Identification and analysis of possible splits for azeotropic mixtures—1. Method for column sections

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ABSTRACT

The identification of possible splits at the finite reflux has been the main challenge for the creation of efficient flowsheets for the separation of azeotropic mixtures. We show in this paper that this problem can be solved by analyzing the mode of infinitely sharp splits, for which trajectories of distillation and pinch lines have special characteristics. The feasibility of sharp splits depends on the relationship of phase equilibrium constants K of components at certain points of the concentration simplex. Pinch branches and bundles of trajectories can arise only when certain relationships of K are satisfied on edges of the concentration simplex. Bundles of trajectories of both sections of column can intersect each other only at complementary relationships of these values at points of components and azeotropes. In this case, there are profiles of concentrations of both sections, which together connect the points of products with each other, i.e., a split is possible. The theory of infinitely sharp split mode determines the mentioned relationships of K. The method of infinitely sharp split mode has been developed on the base of this theory. This method includes the calculation of K at certain points of the concentration simplex. It is not iterative. Therefore, it is very fast, reliable, and can be easily programmed. For the first time, this method covers all n-component azeotropic mixtures, and all types of sharp and half-sharp splits, at which both or one product of column is sharp. This method can find unknown energy-efficient splits for different azeotropic mixtures because it is based on fundamental regularities of distillation. The automatic identification of possible splits is the basis for the synthesis of flowsheets for distillation units and for the conceptual designing of distillation columns. The theory of infinitely sharp split, the method of delimitation of product regions on elements of the concentration simplex for each section of simple columns, and the method of identification of types, characteristics, and terminals of pinch branches are considered in this article.

1. Introduction

The commercial modeling softwares, such as Aspen+, Pro/II, Hysys and others, focus on the simulation and the efficient solving of large systems of nonlinear equations. This is not adequate for the designing of distillation units because they do not provide answers to the fundamental questions of conceptual designing, such as the possible splits, the minimum reflux, and the minimum number of trays. In particular, this is important for the azeotropic mixtures, where the identification of possible splits is of key importance.

Therefore, the numerous studies on the structure of distillation process have been carried out during the last decades. These studies have been focused on the calculation of minimal reflux (Levy et al., 1985; Julka and Doherty, 1990; Doherty and Malone, 2001; Bausa et al., 1998; Bruggemann and Marquardt, 2004) and for the identification of possible splits at the infinite reflux and infinite number of trays (Safrit and Westerberg, 1997). Positive results have been obtained in these two directions. These studies were based on the geometrical approach, which is well suited for azeotropic mixtures. The most promising results for the minimal reflux have been achieved by Bausa et al. (1998), who developed the rectification body method (RBM) using pinch branches. The problem of calculation of minimal reflux has been solved by means of the RBM for n-component azeotropic mixtures for all types of splits including intermediate splits if the possibility of a split is known a priori, and concentrations of components in both products are given.

However, our analysis of all possible types of pinch branches demonstrates that this method is not always effective. Some

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drawbacks of this method are the skipping of the important pinch branches and endless iterations because of jumps of calculated pinch points away from one pinch branch to another in some cases.

For the problem of identification of possible splits, the following factors have important meaning: the type of split, the reflux, and the number of components. There are different classes of splits (the sharp split, the semi-sharp split and the non-sharp split) for different types of sequences of separation (the direct split, the indirect split, the intermediate split, and the split with one or several distributed components). Examples of these classes and types for the four-component ideal mixture of components 1, 2, 3 and 4 serve as the following splits:

(1:2,3,4)—the direct sharp split,
(1,2,3:4)—the indirect sharp split,
(1,2:3,4)—the intermediate sharp split,
(1,2:2,3,4)—the split with one distributed component,
(1,2,3:2,3,4)—the sharp split with two distributed components,
(1,2:1,2,3,4)—the intermediate semi-sharp split,
(1,2,3,4:1,2,3,4)—the non-sharp split.

We will not consider non-sharp splits because they are of less interest for the separation of mixtures.

We will not consider the splits with two and more distributed components too because they are possible only for certain distributions of components between the products. All the other splits are considered in the present article and the subsequent articles. Of course, the sharp splits are of most interest, but such splits are possible only for a small number of structures of the azeotropic mixtures because the internal restrictions exist in the concentration simplex, caused by the azeotropes. These restrictions allow us to use only the semi-sharp splits in most cases.

Direct and indirect sharp and semi-sharp splits are the easiest for identification of separability irrespective of the number of components (see Doherty, and Malone, 2001). These splits are possible if there is the single-component product, which is the unstable or stable node because it can always be separated from the rest of components. For other types of splits, it is necessary to use the more advanced geometrical approaches. The famous geometrical approaches can rather easily be used for three- and four-component mixtures because the visualization is possible only for such mixtures. Wahnschafft et al. (1992) and Castillo et al. (1998) have suggested to use the specific sets of points located between the line of distillation and the pinch branch (the leaves) for a given composition of product. Profiles of concentration of the sections at any reflux are located on these leaves. Therefore the crossing of these leaves for both sections is the criterion of separability for the given split for the given three-component mixture.

Many studies have been done for the identification of possible splits at infinite reflux for the n-component mixtures (Petlyuk et al., 1979; Knight and Doherty, 1990; Rooks et al., 1998) and for the solution of related tasks like the identification and calculation of composition of azeotropes (Fidcowski et al., 1993), the determination and matrix representation by means of the adjacency matrices of structure of azeotropic mixtures, and the determination of boundaries of distillation regions (Petlyuk et al., 1979; Safrit and Westerberg, 1997; Rooks et al., 1998). The separability at finite reflux is the most interesting issue because the most effective splits are possible at finite reflux, but they are impossible at infinite reflux. However, the identification of possible intermediate splits at a finite reflux for the n-component mixtures is the most challenging task. An attempt to solve this problem was made in this work (Thong and Jobson, 2001). The main aim of this work was to excute a test of the possibility of the given split not for the given composition of product, but for the given element of concentration simplex. On the other hand, defects of this method are that it neglects the most interesting splits when the concentration profile crosses the boundary of distillation region, and frequent cases where the product region is located on some part of an element of the concentration simplex.

In summary, the challenge of identification of possible splits at finite reflux in simple and complex columns remains unresolved. Therefore, methods based on feasible splits at infinite reflux are in practice. However, this results in non-optimal flowsheets because the most economical splits in the simple and complex columns exist at the finite reflux.

Another unsolved challenge of conceptual designing is the calculation of the required number of trays for the given reflux. Thus, despite the large number of studies, all the main problems of conceptual design have been only partially solved, and therefore, the mentioned methods are not widespread.

For solving these problems, it is necessary to determine general laws of location of profiles of concentration at finite reflux. In addition, it is necessary to linearize some lines in the simplex, that will allow us to replace geometrical images of these lines using the algebraic expressions.

We will illustrate here that all challenges of conceptual design can be overcome by means of in-depth study of *infinitely sharp mode* of distillation, at which concentrations of impurities in products of column are infinitesimally small at finite reflux. Note that the sharp splits have also been used in works (Bausa et al., 1998; Thong and Jobson, 2001) because it is impossible to specify compositions of products with finite impurities before the calculation. However, these authors have not considered necessary conditions of phase equilibrium at points of tearing-off of distillation trajectories away from boundary elements of concentration simplex that is the basis of theory of infinitely sharp splits. This mode, which is a very powerful tool, has not been deeply investigated before our research in contrast to the infinite reflux mode. In our earlier studies (Petlyuk et al., 1984; Petlyuk and Danilov, 1999, 2000a, 2000b, 2001a, 2001b; Petlyuk, 2004), we have shown simple relationships between the separability of mixtures at the mode of infinitely sharp splits and the relations of inequalities of coefficients K of all components on bounding elements of concentration simplex (short: the elements). This allowed us to identify the regions on these elements where the points of products can be located (the product regions). The necessary condition for the separability is the location of points of both products in these regions.

In this study, we will identify the location of terminals of pinch branches for products of column without calculating them, which can sometimes be difficult. It will be shown in this article that the sufficient condition for the separability is the presence of common terminals of pinch branches for both products of column. It will be proven in this article that the location of these terminals depends only on relations between values of coefficients K at some points of components and azeotropes. We have developed the non-iterative method for the identification of these terminals. This approach allows us to identify efficiently possible splits and to determine their properties. The creation of reliable methods based on the mode of infinitely sharp split is an important step towards automatic designing of distillation units.

In this article, we will first consider the peculiarity of infinitely sharp mode with illustrative examples. We will then show why these peculiarities follow from fundamental regularities of distillation, and we will finally propose the algorithms for the identification and analysis of possible splits, which follow from these regularities.

Methods described in this article are valid for sections of column, while in our next article, we will present methods for simple two-sectional columns.

2. The theoretical base

2.1. Illustrative examples

The mode of infinitely sharp split has some particular properties. Therefore, we need to introduce the new terms and explain them by means of some examples. New terms will be marked by italics. Definitions of these terms can be found in the glossary.

Only a part of feed components is present in the product of column at the infinitely sharp mode (in the infinite column ($N = \infty$) with the finite reflux ($V/L \neq 1$)). These components will be called *present components i*, in contrast to the so called *absent components j*. *Absent and present components* affect the process of distillation in the different ways. According to the rigorous meaning of present and absent components, following correlation is valid, for example, for the bottom section of column:

$$\lim(x_{Bj}/x_{Bi}) = 0 \quad \text{for } x \to x_B, \text{ for all } j \text{ and } i \qquad (1)$$

where x is the arbitrary composition point; x_B is the composition point of bottom product in the simplex; and x_{Bj} and x_{Bi} are the concentrations of absent and present components in the bottom product, accordingly.

To understand the basic features of location of trajectories in the infinitely sharp mode, we consider a few illustrative examples (Figs. 1–9). At the top of each figure is given a sketch of bottom section (Figs. 1–4, 6 and 7, and 9) or the top section (Figs. 5 and 8) with the split, which is studied.
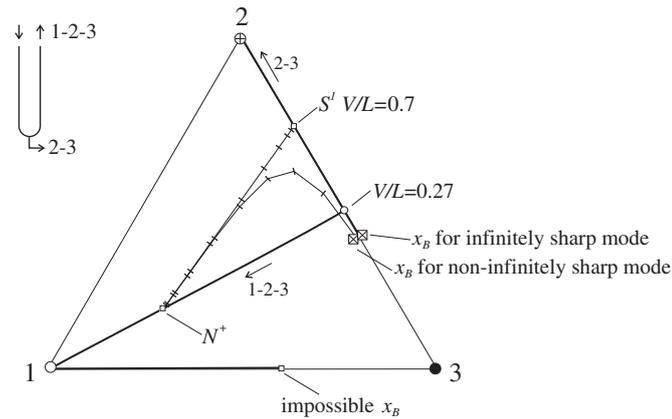

Fig. 1. Trajectories for infinitely sharp and unsharp modes at $V/L = 0.7$, and pinch branches. ($\square$) tearing off point and final point of trajectory; ($\vdash\!\!-\!\!\dashv$) pinch trunk and branch; (——) trajectory; ($\circ$) branching point; ($\rightarrow$) direction of pinch branches; 1-2 element.
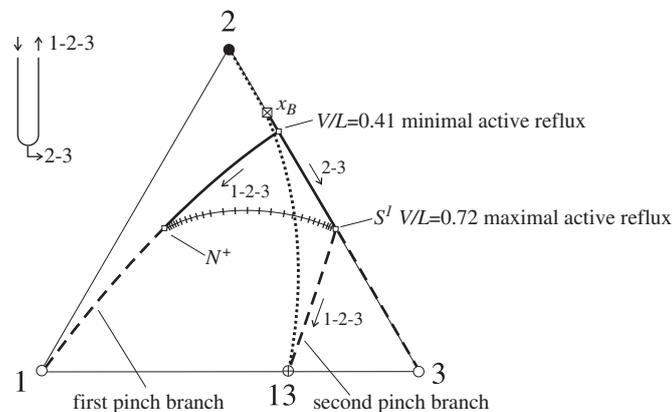
Fig. 2. Active and inactive pinch branches. Reflux interval. (- - -) inactive pinch branches and their segments. Thick dotted line trace of distillation boundary on faces of concentration simplex.
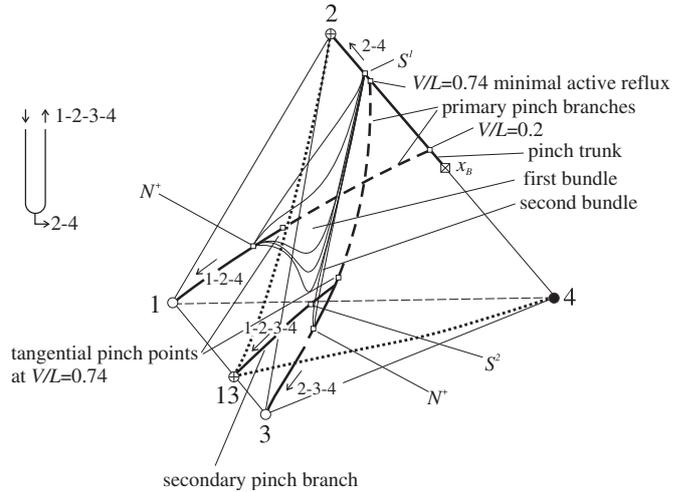
Fig. 3. Two bundles of trajectories. Tangential pinch. Thin lines—trace of distillation boundary on faces of concentration simplex.
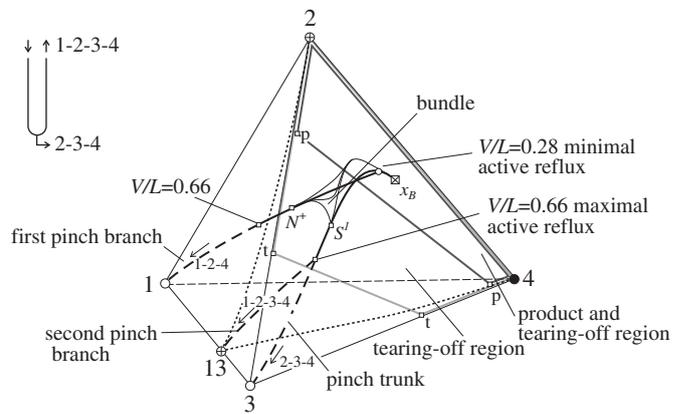
Fig. 4. Tearing off and product regions. Reflux interval. t—limiting tearing-off points. p—limiting product points.
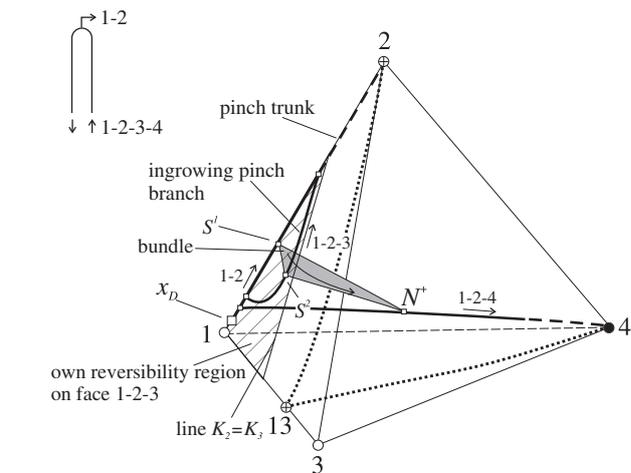
Fig. 5. Ingrowing pinch branch.

In Fig. 1, pinch branches and trajectories of distillation are shown for the given product point of bottom section in the infinitely and non-infinitely sharp modes for the given reflux
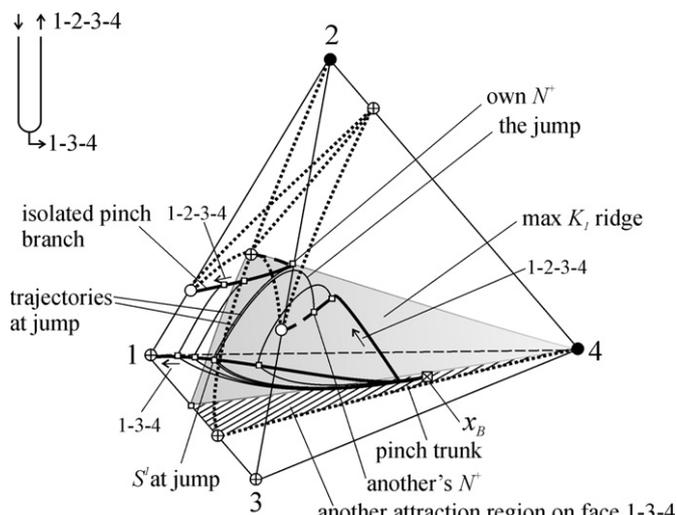
Fig. 6. Jump between pinch branches.

Fig. 9. Six bundles. ⟶ trajectories of bottom section at $V/L=1$; ■ ▨ boundaries of 3D bundles at $V/L=1$.

Fig. 7. Primary, secondary and tertiary pinch branches.

Fig. 8. Pinch bridge.

parameter V/L for the ternary ideal mixture pentane–hexane–heptane (the bottom product point is located on side 2-3). Trajectories at the infinitely sharp mode always consist of two

parts in contrast to trajectories at the non-infinitely sharp mode. The first part, which is located on the bounding element of simplex containing the point of product (on the *product element*), begins at this point and comes to an end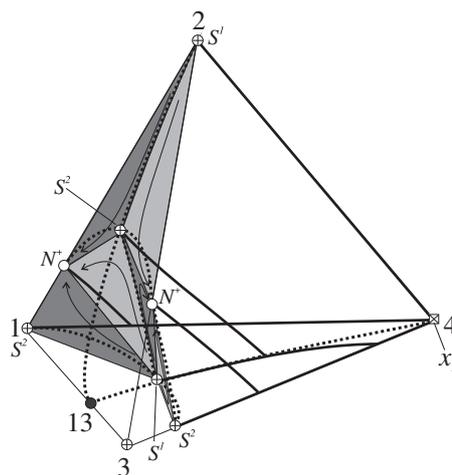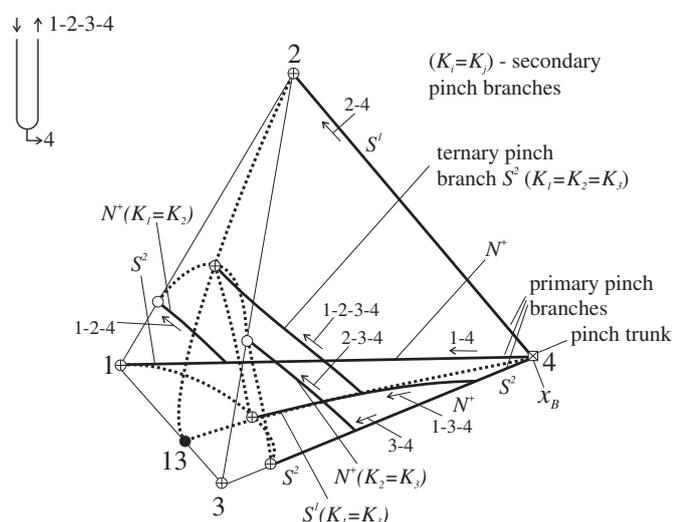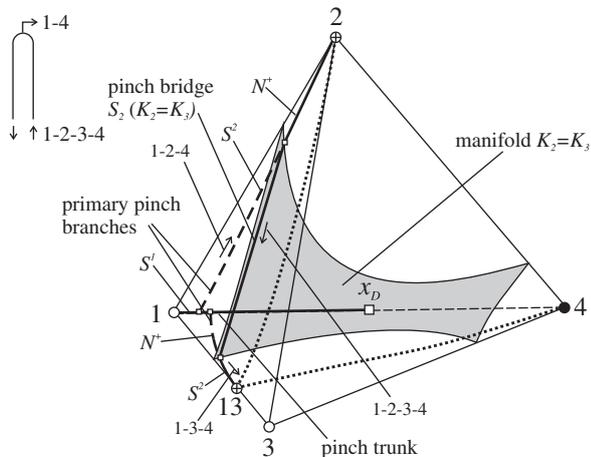 at the point S^1, which we will name the *tearing-off point*. The second part, which is located inside simplex, begins at the point S^1 and comes to an end at the stationary point N^+ on the pinch branch (N^+ is the sign of eigenvector). We will name common points of two pinch branches the *branching points*. The value of reflux parameter V/L increases along with pinch branches in the direction away from the product point x_B, where $V/L=0$. The multitude of pinch branches looks like the pinch tree, the pinch trunk of which is the pinch branch on the product element. In Fig. 1, the *product element* is the side 2-3, and the *product region* is the whole of side 2-3 because any point at side 2-3 can be a *product point*. No point on side1-3, for example, can be the *product point* because it is not in the *product region*. Any trajectories inside the simplex cannot pass through this point (the trajectory is the dotted line going on side 1-3).

In Fig. 2, pinch branches and the trajectory of distillation are shown for the given product point of bottom section in the infinitely sharp mode for the given reflux parameter V/L for the ternary azeotropic mixture of acetone–benzene–chloroform (the bottom product point is on side 2-3). The product region is the segment of side 2-3 from the vertex 2 to the point x3=0.27. The pinch tree consists of *pinch trunk* and two pinch branches. We will denominate the pinch branches, that are located inside the concentration simplex nearer and farther from the product point as the *first and second pinch branches*, accordingly. Points S^1 can be located only between the branching points of *first and second pinch branches*. Therefore, only the segment of pinch trunk between these points is *active*, while its other segments are *inactive*. The *reflux parameter is minimal and maximal* in the first and second branching points, accordingly. In Fig. 2, the trajectory of distillation is represented at the *maximal active reflux*. The whole of second pinch branch and the segment of first pinch branch, that are farther from a product point than the point N^+ at the maximal active reflux, are inactive. Note that the distillation boundary (the thin line between the vertex 2 and azeotrope 13) does not affect this analysis.

We will now consider four-component azeotropic mixtures. These mixtures are the most interesting for understanding the regularities of infinitely sharp mode because of the following two reasons: all regularities of mixtures with any number of

components can appear for four-component azeotropic mixtures, but not for all, they can appear for ternary azeotropic mixtures; pinch branches and trajectories of distillation for four-component azeotropic mixtures can be visible in the concentration simplex in contrast to mixtures having five or more components. In Fig. 3, the pinch tree and two bundles of trajectories are shown for the mixture acetone–benzene–chloroform–toluene (the bottom product point is located on the edge 2-4 of simplex). The product segment is the whole of side 2-3. There are two *primary pinch branches*, which begin at branching points away from the pinch trunk and exist in two different faces of simplex—1-2-4 and 2-3-4 (they are not the first and second pinch branches because they are not located inside the concentration simplex), and one *secondary pinch branch*, which is located inside the simplex and begins at the branching point away from one of two primary pinch branches. Initial segments of primary pinch branches and the pinch trunk are inactive because of *tangential pinch*. One bundle of trajectories appears at the tearing-off point S^1 when the tangential reflux takes place, and then it divides into two bundles when the reflux of secondary branching takes place.

In Fig. 4, the pinch tree, the trajectory, the limited product region, and the limited tearing-off region are shown for the mixture acetone–benzene–chloroform–toluene (the bottom product point is located on the face 2-3-4 of simplex). The pinch tree consists of pinch trunk and two primary pinch branches, which are located inside the concentration simplex in contrast to the primary pinch branches in Fig. 3. They are the *first and second pinch branches* like the pinch branches in Fig. 2. Points S^1 can be located only between the branching points of first and second pinch branches. Therefore, only the segment of pinch trunk between these points is active, while its other segments are inactive. The reflux parameter is minimal and maximal in the first and second branching points, accordingly. In Fig. 4, the trajectory is represented at some active reflux. The whole second pinch branch and the segment of first pinch branch, which are farther from the product point than the point at maximal active reflux, are inactive.

In Fig. 5, the pinch tree and the bundle of trajectories are shown for the mixture acetone–benzene–chloroform–toluene (the top product point is located on limited product segment on the edge 1-2 of simplex). There is the *ingrowing pinch branch* on face 1-2-3, that initially tears off from the pinch trunk in the branching point and then grows up into the pinch trunk at the *point of ingrowing*. The pinch trunk and the ingrowing pinch branch are only active between the branching point and the point of ingrowing. The reflux parameter is minimal and maximal in these points, accordingly.

In Fig. 6, the pinch tree, the *isolated pinch branch*, and the trajectories at different reflux are shown for the mixture acetone–methanol–chloroform–acetonitrile (the bottom product point is located on the face 1-3-4). There is a *jump of pinch point* away from the primary pinch branch up to the isolated pinch branch at a certain reflux (the *reflux of pinch jump*). The primary pinch branch is located in the attraction region to the stable node of distillation region, which does not contain the product point (the *another's stable node*). The segment of primary pinch branch before the jump and the segment of isolated pinch branch after the jump are active. The trajectories are completed at points of primary pinch branch before the reflux of pinch jump; the trajectories after this reflux are completed at points of isolated pinch branch.

In Fig. 7, the pinch tree is shown for the mixture acetone–methanol–chloroform–ethanol (the bottom product point is vertex 4). The pinch trunk coincides with vertex 4. The primary pinch branches are located on the edges 1-4, 2-4, and 3-4; the secondary pinch branches are located on the faces 1-2-4, 1-3-4, and 2-3-4; the tertiary pinch branch is located inside the simplex. The secondary pinch branches are located on univolatility lines, on

which phase equilibrium coefficients of any two components out of absent components 1, 2, and 3 are equal; the tertiary pinch branch is located on univolatility line, on which phase equilibrium coefficients all of absent components 1, 2, and 3 are equal.

In Fig. 8, the pinch tree is shown for the mixture acetone–benzene–chloroform–acetaldehyde (the point of top product is located on the edge 1-4). There is *the pinch bridge* between two primary pinch branches, which are located on the faces 1-2-4 and 1-3-4. The pinch bridge is located on the α_{23}-univolatility surface (the surface $K_2 = K_3$). There is the tangential pinch, too. Therefore, initial segments of pinch branches are inactive.

In Fig. 9, the pinch tree for the mixture acetone–methanol–chloroform–ethanol and the boundaries of the 3D bundles at $V/L = 1$ (the point of bottom product is vertex 4) are shown. The bounding bundles have the differing stationary points S^1, S^2, and N^+ of bundles (the points S^1 are the unstable nodes for the bounding bundles).

2.2. Basic correlations for infinitely sharp splits

The simple and important relations exist between coefficients K_i, K_j and reflux V/L at tearing-off points and on pinch branches (Petlyuk et al., 1984; Petlyuk and Danilov, 2001a; Petlyuk, 2004). These relations follow from the specific character of tearing-off points and branching points away from the product elements. In tearing-off points, concentrations of present components stay constant. However, the concentrations of absent components grow up in the direction away from product elements. Tearing-off points can be characterized as quasi-stationary points. The basic relationship can be obtained for the mode of infinitely sharp split taking into consideration this specific property of tearing-off points. We can consider each point of the pinch branch as the composition point at certain cross-section of *reversible distillation*, i.e. the distillation, at which the ingoing flows of liquid and vapor toward every tray exist in the phase equilibrium. The material balance of the part of bottom section from the bottom product up to this cross-section for any absent component j is the following:

$$Lx_j = VK_jx_j + (L-V)x_{Bj} \qquad (2)$$

Eq. (2) is the equation of material balance for the part of bottom section taking into consideration the liquid–vapor phase equilibrium for the neighboring trays for the reversible distillation.

We will obtain for any point of pinch branches x^{st} after dividing by Vx_j and neglecting the infinitesimal quantity x_{Bj} the following:

$$L/V = K_j^{st} \qquad (3)$$

In the infinitesimal neighborhood of a tearing-off point x^t, concentrations x_i^t of present components i constitute finite constant quantities, but the concentrations x_j^t of absent components j are infinitesimal quantities, and they increase in the direction of a trajectory (this is well visible in Fig. 1):

$$x_{i(m+1)}^t = x_{i(m)}^t \quad \text{for all of components } i \text{ if all } x_j \to 0 \qquad (4)$$

$$x_{j(m+1)}^t > x_{j(m)}^t \quad \text{for all of components } j \text{ if all } x_j \to 0 \qquad (5)$$

where m and $m+1$ are below and above located consecutive trays, accordingly.

The material balance of a part of bottom section from the bottom product up to the cross-section in the point x^t for any *absent component j* neglecting x_{Bj} is the following:

$$VK_{jm}^t x_{j(m)}^t = Lx_{j(m+1)}^t \quad \text{for all of components } j \text{ if all } x_j \to 0 \qquad (6)$$

From (5) and (6) we get the following:

$$L/V < K_j^t \quad \text{for all of components } j \text{ if all } x_j \to 0 \qquad (7)$$

On the other hand, we will obtain from the equations of material balance and phase equilibrium for the cross-section at

the point x^t for *present components i* the following:

$$(L/V)x_i^t = K_i x_i^t + (L/V-1)x_{iB} \quad \text{for all of components } i \text{ if all } x_j \to 0 \tag{8}$$

We will obtain from (8), subject to $x_{iB} > 0$ and $L/V > 1$, the following:

$$L/V > K_i^t \quad \text{for all of components } i \text{ if all } x_j \to 0 \tag{9}$$

Comparing (7) and (9) gives the following:

$$K_i^t < K_j^t \quad \text{for all of components } i \text{ and } j \text{ if all } x_j \to 0 \tag{10}$$

Let us consider now all other points x^{st} of pinch branches. One can consider each of these points as stationary point of trajectory of the adiabatic column working in the infinitely sharp mode at some reflux (N^+, or S^2, or …), i.e., as the point of composition in a cross-section of this column. Therefore, the inequalities and equalities (5)–(9) should be correct for the infinitesimal neighborhood of this cross-section. Thus the following inequality is true for any point x^{st} of pinch branches:

$$K_i^{st} < K_j^{st} \quad \text{for all of components } i \text{ and } j \text{ presented in the point } x^{st} \tag{11}$$

We will call a region, in which the inequality $K_i < K_j$ for the bottom section or the inequality $K_j < K_i$ for the top section is valid, as the *reversibility region* of simplex.

2.3. Types and properties of pinch trees

2.3.1. Pinch trees and reversibility regions

If a split is possible for a given composition of a product x_B and a given value of reflux V/L, there are one or several bundles of trajectories inside the simplex. All vertexes of each bundle are located on different pinch branches (see, for example, Fig. 3). Thus the location of bundles of trajectories depends on the location of pinch branches for the given product x_B and for the given value of reflux V/L (Petlyuk and Danilov, 2001a). The examples of pinch branches and pinch bundles associated with them are shown in Figs. 3, 5, and 9. The separability of a split in the two-sectional column depends on the location of terminals of pinch branches for each section. Therefore, first of all, we will consider all types of location of terminals of pinch branches.

In accordance with Eqs. (2) and (8), the points x^{st}, y^{st}, and x_B should be located in a straight line. If the continuation of this straight line does not intersect with the product element containing a product region, the inequality (11) cannot be satisfied. Therefore, each pinch branch for the given point of product should be located inside the same reversibility region of the corresponding element at $k < n-1$ (see, for the example, the face 1-2-3 in Fig. 5) or inside the reversibility region of simplex at $k = n-1$. Therefore, each bundle of trajectories should be located inside the same reversibility region.

2.3.2. Pinch trunk

The coefficient K of some absent component can monotonously decrease in the direction of pinch branches (in the bottom section) or can have one minimum value if the pinch branch passes through a concave region on the surface of function K of this component. Therefore, the branching points b_j away from the pinch trunk into different elements are located in the direction away from the point of product in decreasing order of values of K_j: b_{j1}, $b_{j2}…b_l$ (here b_{j1} is the branching point toward the element containing the component $j1$ having the largest value of a coefficient K_j, and b_l is the branching point towards the element containing the low-boiling key component l). For example, the components $j1$ and l are the components 1 and 3 in Fig. 3. The

pinch terminal for the pinch trunk is the unstable node of the distillation region containing the point of product (it is the vertex 2 in Figs. 3 and 5, the vertex 3 in Fig. 4, and the vertex 1 in Figs. 6 and 8). The existence of either one or two pinch branches (first and second pinch branches) inside the element (or whole simplex) having the absent component l depends on the shape of function of the coefficient K_l from the reflux V/L. There is one such pinch branch in Figs. 1, 3, 5, 6, and 8 and two pinch branches in Figs. 2 and 4. A limited interval of active reflux exists between the values of reflux parameter in the first b_{l1} and the second b_{l2} branching points (see, Figs. 2 and 4), if there are two such pinch branches. The unlimited interval of active reflux exists if there is one such pinch branch. The branching points are the bifurcation points, the number of eigenvectors along pinch branches is increased or decreased by one after each of these points. In Figs.1, 3, 5, 6, and 8, the pinch trunk is the N^+ before the first branching point, and the S^1 after this point. In Figs. 2, and 4 the pinch trunk is the N^+ before the first branching point, the S^1 between the first and second branching points, and the N^+ after the second branching point.

2.3.3. Primary pinch branches

Bifurcation points appear on primary pinch branches in several cases: on the existence of the tangential pinch, either at crossing certain univolatility manifolds, or on the existence of two unstable/stable nodes for the bottom/top section in the same reversible region.

The tangential pinch occurs if the coefficient K_l has a minimum on the primary pinch branch in element l. The bifurcation occurs in this minimum point, the pinch branch is the S^1 before it, and the N^+ after it. A primary pinch branch in the element l has the inactive segment between the branching point away from the trunk b_l and the pinch point (the *tangential pinch point*) where the value of the coefficient K_l on the primary pinch branch is the same as in this branching point (see, Figs. 3, 5, and 8). The reflux interval is inactive between values of reflux V/L in these two points. Therefore, segments of all pinch branches are inactive in this reflux interval.

The point of intersection of any primary pinch branch with the univolatility manifold, where two components j have equal values of the K_j, is the branching point of secondary pinch branch away from this primary pinch branch. For the primary pinch branch, the number of stable eigenvectors is increased or decreased by one after this point.

Daughter secondary pinch branches are located inside univolatility manifolds in elements having the dimension by one bigger than the dimension of parental primary pinch branches (see the secondary pinch branch on Fig. 3).

The location of primary pinch branches and their terminals depend on the number (0 or 1 or 2) of unstable/stable nodes on the element for the bottom/top section, which are located in the reversibility region, in which the point of product is located (in the own reversibility region of element).

If the own reversibility region of element contains one node, this node is the terminal of primary pinch branch (see, the terminals for the first primary pinch branch on Fig. 2, for the primary pinch branches of elements 1-2-4 and 2-3-4 on Fig. 3, for the first primary pinch branch on Fig. 4, for the primary pinch branches of elements 1-4, 2-4 and 3-4 in Fig. 7, and for the primary pinch branches of elements 1-2-4 and 1-3-4 in Fig. 8).

If the own reversibility region of element does not contain nodes, a primary pinch branch grows into the trunk of pinch tree, and the active reflux interval is limited. The interval of active reflux is the interval between values of $L/V/V/L$ for the top/bottom section in the branching point and in the point of ingrowing. In Fig. 5, there is the ingrowing pinch branch on the face 1-2-3

because on this face the own reversibility region does not have the stable node (the boundary of own reversibility region on this face is the univolatility line where the equality $K_2=K_3$ is valid).

If the own reversibility region of an element contains two nodes, each of the nodes has its *own region of attraction* for pinch branches. The boundary between regions of attraction serves as the manifold $max(K_h)$, i.e. the ridge on the surface or the hypersurface of the coefficient K_h (h is the *heavy-boiling key component*). The primary pinch branch cannot intersect this ridge, which passes through a stable node of the distillation region, which contains the product point (of the *own distillation region*), and through the saddle azeotrope on the boundary of two distillation regions (see Fig. 6). In Fig. 6, the split is 1,2,3,4:1,3,4 (the bottom product is the mixture 1, 3, 4), therefore the heavy-boiling key component is the component 1 ($h=1$). The boundaries of regions of distillation and the attraction do not coincide, the boundary of distillation region serves as the surface having the vertexes 123, 4, and 13, but the boundary of the attraction region is the surface max K_1 passing through the azeotrope 123, the vertex 4, and the point $max(K_1)$ on edge 1-3. There are two sub-cases: (1) the same node serves as for own distillation and attraction regions, and (2) the nodes for own distillation and attraction regions are different.

In the first sub-case, this node is the terminal for the primary pinch branch.

The second sub-case is not ordinary. In this sub-case, the primary pinch branch has the inactive final segment. This case is shown in Fig. 6. The azeotrope 12 is the unstable node at its own distillation region, and the azeotrope 23 is the unstable node at its own attraction region. At some reflux (the *reflux of pinch jump*), the active pinch point makes the jump away from this primary pinch branch through the ridge $max(K_1)$ up to the isolated pinch branch, which is not connected with the pinch tree. The distillation trajectory undergoes discontinuous change at the reflux of pinch jump. The active pinch point (*point of jump*) is located after the jump on the intersection of isolated pinch branch and the boundary between the attraction regions. Thus the jump happens when the *reflux of pinch jump* is equal to $max(K_h)$ on the isolated pinch branch. The isolated pinch branch has the active final segment. Before the jump, points N^+ are located on the primary pinch branch, which goes up to the azeotrope 23, but after the jump, they are located on the isolated pinch branch, which goes up to the azeotrope 12. The active reflux interval is unlimited, but it consists of two parts: one before and one after the reflux of jump.

If the product point is located on the unhatched regions on the face 1-3-4 in Fig. 6, the first sub-case exists.

2.3.4. Secondary, tertiary, etc., pinch branches

The binary, ternary, and so on azeotropes always generate the univolatility manifolds that contain the secondaries, tertiaries, and so on pinch branches, accordingly. These azeotropes are the terminals of corresponding pinch branches (see Fig. 7). These pinch branches begin from intersection points of their parental pinch branches with their univolatility manifolds.

If some pinch branch intersects the univolatility manifold, that is not generated by azeotrope, the pinch bridge arises instead of secondary pinch branch. This pinch bridge connects the parental pinch branch with another pinch branch, which has the same dimension (see, Fig. 8).

2.4. Number of bundles and their allocation

If more than one bundle in one or in both sections exist, and the split is possible, one bundle of one section intersects one bundle of another section. As examples, two bundles in Fig. 3, and

six bundles in Fig. 9 exist. Mixtures that have five and more components, can exist in many bundles. We need to identify only the interactive bundles out of all bundles. The location of interactive bundles depends on the location of product points for both sections of column. One need to identify, firstly, the number of bundles of each section and their allocation relative to the pinch branches. For solving this problem, it is necessary first to identify the types of all pinch points. For this, it is enough to calculate coefficients K in each pinch point without calculation of eigenvalues and eigenvectors of distillation. If the present component having the biggest value of coefficient K in the pinch point (in the bottom section) has the order number m in decreasing order of values of coefficients K out of all components, then the type of this pinch point is S^{n-m} (if $m>1$) or N^+ (if $m=1$). The number of *bundles* is the number of different sequences $S^1 \rightarrow S^2 \rightarrow \ldots \rightarrow S^{n-k} \rightarrow N^+$ (if $k>1$) or $N^- \rightarrow S^1 \rightarrow S^2 \rightarrow \ldots \rightarrow S^{n-k}$ (if $k=1$). For example, in Fig. 7, for the *pinch segment* on the edge 3-4 near to the vertex 4, the decreasing order of values of coefficients K is $K_1 > K_3 > K_2 > K_4$. Component 3, which is present in this segment, is the second component in this order out of all components. Therefore, the type of this segment is S^2 ($n=4$, $m=2$, and $n-m=2$).

Types of final segments of pinch branches are the same as types of their terminals. The bounding bundles of 3D primary pinch bundles, and the types of pinch points are shown in Fig. 9 at the infinite reflux $V/L=1$. Each bundle has its own sequence of points, $S^1 \rightarrow S^2 \rightarrow N^+$. There are the sequences $134 \rightarrow 1 \rightarrow 12$, $134 \rightarrow 123 \rightarrow 12$, $134 \rightarrow 123 \rightarrow 23$, $134 \rightarrow 34 \rightarrow 23$, $2 \rightarrow 123 \rightarrow 12$, and $2 \rightarrow 123 \rightarrow 23$ (the eigenvectors are directed into smaller temperature for the bottom section). The vertexes of these bundles are located on seven pinch branches.

3. Methods for identification and analysis

3.1. Methods for delimitation of tearing-off and product regions

The tearing-off region is the multitude of tearing-off points x^t on the given element for all product points x_B located on this element and for all values of reflux $L/V/V/L$ for the top/bottom section. The inequality (12) should be valid in all the points of tearing-off region. Therefore, boundaries of tearing-off region are univolatility manifolds, at points of which the coefficient K of one of present components i is equal to the coefficient K of one of the absent components j. Therefore, boundaries of the tearing-off region can be obtained by scanning the given product element, and by calculating values of coefficients K_j and K_i for all absent and present components. When the dimension of these elements increases, the required computing time for such scanning rises steeply. The assumption of linearity of boundaries of tearing-off regions leads to the significant reduction in the calculation time. With this assumption it is enough to scan one-dimensional edges of elements only. The loss of accuracy in this case does not have practical importance because the tearing-off points selected for design should be located away enough from the boundary for the guarantee the process stability.

We use the following method of delimitation for tearing-off regions:

(1) We scan edges of element, which are considered, with a certain step, and calculate values of coefficients K_i and K_j for all components in each of the scanned point.
(2) We determine limiting tearing-off points x^t_{lim}, where the equality $K_i=K_j$ is valid.
(3) We connect these limiting tearing-off points on the different edges of element by direct lines.

The example of using this method is shown in Fig. 4, for the face 2-3-4 (x^t_{3lim}=0.62 on the edge 2-3; x^t_{3lim}=0.35 on the edge 3-4; here x^t_{3lim} are the concentrations of component 3 in the limiting tearing-off points on the edges).

The element having the tearing-off region can contain the region of possible points of product (the product region). Trajectories go away from points of product region up to corresponding points of tearing-off region. Every *product point* can be calculated by the Eq. (10) for every *tearing-off point* x^t located in the *tearing-off region* and for every reflux *L/V* inside the *interval of active reflux*. If we scan each point x^t inside the *tearing-off region* and also scan values of reflux *L/V* for each point x^t inside the *interval of active reflux*, we can calculate all possible points of a product x_B on the element considered. If we assume linearity of the boundaries of *product regions*, it is enough to scan only one-dimensional edges of each element considered.

Thus, we use the following method of delimitation for product regions:

(1) We scan tearing-off segments on edges of element, which are considered, at a certain step.
(2) We scan values of parameter *L/V* or *V/L* at a certain step in the interval of active reflux in each scanned point x^t in accordance to the step 1.
(3) We calculate concentrations x_{iB} by Eq. (10) for all components i for each scanned point x^t in accordance to step 1 and each scanned value of parameter *L/V* or *V/L* in accordance to step 2.
(4) We identify limiting points of product x_{iBlim} on edges of element, which is considered, for each component i.
(5) We determine total limiting product points x_{Blim} for all components i on edges of element, which is considered.
(6) We connect by direct lines total limiting product points x_{Blim} on different edges of an element, which is considered.

The example of using this method are shown in Fig. 4 (x_{B3lim}=0.28 on the edge 2-3; x_{B3lim}=0.08 on the edge 3-4; here x_{B3lim} are the concentrations of component 3 in the total limiting product points).

Regions of possible product points for the given impurities in the products are always bigger than product regions for the infinitely sharp mode. However, if the product region inside some element is absent, the corresponding split is impossible for any allowable impurities.

3.2. Identification of terminals and characteristics of pinch branches

Our approach allows us to identify terminals of pinch branches without their calculation. This is necessary for accurate, fast, and error-free check-up for the sufficient conditions of separability in two-sectional columns. Moreover, if the split is possible, then this approach allows us to determine characteristics of column that is important for designing. In addition, the knowledge of terminals of pinch branches ensures the following error-free calculation of pinch trees at the stage of determination of minimal reflux. The novel procedure for the identification of terminals and of characteristics of pinch branches is given below (for the bottom section):

(1) We calculate values of coefficients K at the point x_B and identify the key components l and h in the list of components for the given split.
(2) We determine the unstable node for the point x_B in the product element by means of calculation of line of conjugate tie liquid-vapor (for each liquid point, we calculate the phase equilibrium, i.e. the temperature and the vapor point, which is the liquid point for the next tie liquid-vapor). If the inequality $K_i < K_j$ is valid in the unstable node for all components, the

interval of active reflux is unlimited (for example, in Fig. 3 in the vertex 2 on the product element 2–4 i=2, 4, j=1, 3, $K_2 < K_1$, $K_2 < K_3$, $K_4 < K_1$, $K_4 < K_3$), and is limited if not (for example, in Fig. 4 in the vertex 3 on the product element 2-3-4 i=2, 3, 4, j=1, $K_2 < K_1$, $K_3 > K_1$, $K_4 < K_1$).

(3) We calculate values of coefficients K in vertexes of simplex and in points of azeotropes except when they are located in the product element.
(4) We identify each point mentioned in step 3 as the terminal of primary pinch branch if it is the unstable node in any j-element (in the element containing all present components i and one certain component j), and the inequality $K_i < K_j$ is valid for the all components, which are present at this point (see, for example, the terminals 1, 2, 23, 34, 123, and 134 in Fig. 7).
   a. If the terminal of primary pinch branch in a j-element is absent, there is the *ingrowing pinch branch*, which grows into the pinch trunk, and the active reflux interval is limited (the example is shown in Fig. 5).
   b. If there are two possible terminals in a j-element, and the product point is located in the *another's attraction region*, the pinch point makes the jump away from the primary pinch branch up to the *isolated pinch branch* at the *reflux of pinch jump* (the example is in Fig. 6). The initial segment of primary pinch branch and final segment of isolated pinch branch are active.
   c. If there are two terminals in a j-element, and one of those is located concurrently in the own attraction region and the own distillation region, it is the terminal of pinch branch.
(5) We identify azeotropes of two or more components j as terminals of non-primary pinch branches if they are not the terminals of primary pinch branches, and the inequality $K_i < K_j$ is valid for all components i and j that are present in these azeotropes (the examples are: point 13 in Fig. 3, and points 1, 2, 12, 23, 34, 123, and 134 in Fig. 7).
(6) If there is the univolatility manifold where two or more of component j have equal values of coefficients K_j, and the inequality $K_i < K_j$ is valid for all the components, which are present on this manifold, but the azeotrope of these components is absent, then pinch bridge on this manifold exists (an example is shown in Fig. 8).
(7) If there is the $min(K_l)$ manifold on the l-element in the reversibility region, a tangential pinch can exist (an example is the point min (K_3) in Fig. 3).
(8) We determine the number of bundles of trajectories at the infinite reflux V/L=1 and their allocation relative to pinch branches:
   a. We determine for each active terminal of pinch branch for the component, which is present in this pinch terminal and has the biggest value of coefficient K, the order number m in the decreasing order of values of coefficients K out of all the components of mixture. The type of pinch terminal is S^{n-m} (if $m > 1$) or N^+ (if m=1).
   b. Determine the number of bundles as the number of different sequences $S^1 \rightarrow S^2 \rightarrow \ldots \rightarrow S^{n-k} \rightarrow N^+$ (for $k > 1$) or $N^- \rightarrow S^1 \rightarrow S^2 \rightarrow \ldots \rightarrow S^{n-k}$ (for k=1). Each sequence corresponds to one pinch bundle out of all pinch bundles.

Our method is described here only for bottom section, but can be easily modified for the top section.

4. Conclusion

The method of infinitely sharp mode requires only the calculation of coefficients K in product points, in vertexes of simplex, in

points of azeotropes, and in points of one-dimensional edges of simplex. It is a quick, non-iterative and foolproof method in contrast to other used methods. This approach allows us to identify possible splits in the section and to investigate their characteristics like the limited interval of active reflux, the tangential pinch, and the jump of trajectory. The delimitation of product regions and the identification of terminals of pinch branches allow us to identify possible splits in the column in the sequel. Besides, the identification of terminals of pinch branches and the determination of location of bundles allow us to identify the interactive bundles of trajectories for both sections of column in the sequel. The delimitation of product regions allows to us automatically calculate the recycles, which are necessary for the separation of azeotropic mixtures. The linearisation of important bounding manifolds allows us to apply the method of infinitely sharp mode for mixtures having any number of components.

This method is universal because any column consists of sections. However, it is necessary to allow the specific distinctions for extractive, heteroazeotropic, and reactive sections. Description of our method for extractive sections will be presented in one of future articles.

This method allows us to create the new more energy-efficient flowsheets for the distillation units because it is based on the general regularities of distillation.

In our next article will be described the method for two-sectional columns based on the principles described in the present article.

Notation

K	coefficient of phase equilibrium
N^+	stable node of bundle of section profiles
N^-	unstable node of bundle of section profiles
$S^1, S^2 \dots$	saddle of bundle of section profiles in ascending order number of arriving eigenvectors
L	liquid flow rate
V	vapor flow rate
L/V	liquid-vapor ratio
V/L	vapor-liquid ratio
i	component present in product
j	component absent in product
k	number of components in product
n	number of components in mixture
x	concentration of component in liquid phase
y	concentration of component in vapor phase
1, 2, 3 …	numbers of components
12, 13 … 123 …	azeotropes
(1), (2)	pinch points having identical type
1-2, 1-3…1-2-3, 1-2-4…	elements of simplex
b	branching point
b_{l1}	first branching point
b_{l2}	second branching point
x^t_{lim}	limiting tearing-off points
x_{iBlim}	limiting points of product for component i
x_{Blim}	limiting product points

Subscripts

D	top product
B	bottom product
i	present component
j	absent component
r	top section
s	bottom section
m	tray number ($m=0$ for product cross-section)

$j1$	the most low-boiling absent component
l	low-boiling key component
h	heavy-boiling key component

Superscripts

st	pinch point
t	tearing-off point
m	the order number of component in decreasing order of values of coefficients K

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Glossary with examples from figures

Bundle: the infinitely manifold of trajectories having the same unstable and stable nodes, and saddles (see, for example, in Fig. 9 the bundles at $V/L=1$: $4\to2\to123\to12$, $4\to2\to123\to13$, $4\to134\to1\to12$, $4\to134\to34\to23$, $4\to134\to123\to12$, and $4\to134\to123\to23$);

Bounding bundle: the bundle, which is located on a bounding element of primary bundle (see, for example, the filled in triangles in Fig. 9);

Components:

Present components: the components, which are contained in the product of section (see, for example, the components 2, 4 in Fig. 3);

Absent components: the components, which are absent in the product of section (see, for example, components 1, 3 in Fig. 3);

Low-boiling key component: the most heavy-boiling component of present components of the top product (see, for example, the component 3 in Fig. 3);

Heavy-boiling key component: the most light-boiling component of present components of bottom product (see, for example, component 2 in Fig. 3);

Component order: the decreasing order of values of phase equilibrium coefficients of components;

Distillation edges: edges of distillation regions at V/L=1 (see, for example, the lines 2-13 and 4-13 in Fig. 3);

Elements: vertexes, edges, faces, hyperfaces of concentration simplex;

Elements:

product element: the element, which contains all the present components and does not contain the absent components (see, for example, the edge 2-4 in Fig. 3);

j-element: the element containing all present components i and one certain component j (see, for example, the element 1-2-4 in Fig. 3);

l-element: the element containing all the present components i and one light-boiling key component l (see, for example, the element 2-3-4 in Fig. 3);

h-element: the element containing all the present components i and one heavy-boiling key component h (see, for example, the element 1-2-3 in Fig. 5);

Manifolds:

α_{ij}-*manifold, α_{ijk}-manifold* …: the univolatility manifolds, in points of which phase equilibrium coefficients for the components i and j or i, j and k… are equal, correspondingly (see, for example, the surface $K_2 = K_3$ in Fig. 8);

Min(K_l)-manifolds: the manifolds, in points of which phase equilibrium coefficients for the low-boiling key component l are minimal (the valley);

Max(K_h)-manifolds: the manifolds, in points of which phase equilibrium coefficients for the heavy-boiling key component h are maximal (the ridge) (see, for example, the surface $maxK_1$ in Fig. 6);

Modes of distillation:

infinite sharp mode: the mode, in which some components of feed have infinitesimal concentrations in the product of section of column, in the infinite column ($N = \infty$) at the finite reflux ($V/L \neq 1$);

Pinch trunk: the line, which consists of pinch points located on the product element (see, for example, the line $x_B \rightarrow 3$ on the face 2-3-4 in Fig. 4);

Pinch branches: the lines, which consist of pinch points located on elements other than the product element (see, for example, the lines away from the edge 2-4 up to the vertexes 1 and 3 in Fig. 3);

Pinch branches:

primary, secondary, tertiary… pinch branches: the pinch branches, which contain one, two, three… absent component, correspondingly (see, for example, primary the ones on the edges 1-4, 2-4, 3-4, secondary the ones on the faces 1-2-4, 1-3-4, 2-3-4, and tertiary the one inside simplex in Fig. 3);

N^+ *pinch branches*: the pinch branches, in points of which all eigenvectors are entering (see, for example, the pinch branches on the faces 1-2-4, and 2-3-4 in Fig. 7);

S^1, S^2, S^3… *pinch branches*: the pinch branches, points of which have one, two, three… entering eigenvectors, correspondingly (see, for examples, S^1 the one on edge 2-4, and S^2 the one inside simplex in Fig. 7);

active pinch branches: the pinch branches, points of which can be points of ends or contact of trajectories (see, for example, the one inside simplex in Fig. 3);

inactive pinch branches: the pinch branches, points of which cannot be points of ends or contact of trajectories(see, for example, the one inside simplex in Fig. 4);

first pinch branch: the pinch branch, which is located in the same element nearer from the point of product than another pinch branch if there are two pinch branches in the same element (see, for example, the one, which goes up to the vertex 1 in Fig. 4);

second pinch branch: the pinch branch, which is located in the same element farther from the point of product than another pinch branch if there are two pinch branches in the same element (see, for example, the one, which goes up to the azeotrope 13 in Fig. 4);

isolated pinch branch: the pinch branch unconnected with the pinch trunk (see, for example, the line, which connects the azeotropes 12 and 123 in Fig. 6);

ingrowing pinch branch: the primary pinch branch, which returns to the pinch trunk (see, for example, the one on the face 1-2-3 in Fig. 5);

Pinch bridge: the pinch line, which connects two pinch branches located on two different elements having the same dimension (see, for example, the one, which connects the faces 1-2-4 and 1-3-4 in Fig. 8);

Pinch segment: the part of pinch branch located between two the nearest branching points (see, for example, the segment between the branching points to the faces 1-3-4 and 2-3-4 on the edge 3-4 in Fig. 7);

Pinch jump: the jump of pinch point away from one pinch branch up to another (see, for example, the one between the pinch branches, which go up to the azeotropes 23 and 12 in Fig. 6);

Pinch chain: the chain, which goes away from the pinch trunk up to the stable node or the final saddle, and consists of pinch segments having different dimension (see, for example, the one $4 \rightarrow 3\text{-}4 \rightarrow 1\text{-}3\text{-}4 \rightarrow 1\text{-}2\text{-}3\text{-}4 \rightarrow 123$ in Fig. 7);

Pinch tree: the collection of pinch chains (see, for example, the pinch chains: $4 \rightarrow 34$, $4 \rightarrow 23$, $4 \rightarrow 123$, $4 \rightarrow 134$, $4 \rightarrow 1$, $4 \rightarrow 12$, $4 \rightarrow 2$ in Fig. 7);

Points:

pinch points: the points of composition on trays of column, for which counter flows of liquid and vapor are in phase equilibrium;

product point: the point of composition of product of column (see, for examples, the points x_B or x_D in Figs. 1–9);

tearing-off point: the point, in which the trajectory tears off away from the product element at the given reflux (see, for examples, the points S^1 in Figs. 1–3);

limiting tearing-off point: the tearing-off point, which is located on intersection of edge with the boundary of tearing-off region (see, for example, the points t on the edges 2-3 and 3-4 in Fig. 4);

limiting point of product: the limiting concentration of certain present component i in the product region;

total limiting product point: the product point, which is located on intersection of edge with the boundary of product region (see, for example, the points p in Fig. 4);

branching point: the point, which contains in two pinch branches (see for examples, the points of intersection of edge 3-4 with the pinch branches on the faces 1-3-4 and 1-2-4 in Fig. 7);

pinch terminal: the point, in which the pinch branch finishes (see, for examples, the vertexes 1 and 3, and azeotrope 13 in Fig. 3);

tangential pinch point: the point of pinch branch, in which the reflux is the same as in the tearing-off point (see, for examples, the ones in Fig. 3);

terminal of pinch bridge: the point, in which the pinch bridge finishes (see, for example, the one in Fig. 8);

starting point of pinch jump: the last point of pinch branch of pinch tree before the pinch jump (see, for example, the one in Fig. 6);

terminal of pinch jump: the starting point of active segment of isolated pinch branch after the pinch jump (see, for example, the one in Fig. 6);

own stable node: the N^+ terminal of own distillation region (see, for example, the azeotrope 12 in Fig. 6);

another's stable node: the N^+ terminal of another's distillation region (see, for example, the azeotrope 23 in Fig. 6);

point of ingrowing: the point, in which the pinch branch grows into the pinch trunk (see, for example, the one in Fig. 5);

Reflux:

reflux parameter: the relation of rate of liquid and vapor (L/V) for the top section or of vapor and liquid (V/L) for the bottom section;

minimal active reflux: the reflux in the branching point of first pinch branch or ingowing pinch branch away from the pinch trunk (see, for examples, the ones in Figs. 4 and 5);

maximal active reflux: the reflux in the branching point of second pinch branch away from the pinch trunk or in the point of ingrowing (see, for example, the ones in Figs. 4 and 5);

interval of active reflux: the interval of reflux parameter between minimal and maximal active refluxes;

reflux of pinch jump: the reflux, at which the pinch point jumps away from the pinch tree up to the isolated pinch branch;

Regions:

tearing-off regions: the regions, points of which can be tearing-off points (see, for example, the one restricted of edges 2-3, 2-4, 3-4, and of line between points t in Fig. 4);

limited tearing-off regions: the tearing-off regions, points of which fill up the part of element (see, for examples, the one restricted of edges 2-3, 2-4, 3-4, and of line between points t in Fig. 4);

unlimited tearing-off regions: the tearing-off regions, points of which fill up the whole of element (see, for example, the edge 2-4 in Fig. 3);

product regions: the regions, points of which can be product points (see, for example, the one restricted of edges 2-3, 2-4, 3-4, and of line between points p in Fig. 4);

product segment: the one-dimensional product region (see, for example, the edge 2-4 in Fig. 3);

limited product regions: the product regions, points of which fill up a part of element (see, for example, the one restricted of edges 2-3, 2-4, 3-4, and of line between points p in Fig. 4);

limited product segment: the one-dimensional limited product region (see, for example, the one on the line 1-2 in Fig. 5);

unlimited product regions: the product regions, points of which fill up the whole of element;

attraction regions: the product regions, away from points of which primary pinch branches come to certain stable node (see, for example, the hatched region in Fig. 6);

own attraction region: the attraction region containing the product point (see, for example, the region, the vertexes of which are 1, 4, and the point $max K_1$ in Fig. 6);

another's attraction region: the attraction region, in points of which his stable node and the stable node of distillation region are different (see, for example, the one hatched in Fig. 6);

distillation region: the region, in which all trajectories have the same unstable and stable nodes (see, for examples, regions: $(N^-) \rightarrow 12(N^+)$, $(N^-) \rightarrow 23(N^+)$ in Fig. 9);

own distillation region: the distillation region containing the product point (see,for example,the one $12(N^-) \rightarrow 4$ (N^+) in Fig. 6);

own distillation region of element: the distillation region of element containing the product point(see, for example, the one on the face 1-3-4 $4(N^-) \rightarrow 1(N^+)$ in Fig. 6);

reversibility region: the region, in points of which the phase equilibrium coefficients of present components have larger/smaller values than the ones of absent components for top/bottom sections, correspondingly (see, for example, the one, which vertexes are 1, 2, 4, 13, and the points t ($K_2 < K_1$, $K_3 < K_1$, $K_4 < K_1$) in Fig. 4);

own reversibility region: the reversibility region containing the product point (see, for example, the one, which vertexes are 1, 2, 4, 13, and the points t ($K_2 < K_1$, $K_3 < K_1$, $K_4 < K_1$) in Fig. 4);

own reversibility region of element: reversibility region of element containing the product point (see, for example, the one hatched in Fig. 5);

Simplex: the concentration simplex, every point of which correspond to certain composition of mixture (see, for examples, the triangles on Figs. 1–2, and the tetrahedrons in Figs. 3–9);

Split: lists of components of products of each section (For example, 1,3 (the top product):2,4 (the bottom product) in Fig. 3);

Splits:

direct or indirect split: the split, at which the product of top or bottom section contains one product component (see, for example, indirect split 1,2,3,4:4 in Fig. 7);

intermediate split: the split, products of which contain more than one component (see, for example, intermediate split 1,2,3,4:2,4 in Fig. 3);

Trajectory of section: the line passing through the composition points, for which the equations of phase equilibrium and material balance are true for the given product point (see, for examples, the ones in Figs. 1 and 6).