Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Distillation limit dependence on feed quality and column equipment

Lechoslaw J. Krolikowski*

Department of Chemical Engineering, Wroclaw University of Technology, Norwida 4/6, 50-373 Wroclaw, Poland

ARTICLE INFO

Article history:
Received 3 October 2014
Received in revised form 4 March 2015
Accepted 6 March 2015
Available online 26 March 2015

Keywords:
Feasible separation region
Distillation boundary
System synthesis

ABSTRACT

A feasible separation region is bounded by the product composition multitude (i.e., the distillate and bottoms composition points at total reflux and infinite number of stages) and by the distillation limit, which is defined for total condenser, partial reboiler and saturated liquid feed only. The present work addresses the dependence of the distillation limit on feed quality and column equipment and is based on material balances for a stripper or rectifier (with the envelope going through the pinch zone). Simple relationships for the distillation limit (in cases of saturated liquid/vapor feed and total/partial condenser or reboiler) were obtained. The application of generalized distillation limits to process synthesis may yield new, more efficient distillation systems. Furthermore, suitable selection of column equipment type, and thermodynamic state of the feed, may lead to extended possibilities for crossing distillation boundaries. In certain cases, the location of the distillation limit allows a composition profile to cross a pair of distillation boundaries: the total-reflux boundary and the pitchfork distillation boundary.

1. Introduction

In the course of process synthesis of separation systems for azeotropic mixtures, the need for quick identification of feasible separations arises. For a given feed composition, feasible separations are described by a set of possible distillate and bottoms compositions, which is called a *product composition set*. This set is called the *feasible separation region* if it includes all possible products' compositions. A number of studies determining attainable regions for homogenous azeotropic mixtures have been performed (Petlyuk and Serafimov, 1983; Laroche et al., 1992; Stichlmair and Herguijuela, 1992; Wahnschafft et al., 1992; Fidkowski et al., 1993; Poellmann and Blass, 1994), though, in most cases, these have usually been limited to total reflux, as the feed quality and thermodynamic state of the products are not relevant for total reflux. From a practical point of view, the feasible separation regions for finite reflux are more relevant.

A border of the product composition set at total reflux consists of two elements (Fig. 1). According to Serafimov (1968b), the first element of the set is a product composition multitude (PCM) – i.e., the distillate and bottoms composition points at total reflux and an infinite number of stages. The second element is a distillation line, going from the feed composition point $\mathbf{z}_F$ to unstable and stable nodes of the distillation region, which includes the given feed composition. This line is called the *feed distillation line* (FDL). As was shown by Petlyuk and Avetyan (1971), a part of the feed distillation line located between the feed composition point and unstable node restricts the distillate compositions at total reflux, while a part of the FDL limited by the feed composition point and stable node restricts the bottoms compositions at total reflux.

A feasible separation region is bounded by the product composition multitude and by the pinch point curve (PPC), which goes through the feed composition point (according to Wahnschafft et al., 1992) or by the distillation limit (according

* Tel.: +48 71 320 3334; fax: +48 71 328 0475.
E-mail address: lechoslaw.krolikowski@pwr.edu.pl
http://dx.doi.org/10.1016/j.cherd.2015.03.005
0263-8762/

Nomenclature

D	molar flow rate of distillate
F	molar flow rate of feed
L	molar flow rate of liquid phase
N	number of stages
q_L	molar fraction of the feed that is liquid
R	reflux ratio
S	reboiler ratio
V	molar flow rate of vapor phase
$\mathbf{x}$	vector of mole fractions in liquid phase
$\mathbf{y}$	vector of mole fractions in vapor phase
$\mathbf{z}$	vector of mole fractions in feed or product

Subscripts

B	bottom
D	distillate
F	feed
p	pinch
r	rectifying section
s	stripping section

Acronyms

CMO	constant molar overflow
DL	distillation limit
FDL	feed distillation line
FTLS	feed tie-line split (transition line)
PCM	product composition multitude
PDB	pitchfork distillation boundary
PPC	pinch-point curve
S	saddle
SN	stable node
TRB	total-reflux boundary
UN	unstable node
VLE	vapor–liquid equilibrium

to Fidkowski et al., 1993). For both cases, the following question arises: what is the influence of feed quality and distillation column equipment on the borderline between sloppy splits and regions not accessible by distillation? A change in the borderline will immediately have an effect on the feasible separation region (addressed in this study) and may have an indirect effect on system synthesis. In other words, it may influence the system structure, the design and the operating parameters of individual columns.

In the current study, continuous distillation in trayed columns was modeled by theoretical stages. Constant molar overflow in each section of the column, constant pressure along the column, and the products in the form of saturated liquid or vapor were all assumed. An ideal vapor phase and an activity coefficient model (using the Wilson equation) for the liquid phase were used in all calculations. The references for vapor–liquid equilibrium data are given in Table 1. MATLAB and Aspen Plus were used for calculations.

2. Wahnschafft's feasible separation region

Wahnschafft et al. (1992) indicated that the feasible separation region is bounded by the product composition multitude at $R=\infty$ and $N=\infty$ and by the feed pinch-point curve going from the feed composition point in both directions (to unstable and stable nodes), where the feed pinch-point curve was defined as the liquid-phase PPC (liquid PPC). They assumed that the feasible separation region is a sum of the product composition set at total reflux and its extension with the reachable products at finite reflux. The feasible separation region for a ternary zeotropic mixture with C-shaped distillation lines is shown in Fig. 2. The continuous feed distillation line (FDL) is approximated by the discrete feed distillation line in the figure for practical reasons (this approximation is used in other figures). It should be noted that Wahnschafft and co-workers did not give any assumptions relative to feed quality, column equipment (type of condenser and reboiler) or thermodynamic state of the products. If one assumes a saturated liquid feed, total condenser, and a partial reboiler (the most frequently occurring case), then Wahnschafft's feasible separation region contains a distillate composition subset enclosed by feed-vapor PPC and feed-liquid PPC, which cannot be obtained (based on observations of process simulation results), whereas the bottoms composition set is defined correctly.

3. Fidkowski's feasible separation region

Assuming that the rectifying section is responsible for the distillate composition, and the stripping section is responsible for the bottoms composition, Fidkowski et al. (1993) considered an instance when a saturated liquid mixture is fed into a column equipped with a total condenser and partial reboiler. The authors concluded that sloppy separations were demarcated from regions not accessible by distillation by two curves: the feed-vapor PPC, which restricts distillate composition, and the feed-liquid PCC, which limits bottoms compositions, with these curves denoting the *distillation limit*. According to Fidkowski and co-workers, feasible separation regions are determined by the product composition multitude at $R=\infty$ and $N=\infty$ and the distillation limit together with the mass balance line of *feed tie-line split* (transition line). The transition line divides the *direct geometry* (where there is a pinch

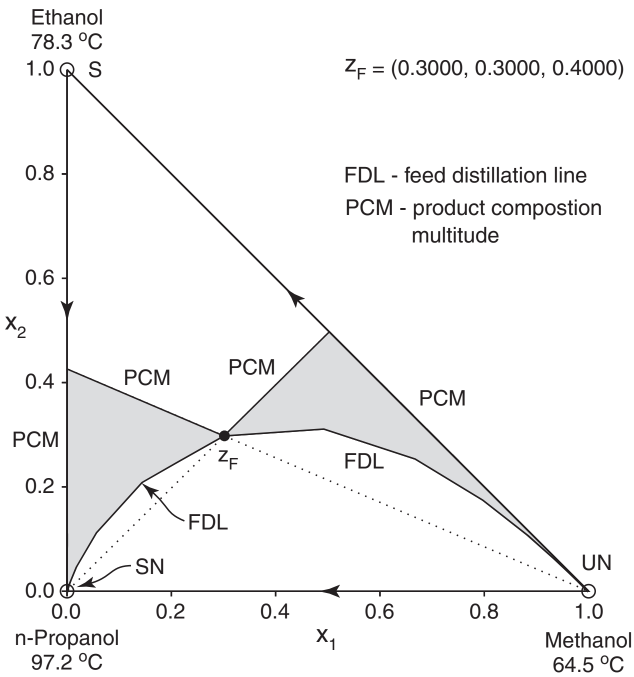

Fig. 1 – Product composition set for a zeotropic mixture with C-shaped distillation lines and total reflux.