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Identification and analysis of possible splits for azeotropic mixtures. 2. Method for simple columns

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ABSTRACT

A new method for the design of distillation units based on the behaviour of the mode of infinitely sharp split is presented. The method is non-iterative, fail free and fast. It can lead to the creation of more optimised process flow sheets, and can automate the design process. The first step of the method consists of fast delimitation of the product regions in the concentration simplex and the identification of the ends of the pinch branches at each section. In this way a qualitative evaluation of the arrangement of the pinch branches and the bundles of trajectories can be obtained as the bundles of trajectories depend only on the relations between the values of the coefficients of the phase equilibrium of components at certain points in the concentration simplex. This first step of the method was described in a previous article. In the present article, the second step is described, namely the identification of the possible splits in simple two-sectional columns. If some split is possible, trajectories of both sections intersect each other. The simple, necessary and sufficient condition of the separability has been established: trajectories of both sections intersect each other if pinch branches of both sections have common terminals (ending points). The check-up of this simple condition does not request the calculation of pinch branches and trajectories. The identification of the possible splits is the basis for any algorithm in the synthesis of flowsheets. An algorithm for the identification of one interactive bundle at each section among many is presented here. The interactivity of bundles depends on the location of the point of products. This information about the interactive bundles will be used for subsequent steps of designing e.g. for the calculation of minimal reflux and necessary trays for given reflux.

1. Introduction

In a previous article Petlyuk et al. (2011), have pointed out the main disadvantages of the conventional cut-and-try method for the design of distillation columns used in commercial modelling software, namely non-optimal flowsheets and lengthy design processes. On the other hand, many proposed methods for conceptual design are useful only for special cases such as the infinite reflux, the *direct* or *indirect splits*, which are often impossible or non-optimal (Doherty and Malone, 2001; Safrit and Westerberg, 1997; Rooks et al., 1998; Thong, and Jobson, 2001). The method presented here (Petlyuk and Danilov, 1999, 2000a, 2000b, 2001a, 2001b; Petlyuk, 2004; Petlyuk et al., 2011) uses the regularities of the *infinitely sharp split mode* (the terms in italics are explained in the "Glossary"), in which each product of the column contains only some of the feed components. The components present in the product are called *present components* (noted with subscript i), in contrast to the components not present in the product which are called *absent components* (they have the subscript j). The *product points* are located on the boundary of the concentration *simplex*. In the infinitely sharp split mode, only the present components exist in the product point, while the absent components exist in the infinitesimal neighbourhood of it. The infinitely sharp split mode is only possible in infinite columns. However, if some split is possible in the infinitely sharp split mode, it is possible for any product purity in finite columns. The split is possible if the product points are connected to each other by *section trajectories*. The main regularities for the infinitely sharp split mode for a single section are described and illustrated in our previous article (Petlyuk et al., 2011). Important differences exist between the location of the section trajectories at infinitely sharp and non-infinitely sharp splits. The section trajectory for the non-infinitely sharp mode is everywhere a smooth line. In contrast, the

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section trajectory for the infinitely sharp mode consists of two segments. The first segment is located between the *product point* and the *tearing-off point* on the product element in the concentration simplex. The second segment is located inside the simplex. The tearing-off point is a sharply salient point of the section trajectory. In addition, infinite multitude of segments of section trajectories (the *bundle* of trajectories) exist inside the simplex at the infinitely sharp mode for any given product point and for any the given reflux. The location of the bundles depends on the location of the pinch lines for the given product point. Important differences between the location of pinch lines at the infinitely sharp and the non-infinitely sharp split exists in the same way as for the section trajectories. The pinch line for the non-infinitely sharp mode is a smooth line. In contrast, a tree of pinch lines (*pinch tree*) exist at infinitely sharp mode. The root of this tree is the product point; the *pinch trunk* is the pinch line on the product element of the simplex; the *pinch branches* are the pinch lines on other elements of the simplex and inside it. The bundle of trajectories is a polyhedron, the vertexes of which are located on the pinch tree. In our previous article, we have presented a new non-iterative method of the identification of beginning and ending points (*terminals*) of pinch branches by calculating the phase equilibrium coefficient K of all components (present and absent components) in the points of the pure components and azeotropes. In this way, difficulties in the calculation of pinch branches were avoided, and a quick qualitative evaluation of the location of pinch branches and bundles of trajectories was provided.

In this article we go a step further by describing a method for the determination of possible splits in simple columns. We consider here the connection and interaction between the sections of the column. If some split is possible, only one trajectory of a bundle of section exists, which interacts with a trajectory of another section, and only one bundle of section exists, which interacts with a bundle of another section. If some split is possible, certain trajectories (*interactive trajectories*) of both sections intersect each other (Levy et al., 1985). We show that the existence of common terminals of pinch branches of both sections is a sufficient condition for this intersection at a reflux higher than minimal reflux (interactive trajectories will be calculated at subsequent design steps). In addition, we describe the method for identifying one of the many bundles of trajectories (an *interactive bundle*) in each section, which is involved in the process of distillation at the given composition of both products.

Some other methods of conceptual designing include the calculation of pinch branches. The most known of these is the method of RBM (Bausa et al., 1998). There are a few differences between our method and the RBM method. Our method checks, whether a split is possible, but the RBM method calculates the minimal reflux if this split is possible. This is a different stage of conceptual design. Our method takes into account all types of locations of pinch lines of sections, which are shown in a previous article, which is not the case for the RBM method. Moreover, our method determines the active pinch branches for the calculation, while the RBM method does not. Some important disadvantages of the RBM method are specified by Ruiz et al. (2010): trajectories intersect, but rectification bodies do not; rectification bodies intersect, but trajectories do not. There are also significant differences between bundles and rectification bodies. The bundle is located only inside the simplex, but not on its bounding elements in contrast to the rectification body, which is located on both. Therefore, the rectification body has the dimension more by one than the bundle, and it is partly empty. Bundles of trajectories contain elements having the different dimension, which depend on numbers of components in products and in the feed. These elements are curved (in our following examples very small). They are shown as linear for simplification in figures. In contrast to the bundles of trajectories, rectification bodies have linear edges.

Another recent pinch-based method is the PDB method (Brüggemann and Marquardt, 2011) for the determination of the distillation boundary for the given purity of the product, which is based on the concept of reversible distillation.

Some new methods of synthesis of distillation flowsheets were proposed in the article by Ruiz et al. (2010) with the method of temperature collocation, which requires the solution of a system of nonlinear equations. The method is however only illustrated for the case of an ideal mixture.

A more general method, that of the shortest stripping line for finding the minimum energy requirements (Lucia et al., 2008) also requires the solution of a system of nonlinear equations.

Unlike all other methods of conceptual distillation design, which solve complex systems of nonlinear equations, our method does not require it, and it does not even require the calculation of pinch branches and distillation trajectories, because it uses, instead, the regularities of distillation at infinite sharp splits. Therefore, it is very fast and error-free.

2. The theoretical base

2.1. Illustrative examples

First, let us consider a few illustrative examples of the interaction of bundles of trajectories in both sections for some four-component mixtures for all types of splits (*direct*, *indirect*, *intermediate*, and *with distributed components*). The following figures show the material balance lines in the columns: the feed point can be on any point on these lines, and the product points are the intersection points of these lines with the boundaries of the simplexes. The corresponding split is shown in a small sketch in each figure. Fig. 1 shows the pinch branches for both column sections and the bundles of trajectories at the given finite and the infinite reflux for the intermediate split 1,2:3,4 for the ideal mixture of pentane–hexane–heptane–octane. The bundles of trajectories arise at different refluxes (the *minimal active reflux*) for each section. The *intervals of active reflux* are unlimited for both sections (the *maximal active reflux* is infinite). The bundles do not intersect at the given finite reflux. However, if the reflux increases, the pinch points move on the pinch trees in the direction of the arrows away from the product points of two sections, and thus the bundles are increased. They begin to intersect each other at some reflux (at *minimal reflux*). The pinch points of two sections come in the vertexes 2 and 3 (the *common terminals* of pinch branches) at the infinite reflux. The edge 2–3 is the line of the intersection of two bundles at infinite reflux.

Fig. 2 shows the pinch branches and the bundles for the intermediate split 1,3:2,4 of azeotropic mixture acetone–benzene–chloroform–toluene. Two lines are shown for the material balance: the first line for the product points x_D and x_B, and the second line for the product points x_{D1} and x_B. The common terminals are the vertex 2 and the azeotrope 13 in both cases, and the intersection line of the two bundles at infinite reflux is the boundary of the distillation regions on the face 1–2–3. The *interactive bundles* of each section have different location in each case. They are shown for the finite reflux for the product points x_D and x_B in this figure. We see their intersection line, i.e. the given reflux is higher than the minimal reflux. In order not to make the figure too complex, the bundle of the top section for the product point x_{D1} is not shown. The tangential pinch exists in two sections. Therefore, the beginning *segments* of all primary pinch branches are *inactive*. Other possible splits of this mixture are 1,2,3:4 (for any feed point x_F on the lines $x_D - x_B$ and $x_{D1} - x_B$) and 1:2,3,4 (for some feed point x_F on the lines $x_D - x_B$ and $x_{D1} - x_B$; see Fig. 3).

Fig. 3 shows 3D bundle of the top section, 1D bundle of the bottom section, the product simplexes of the bottom section,