2011) to develop the basic design of RD columns with systems where the transformed compositions space has two dimensions (two degrees of freedom to calculate the reactive phase equilibria). The development of this viewpoint has few previous publications in the open literature (Avami et al., 2012; Sánchez et al., 2013) and contributes to the conceptual design of RD units for the synthesis of acetates.

At the end this work two conclusions are highlighted: 1) the minimum reflux within the best separations of RD columns with an ahead decanter corresponds either with two active pinch points located in different column sections or with a single active pinch point located in the feed tray and 2) the configurations with multiple heterogeneous stages condition the minimum reflux geometry and may reduce the minimum energy consumption.

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