Analytical Determination of Distillation Boundaries for Ternary Azeotropic Systems

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In the past, many strategies have been searched to define the distillation boundaries present in a multicomponent system with azeotropic compositions. In this sense, basic theory and different necessary but not sufficient properties have been published [1]. In addition, several topological and approximated methods have been developed to predict the general location of these boundaries [2-3], having in mind their importance when dealing with azeotropic distillation processes. Nevertheless, no direct procedure has been developed up to date.

In the present work, we present a new algorithm to directly and analytically calculate the distillation boundaries present in ternary azeotropic systems, simply using the concept that such boundaries are distillation trajectories passing through specific singular points. To generate the tested distillation trajectories, that after the optimization process will be the searched boundary, we use cubic splines (although any other adequate equation could be used). Additionally, and in order to simplify the calculation, an empirical but very accurate equation to reproduce the VLE has been used.

The proposed procedure, which has been tested for different ternary systems, consists in:

1. To classify the different singular points of the composition diagram, i.e. the azeotropic compositions and pure components present in the system, as stable, unstable or saddle points [4].
2. To define the origin and ending of the boundary ***t***rajectory searched and its ***n***umber of ***i***ntermediate ***p***oints to be calculated (*nipt*).
3. To define the composition of the component that will be the independent variable (e.g. 2) for each point of the trajectory: $x_{2,k}$ $(1 \le k \le nipt)$
4. To calculate, using the corresponding cubic spline (*cs*) and $x_{2,k}$, the value of: $x_{1,k}^{cs}$.
5. To calculate, the LV equilibrium of each liquid point $x_{i,k}$: $y_{i,k}^{eq.}$.
6. To calculate, using the corresponding cubic spline and $y_{2,k}^{eq.}$, the value of: $y_{1,k}^{cs}$.
7. To find, using an optimization solver over the cubic spline used, the trajectory (passing through the selected singular points of origin and ending) that satisfies the following objective function: $\sum_{k=1}^{nipt}\left(y_{1,k}^{eq.} - y_{1,k}^{cs}\right)^2$ =0.

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