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A novel method for the search and identification of feasible splits of extractive distillations in ternary mixtures

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ABSTRACT

This article describes a novel general method for the search and identification of possible splits of extractive distillations in any ternary azeotropic mixture – the method of infinitely sharp splits. This method finds all feasible product compositions that can be obtained in an extractive column at infinite height and finite reflux. Limiting parameters of mode for the entrainer flow rate and the reflux ratio are determined fast and robustly from the local K-values (vapor–liquid distribution coefficients) of all three components along the sides of the concentration triangle. For the given product specifications the method additionally determines the required number of trays in all the column sections. Hence, both operating and investment costs can quickly be analyzed without cumbersome simulations. The method can be extended to multi-component mixtures.

1. Introduction

Extractive distillation is the main method for the separation of homogeneous azeotropic mixtures. An extractive distillation column consists of three sections: the top, the bottom and the intermediate extractive section that is between the inlets of the feed and the entrainer. The entrainer is withdrawn from the column in the bottom product together with one or more components of the feed and usually recycled in additional apparatus, e.g. a distillation column. The conceptual design of this process is challenging due to its large number of process parameters (e.g. tray numbers of the feed and entrainer, the reflux ratio, entrainer/feed ratio). Finding optimal splits and operation modes by “trial and error” using commercial modeling systems for chemical plants is cumbersome. Therefore, systematic approaches for the conceptual design of this process have been studied in many articles.

Doherty and Caldarola (1985) introduced ternary maps and residue curve map analysis to decide if a separation of an azeotropic mixture in extractive distillation sequence is feasible. Based thereon methods for entrainer screening were presented (Foucher et al., 1991; Laroche et al., 1991).

Wahnschafft and Westerberg (1993) presented a method to decide whether a proposed split defined by a feed composition and desired product purity is feasible in a continuously operated extractive distillation column. Their method is based on a geometric approach, which requires a detailed residue curve maps and is limited to ternary systems. They used pinch curves and geometric conditions to establish the existence of a minimum flow rate of the entrainer. Knapp and Doherty (1994)

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Notation

B	bottom product flow rate, kmol/s
D	top product flow rate, kmol/s
E	entrainer flow rate, kmol/s
K	coefficient of phase equilibrium
L	liquid flow rate, kmol/s
N^+	stable node of bundle of trajectories
N^-	unstable node of bundle of trajectories
S	saddle of bundle of trajectories
T	boiling temperature
V	vapor flow rate, kmol/s
i	ordinal number of the component present in extractive element
iB	ordinal number of the component present in bottom product
iD	ordinal number of the component present in top product
iE	ordinal number of the component present in entrainer
j	ordinal number of the component absent in extractive element
x_i	concentration of component in liquid phase
x_{iD}^{Δ}	concentration of component of top product in delta point
x_{iD}^{r}	concentration of component of top product in root
x_{iD}^{rb}	concentration of component of top product in bounding root
x_{iD}^{sec}	concentration of component of top product in starting point of secondary pinch branch
x^B	composition of the bottom product
x^D	composition of the distillate (top product)
x^F	composition of the feed
$x^{\underline{F}}$	composition of the overall feed
η	impurity of a component
1, 2, 3, ...	ordinal numbers of components
12, 13, 23, 123	azeotropes of components
1-2, 1-3, 2-3	sides of concentration triangle

Subscripts

b	bottom section
e	extractive section
iB	ordinal numbers of a component present in bottom product
iD	ordinal numbers of a component present in top product
iE	ordinal numbers of a component present in entrainer
j	ordinal numbers of component absent in extractive element
m	tray number
t	top section
min	minimum
max	maximum

Superscripts

D	distillate (top product)
E	input of entrainer
mK	point of extreme K
$m\Delta$	point of extreme x_{iD}^{Δ}
r	root
rb	bounding root
sec	starting point of secondary pinch branch
st	stationary point
Δ	point of delta region
Δb	boundary point of delta region
tang	end the inactive segment of reflux due to tangential pinch

employed complex mathematical singularity theory to decide whether a given split defined by a feed composition, product purity and an entrainer to feed ratio is feasible or not. Rodríguez-Donis et al., 2009a,b, 2012) extended the method to study the feasibility of the extractive distillation in the batch operation mode by iso-volatility lines. Recently, Shen et al. (2013) and Shen and Gerbaud (2013) used the framework of Rodriguez-Donis et al. and residue curve maps to study the feasibility continuous extractive distillation columns for certain classes of ternary mixtures with both high-boiling entrainers (for minimum azeotropes) and low-boiling entrainers (for maximum azeotropes).

Brüggemann and Marquardt (2004) presented a short-cut method to determine the minimum entrainer flow rate and limits for the reflux ratio for the given feed and the split based on a non-linear analysis of the extractive section. This method is presented for ternary systems of binary feed mixtures having a minimum azeotrope and high-boiling entrainers. Ternary mixtures comprising of these features are called “mixtures of the extractive type” (class 1.0-1a in the classification of Serafimov (1970)). The splits in the three column sections for mixtures of the extractive type are shown in Fig. 1. A split named, e.g., (1,2:1,2,3) means that, at the top of the section, components 1 and 2 are present, while at the bottom components 1, 2 and 3 are present. Thus, for the component 3 a sharp split is achieved in the section. The entrainer strips one component out of the feed mixture and takes it to the bottom product while the other component is obtained in the distillate. The component obtained at the top of the column can

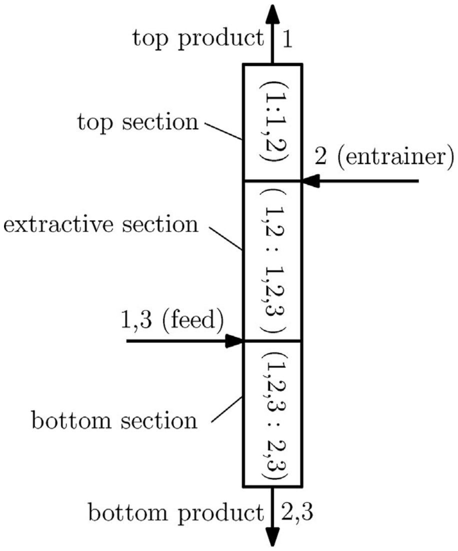

Fig. 1 – Splits in the three sections of an extractive column for a separation of a binary feed in the ternary mixture of the extractive type.