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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,

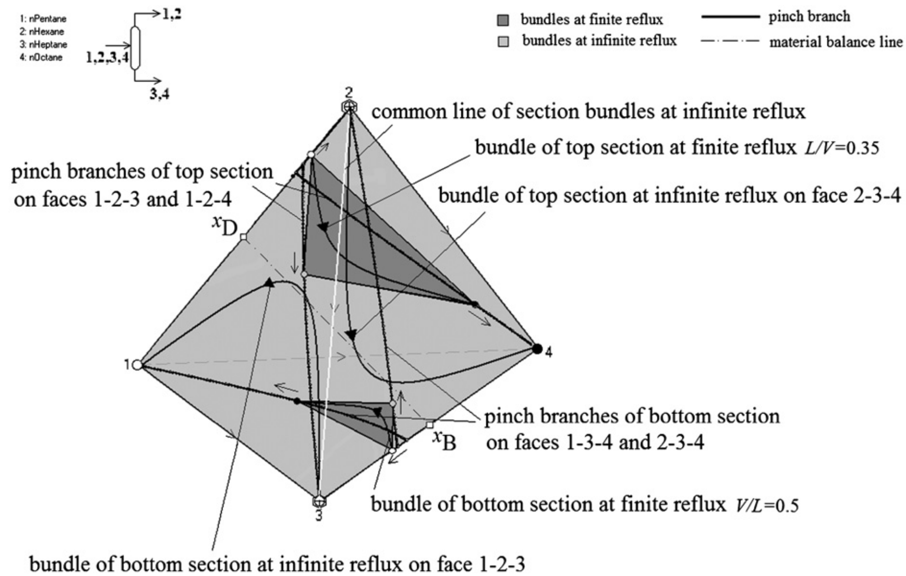

Fig. 1. Bundles of two sections at the given finite and infinite refluxes for intermediate split of ideal mixture.

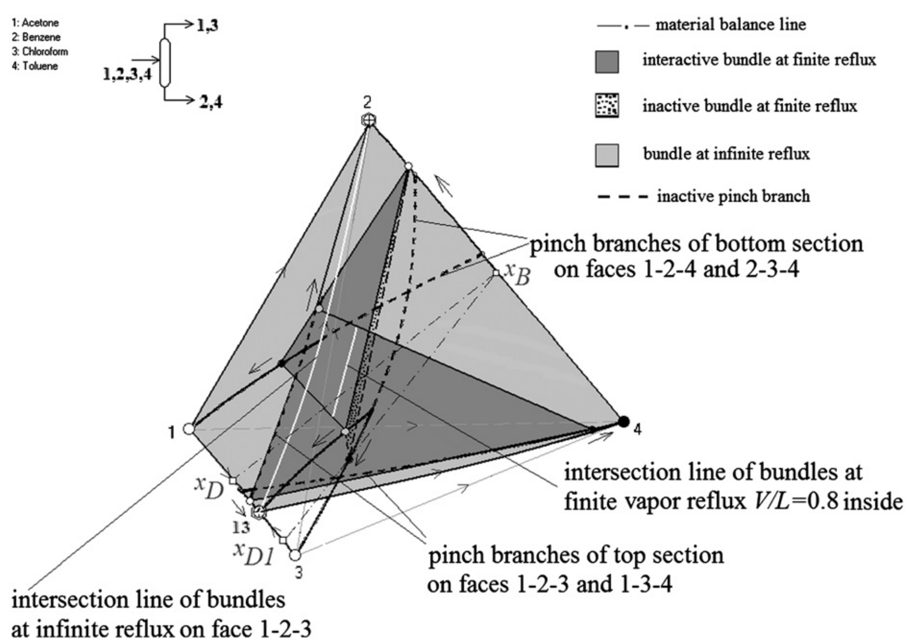

Fig. 2. Bundles for the intermediate split of azeotropic mixture.

and the small sketches of the direct split in one column 1:2,3,4 and in the flowsheet 1:2:3:4 for the mixture acetone–benzene–chloroform–toluene. The product point of the top product x_D is the unstable node of one of the two *distillation regions* (of the region $1\rightarrow13\rightarrow2\rightarrow4$), and the product point of the bottom product x_B is located in the *product region* in the other distillation region (in the region $3\rightarrow13\rightarrow2\rightarrow4$). Although, this split is infeasible at the infinite reflux as the product points are located in different distillation regions, it is feasible at finite reflux, as shown in the figure. 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). This reflux ($V/L=0.66$) is the *maximal active reflux* for the bottom section because it conforms to the branching point of the *second primary branch* (see the previous article). The reflux $L/V=0.8$ is *minimal active reflux* of the top section because its bundle does not exist if $L/V<0.8$. The bundles of two sections exist at these refluxes and intersect each other as shown in the figure. If the product point of the bottom section is located out of the product region (for example, the point x_{B1}), this split is possible by recycling as shown in the sketch.

Fig. 4 is an example of the infeasible split (the azeotropic mixture acetone–methanol–chloroform–acetonitrile; the split with the distributed component 1,2,3:24). Although the product points are located in their product regions (the product region of top section is the grey part of face 1,2,3, and the product region of top section is the segment 24–4), the bundles of trajectories cannot intersect each other at any reflux because the pinch points of two sections are located far apart (the terminals of the bottom section are the points of azeotropes 12, 23, 123, and the terminals of top section are the point of azeotrope 13 and the vertex 4, i.e. the common terminals are absent).

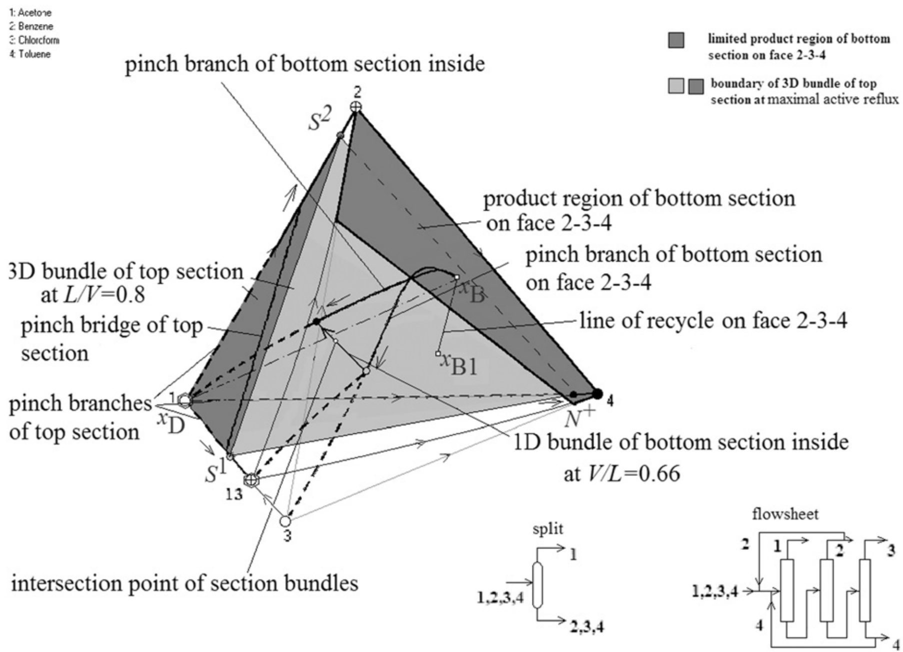

Fig. 3. Split of the azeotropic mixture into the pure component and the zeotropic mixture.

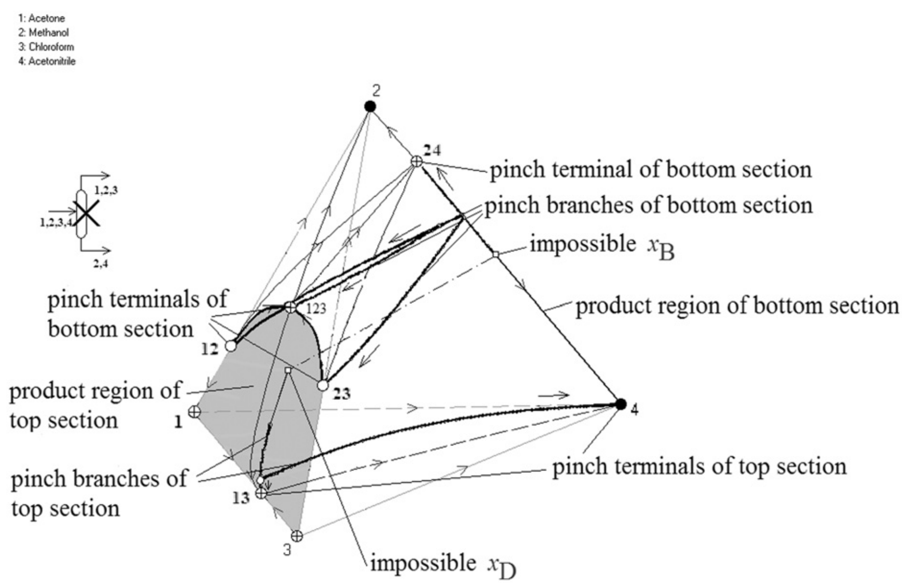

Fig. 4. Potentially possible, but impossible split (common terminals are absent).

Fig. 5 is another example of an infeasible split with the distributed component 2,3:1,3,4 for the same mixture as in Fig. 4. The product point of top section is located in its product segment 23–3, and the product point of bottom section is located in its product region, which is whole face 1–3–4. The bundles of two sections cannot intersect each other at any reflux because the common terminals of sections are absent (the terminals of top section are the point of azeotrope 13 and the vertexes 3 and 4, and the terminals of bottom section are the points of azeotropes 12 and 23 and the vertex 1), and the bundles of sections (the 2D bundle of the top section and 1D bundle of bottom section) are located far apart as shown in the figure.

Fig. 6 shows the possible intermediate split 1,4:2,3 of the mixture acetone–benzene–chloroform–acetaldehyde to two zeotropic mixture (there are the common terminals: the points 1 and 13). The pinch tree of the top section contains the *pinch bridge*. The reflux interval of the bottom section is limited because of existence of the second pinch branch. One of the products of the other possible splits 1,3,4:2 and 4:1,2,3 contains azeotrope 13.

Fig. 7 shows the possible indirect split of the mixture ethyl acetate–propylene glicol–ethanol–water (there are the common terminals: the points 2 and 4). There are the six 3D bundles of the bottom section, one of which is interactive for the given product point of the bottom section. The boundary of the interactive bundle of the bottom section at infinite reflux is the *interactive product simplex* of top section. Its vertexes are the terminals of *interactive pinch branches* of the bottom section. This product simplex and these pinch branches are shown in the figure. The boundary of the interactive bundle of the bottom section at the given reflux ($V/L=0.3$) is shown too.

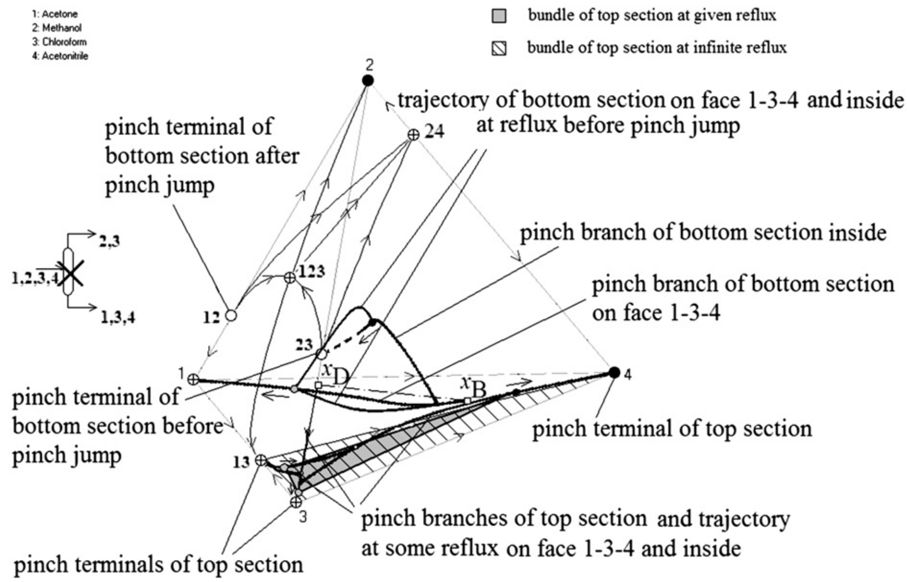

Fig. 5. Potentially possible, but impossible split (common terminals are absent).

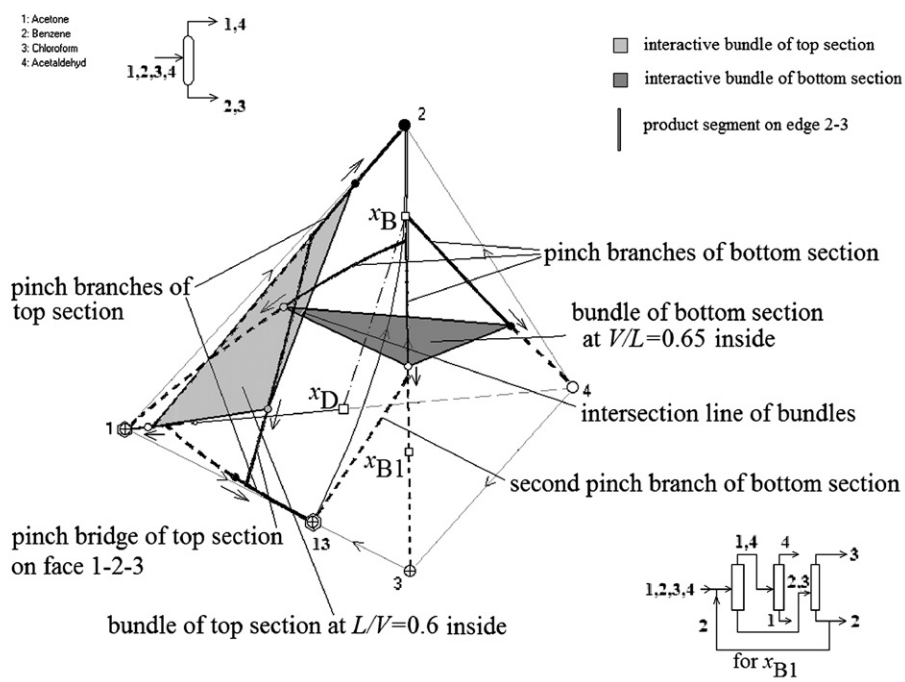

Fig. 6. Split of the azeotropic mixture into two zeotropic mixtures.

Fig. 8 shows the split with the distributed component 2,4:1,3,4 for the same mixture. This split is possible, and the given reflux is bigger than the minimal reflux because there is the *intersection point* of the 1D bundle of the top section and the 2D bundle of the bottom section (the common terminal is the vertex 4).

Fig. 9 shows the example of a *half-sharp split* 1,2,3,4:4 (in the top section the unsharp split, and in the bottom section the infinitely sharp split) for the mixture acetone–methanol–chloroform–ethanol. This split is possible for the given top product point because a common terminal (the vertex 4) of the trajectory of the top section and the bundle of the bottom section exists. The given reflux is higher than the minimal reflux because there is the intersection point of the trajectory of the top section and the bundle of the bottom section.

2.2. Conditions for possible splits

2.2.1. Conditions for the existence of bundles in two-section columns

A split is often possible (*potentially possible split*) if there are bundles in two sections of simple column. A bundle in a section can exist if the product point is located in a product region as indicated in the previous article. Therefore, the material balance line must intersect the opposite elements of the simplex in points, located in product regions. This is the necessary condition of the possibility of the split. It is satisfied in Figs. 1–8. The potentially possible splits for the ideal mixture in Fig. 1 are the direct and indirect splits 1:2,3,4 and 1,2,3:4 (not shown), the intermediate split (it is shown on Fig. 1), and the splits with distributed

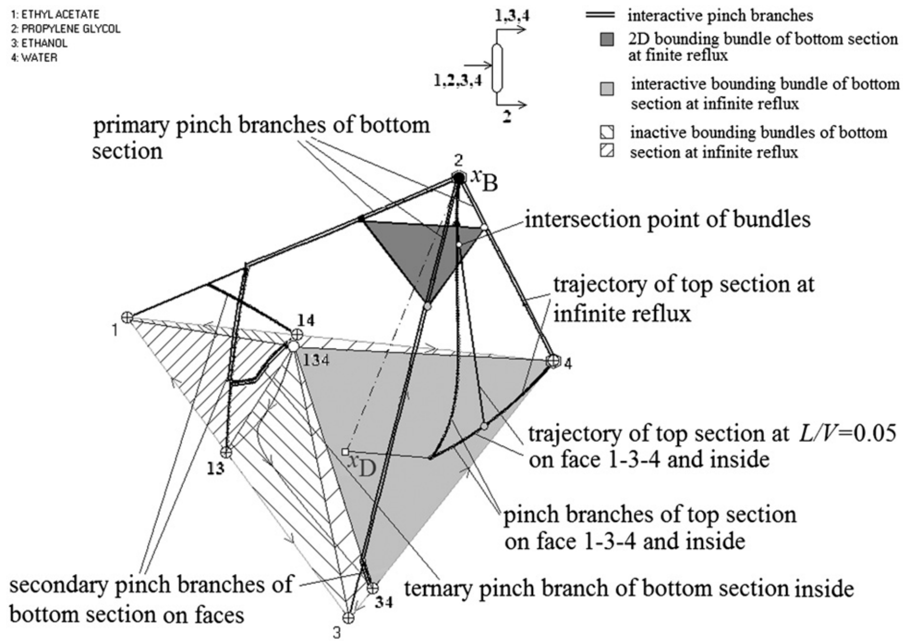

Fig. 7. One active and five inactive product simplexes.

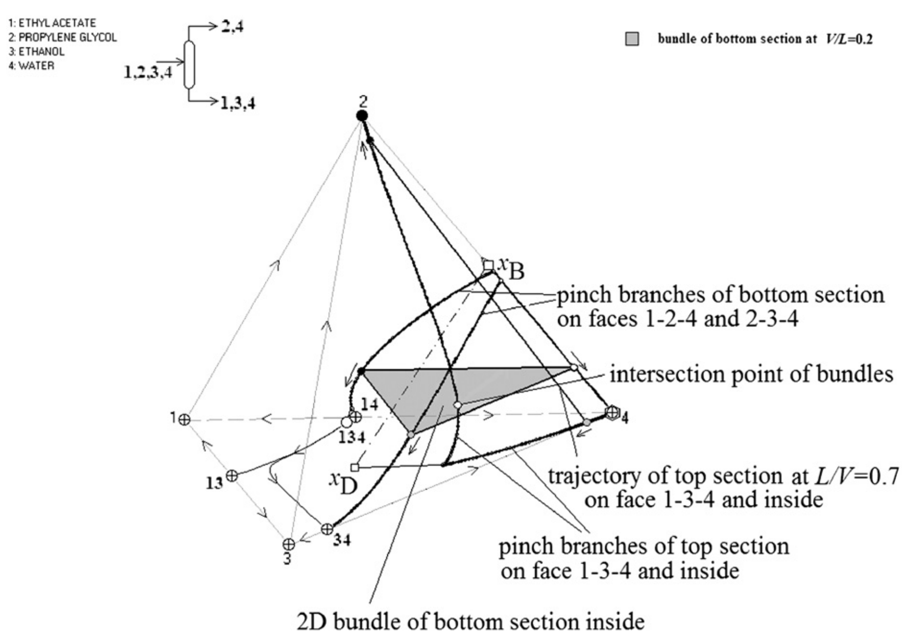

Fig. 8. Split with the distributed component.

components 1,2:2,3,4, and 1,2,3:3,4, and 1,2,3:2,3,4 (not shown). The possible splits for the mixture acetone–benzene–chloroform–toluene are the direct 1:2,3,4 (shown on Fig. 3), and intermediate splits 1,3:2,4 (shown on Fig. 2), and the split with the distributed component 1,3:2,3,4 (not shown). The potentially possible splits for the mixture acetone–methanol–chloroform–acetonitrile (see Figs. 4 and 5) with a distributed component exist because both product points are located in product regions. The possible splits for the mixture acetone–benzene–chloroform–acetaldehyde are the indirect 1,3,4:2 (it is not shown) and intermediate 1,4:2,3 (shown in Fig. 6) splits, and the split with the distributed component 1,3,4:2,3 (not shown). The possible splits for the mixture ethyl acetate–propylene glycol–ethanol–water are the indirect split 1,3,4:2 (it is shown in Fig. 7) and the splits with the distributed components 1,3,4:2,4 (it is shown in Fig. 8), 1,3,4:2,1 (it is not shown), and 1,3,4:2,3 (it is not shown).

The possible split for the mixture acetone–methanol–chloroform–ethanol is the indirect split 1,2,3:4 (shown in Fig. 9) if the product point of the top section is located in its product region (x_{D1}). Otherwise (x_D), there are two ways for this separation: the indirect unsharp split in one simple column (the unsharp split in the top section and the infinitely sharp split in the bottom section), and the separation in two simple columns with recycle (see figure). The first way is cheaper if one needs to extract only one pure component 4, but the second way is necessary if one needs to extract two pure components 2 and 4. If we choose the unsharp split in one section, one needs to determine the *maximal split* when points of products are maximally far apart (see Fig. 9).

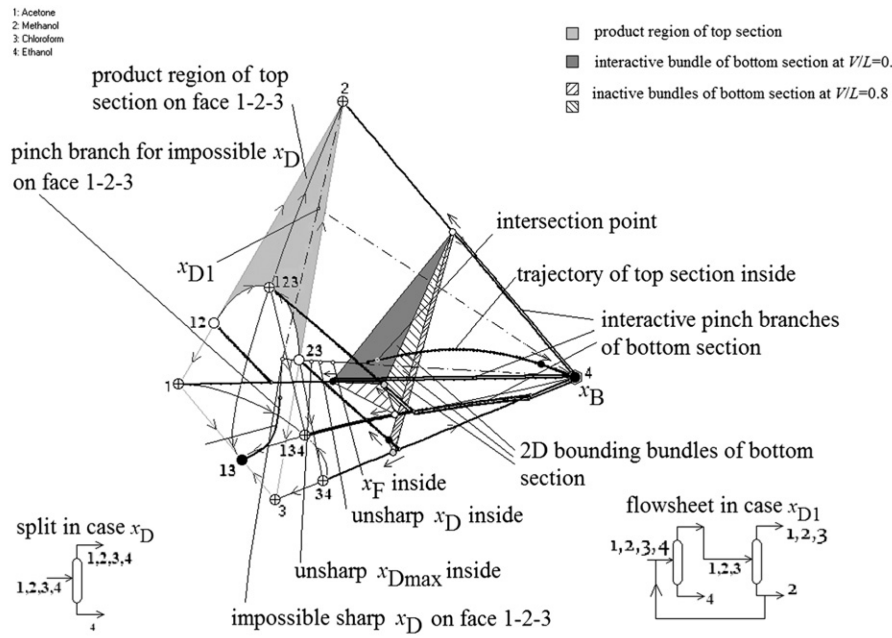

Fig. 9. The half-sharp split.

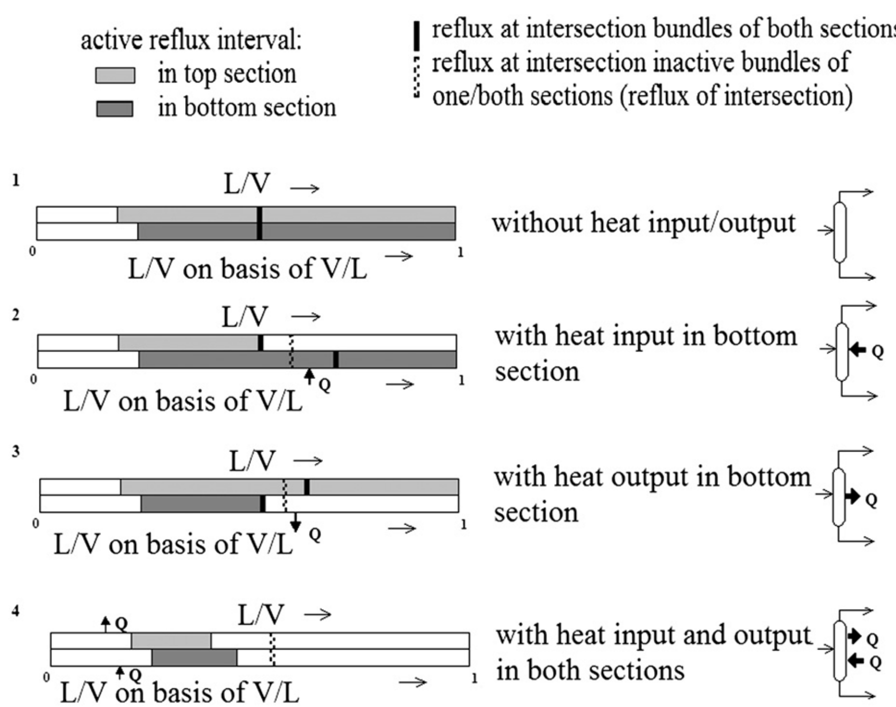

Fig. 10. Necessity of the intermediate heat input or output.

We see from the examples that certain four-component mixtures with one azeotrope can be separated to pure components by means of a flow sheet containing three simple columns (see Figs. 3 and 6). Let us note that these separations are possible only at finite reflux.

2.2.2. Condition of intersection of two bundles

The examples above show that the condition of the existence of bundles of two sections is insufficient for the intersection of each other. In Figs. 4 and 5 two bundles exist, but do not intersect each other at any reflux. If two bundles intersect each other at some reflux, they intersect each other at any higher reflux including the infinite reflux. If two bundles intersect each other at infinite reflux, the pinch branches of two sections must have common terminals. Therefore, the existence of common terminals of pinch branches of two sections is the sufficient condition for the intersection of their bundles with each other. The existence of common terminals of both sections does not mean that a split is possible at infinite reflux. It is possible if these terminals are active, else a split is possible only at finite reflux. For example, the possible split only at finite reflux is shown in Fig. 3 (the common terminals are the points 1 and 13). The intersection of bundles of sections at finite reflux is shown. However, the split is impossible at infinite reflux because the product points are located in the different distillation regions (x_B in $3\rightarrow13\rightarrow2\rightarrow4$, and x_D in $1\rightarrow13\rightarrow2\rightarrow4$). The splits in Figs. 4 and 5 are impossible because the common terminals are absent.

The splits in Figs. 1–3 and 6–9 are possible because the common terminals are present (one common terminal for splits with one distributed component, and two common terminals for other types of splits).

2.2.3. Condition of intersection of reflux intervals

The existence of common terminals is the sufficient condition for the possibility of infinitely sharp and half-sharp splits in most cases. However, this condition is insufficient in few cases because the reflux in one or both sections can not be in their active reflux intervals. Fig. 10 shows the different relations between intervals of the active reflux in the case when the refluxes of sections are connected by means of equations of material and heat balance. We will name the reflux, at which the bundles in the two sections begin to intersect each other, the *reflux of intersection*.

If the reflux of intersection is in the interval of active reflux for each section, it is the minimum reflux (see case 1 in Fig. 10). This case always exists if intervals of the active reflux are unlimited, i.e. if the second pinch branch is absent (see Figs. 1 and 2 and 7 and 8). In case 3, the interval of the active reflux in the top section is unlimited, while in the bottom section is limited. If the reflux of intersection is smaller than the maximal active reflux, the split is possible even without the intermediate input or output of the heat (see Figs. 4 and 6). If not, it is necessary to increase the reflux in the top section by increasing the heat input in the feed cross-section (see case 3 in Fig. 10). Analogically, it is necessary to remove heat in the feed cross-section in case 2 in this figure. However, if the reflux of the intersection is bigger than the maximal active refluxes in two sections (see case 4 in this figure), the split is impossible with heat input or removal in the feed cross-section. In this case, the split is possible by heat input or removal in the intermediate cross-sections. Thus, if there is the second pinch branch in one or two sections, it is necessary to check up the reflux of intersection and the maximal active reflux in the corresponding sections at the calculation of the minimal reflux.

2.3. Interactive bundles and pinch branches

If the split is possible and the reflux is sufficiently high, there are often many bundles and pinch branches in each section. Their number sharply increases with the number of components and azeotropes. For example, there is only one azeotrope and two bundles in Fig. 3, while there are four azeotropes and six bundles in Fig. 7. Only one of the bundles (the *interactive bundle*) participates in distillation for the given product points in each section. Let us consider the bundles at infinite reflux in order to identify the interactive bundle. Boundary elements of bundles at infinite reflux are located on the product element of the opposite section and they are *product simplexes* (see, Figs. 3 and 7). Vertices of each product simplex are points of components and azeotropes, which form sequences $N^- \rightarrow S^1 \rightarrow S^2 \rightarrow \cdots \rightarrow S^{n-k} \rightarrow N^+$ having the proper dimension. Here the types of stationary points are considered with regard to the product element of the opposite section.

For example, in Fig. 3 the vertices of two 1D product simplexes are the points 1, 3, and 13. They form two sequences $N^- \rightarrow N^+$: 1→13 and 3→13. For another example, in Fig. 7 the vertices of six 2D product simplexes are the points 1, 3, 4, 13, 14, and 134. They form six sequences $N^- \rightarrow S^1 \rightarrow N^+$: 134→13→1, 134→14→1, 134→13→3, 134→34→3, 134→34→4, and 134→14→4. The *interactive product simplex* contains the product point of the opposite section because one is the boundary element of the bundle containing the trajectory joining at the infinite reflux the product points of two sections. Other *product simplexes* are *inactive*. The interactive product simplex is the simplex 13–1 in Fig. 3 (the point x_D is located on the segment 13–1), and the simplex 134–14–4 in Fig. 7 (the point x_D is located on the triangle 134–14–4). Let us, for example, consider the trajectory joining the product points x_B and x_D at the infinite reflux in Fig. 7. It goes from the product point of the bottom section x_B along the edge 2–4 to the vertex 4, and then inside the interactive product simplex from vertex 4 to the product point of the top section x_D.

Pinch branches going to vertexes of the interactive product simplex are the *interactive pinch branches* because vertexes of the interactive bundle are located on these pinch branches at any reflux. The interactive pinch branches are shown in Fig. 7 with double lines. The first interactive pinch branch goes to the azeotrope 134 and contains the segment on the edge 1–2, the segment on the face 1–2–3, and the segment inside the simplex; the second interactive pinch branch goes to the azeotrope 34 and contains the segment on the edge 2–3, and the edge on the face 2–3–4; the third interactive pinch branch goes to the vertex 4. In Fig. 7, the interactive bundle is shown at some finite reflux, at which its vertexes are located on the segments of the interactive pinch branches—on the edges 1–2, 2–3, and 2–4. At the subsequent design step, we must take into account only interactive bundles for calculating minimum reflux. This dramatically reduces the required number of calculations.

3. Identification and analysis of possible splits

The theoretical basis above allows us to develop a new method of the identification and analysis of possible splits for any azeotropic mixture with any number of components. This method requires only the calculation of the equilibrium coefficients (*K*-values) in points of pure components and azeotropes, and in points located on edges of the simplex. These calculations can be done fast and easily as they do not require iterations.

3.1. Method for identification of possible splits

1. Sequentially consider all opposite couples of elements of the simplex, and choose the couples, each element of which contains the product region (*potentially possible splits*) (see, Figs. 1–9).
2. If the potentially possible splits are absent, go to step 9. If not, go to step 3.
3. Check whether the product point at each section is located in its product region or not by solving the system of linear equations with regard to the concentrations in the product point and in the vertexes of the product region.
4. If one or two product points of the sections are not located in their product regions, calculate the necessary recycle in order to move them to their product regions using their distances to the boundaries of the product regions (see Fig. 3: $x_{B1} \rightarrow x_B$, Fig. 6: $x_{B1} \rightarrow x_B$; Fig. 9: $x_{D1} \rightarrow x_D$). Determine the new locations of the product points.
5. Identify the terminals of two sections (see the previous article), and check the existence of common terminals (see, Figs. 1–3 and 6–9).
6. If common terminals are absent (see, Figs. 4 and 5), go to the next potentially possible split. If the examined split is final, go to step 9.
7. If common terminals are present, determine the characteristics of the examined split for each section (see the previous article), and identify the interactive bundles and pinch branches (see next section of this article).
8. If the terminals of two sections for the examined split are active, this split is possible without the intermediate input or output of the heat (see, Figs. 1 and 2 and 7–9). If they are inactive (see Figs. 3 and 6), calculate the necessary reflux of the intersection and the maximal active reflux on the step of the calculation of the minimal reflux (to be described in future articles).

9. Choose the elements of the simplex, which contain the product regions (the *potentially possible half-sharp splits*), for the identification of possible half-sharp splits.
10. Execute steps 3, 4, 7, and 8 for the infinitely sharp section, and steps 5, and 6 for two sections of each potentially possible half-sharp split (see, Fig. 9).

We illustrate the main steps of this algorithm on the example of the mixture, which is shown in Fig. 6. Let the feed point be located in the middle of the segment $x_D - x_{B1}$.

1. Opposite couples of elements of the simplex are the vertex 1 and the face 2–3–4, the vertex 2 and the face 1–3–4, the vertex 3 and the face 1–2–4, the edges 1–2 and 3–4, 1–3 and 2–4, and 1–4 and 2–3. The possible top product vertex is the vertex 4 (the unstable node), and the possible bottom product vertex is the vertex 2 (the stable node). The possible top product segment is only the segment of the edge 2–3 close to the vertex 2, and the possible bottom product segments are the segments of the edges 1–4 and 3–4 close to the vertex 4. The possible top product region is the whole face 1–3–4, and the possible bottom product region is the whole face 1–2–3 (the delimitation method of product regions is described in the previously article). Therefore, the potentially possible splits are the splits 4:1,2,3, 1,3,4:2, and 1,4:2,3.
2. There are potentially possible splits: 3.
3. For the split 1,4:2,3, the product point x_D is located inside the product region on the edge 1–4, and the product point x_{B1} is located outside the product region on the edge 2–3.
4. We can move the point x_{B1} to point x_B, which is located inside the product region on the edge 2–3, by means of the recycle of component 2. The value of the recycle can be calculated out of the segments $2 - x_B$ and $x_B - x_{B1}$ by the rule of the lever. The total feed point after the recycle moves to the middle point of the segment $x_D - x_B$.
5. For the point x_D, the terminals of the pinch branches are the vertexes 1 and 2, and the azeotrope 13. For the point x_B, the terminals of the pinch branches are the vertexes 1, 3, and 4, and the azeotrope 13. Therefore, the common terminals of both sections are the vertex 1 and the azeotrope 13.

Therefore, the split 1,4:2,3 is possible for given feed point by means of the recycle of the component 2 as it is shown in the sketch.

3.2. Method of identification of interactive bundles and pinch branches

1. Identify all vertexes of each product simplex from all vertexes of the product region of the opposite section by the extraction of different sets of kind N^-, S^1, …, N^+ (see Fig. 7).
2. Sequentially check all product simplexes to identify if the product point is located inside by solving the system of linear equations including concentrations in vertexes of this product simplex (see Fig. 7).
3. Consider whether each vertex of the interactive product simplex is a terminal of an interactive pinch branch. Find the interactive segment of its *parent pinch branch*. The interactive segment of the parent pinch branch has the same type of pinch points as the initial *daughter pinch branch*, and is located on the element having one dimension smaller than this pinch branch (see, the previous article).
4. Repeat step 3 until the branching point from the pinch trunk. Then move to the next vertex of the interactive product simplex.

We illustrate the main steps of this algorithm in the example of the split, which is shown in Fig. 7.

1. The vertexes of the product simplexes of bottom section are 1) 134, 14, 1; 2) 134, 13, 1; 3) 134, 13, 3; 4) 134, 34, 3; 5) 134, 34, 4; 6) 134, 14, 4.

2. The check-up shows that the point x_D is located inside the product simplex 134, 34, 4. Therefore, it is the interactive simplex.

3 and 4. The terminals of the interactive pinch branches are the azeotropes 134 and 34 and the vertex 4. For the interactive pinch branch, which has the terminal 134, the parent pinch branch has the terminal 13, and its parent pinch branch has the terminal 1 (we go from the azeotrope 134 to the pinch branch inside the simplex, then we go to the pinch branch on the face 1–2–3, then we go to the pinch branch on the edge 1–2). For the interactive pinch branch, which has the terminal 34, the parent pinch branch has the terminal 3. Therefore, the pinch branches, terminals of which are the points 134, 34, 4, 13, 1, and 3, are the interactive pinch branches.

4. Conclusions

There are two important theoretical and methodical results in this article.

1. *A split is possible if common terminals exist*. This condition is universal. It includes splits, which are possible at infinite or finite reflux, with or without recycles and with or without intermediate heat input or removal. For each of the above cases additional conditions exist. A non-iterative method, based on the method of the identification of terminals, for checking whether the above conditions are satisfied was described in our previous article.
2. *The interactive bundle at the infinite reflux contains the product point of the opposite section*. This condition can be easily checked under the approximating assumption of linearity of boundaries of product simplexes.

The theory and methods described in this and previous article are the basis for the creation of software for the determination of possible splits in complex column of different types, for the synthesis of distillation flowsheets, for the determination of the minimal reflux, and for the determination of the necessary number of trays. This software can find new effective flowsheets and integrate them into the system of the automatic design of distillation units for azeotropic mixtures. We will describe our method for extractive sections in next article.

Nomenclature

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…	saddle of bundle of section profiles in ascending order number of arriving eigenvectors
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
1, 2, 3 …	components
12, 13, … 123, …	azeotropes
1–2, 1–3…1–2–3, 1–2–4…	elements of simplex

Subscripts

D	top product
B	bottom product

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Glossary with examples from figures

Bundles

Bundle: the infinitely manifold of trajectories having the same unstable and stable nodes, and saddles (see, for example, Figs. 1–3 and 6–9);

interactive bundles: the bundles of two sections, which intersect each other (see, for example, Figs. 1–3 and 6–9);

bounding bundle: the bundle, which is located on a bounding element of primary bundle (see, for example, the triangles on face 1–3–4 on Fig. 7).

Components

present components: the components, which are contained in the product of section (see, for example, the components 1–2 for top section, and 3–4 for bottom section in Fig. 1);

absent components: the components, which are absent in the product of section (see, for example, components 3–4 for top section, and 1–2 for bottom section in Fig. 1).

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 edge 1–2 for top section in Fig. 1);

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. 2).

Pinch branches

interactive pinch branches: the pinch branches, points of which are points of ends or contact of trajectories at different reflux (see, for example, Fig. 7);

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. 3);

isolated pinch branch: the pinch branch unconnected with the pinch trunk;

ingrowing pinch branch: the primary pinch branch, which returns to the pinch trunk;

parent pinch branch: the pinch branch, from which branches off the daughter pinch branch (see, for example one located on the face 1–2–3 in Fig. 7);

daughter pinch branch: the pinch branch, which branches off from the parent pinch branch (see, for example one located inside simplex in Fig. 7);

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. 6);

Pinch segment: the part of pinch branch located between two nearest branching points (see, for example, one on the face 1–2–3 in Fig. 7);

inactive pinch segment: the pinch segment, points of which cannot be points of ends or contact of trajectories (see, for example, the ones in Fig. 2);

Pinch tree: the collection of pinch chains (see, for example, the pinch chains: $2\to 13$, $2\to 14$, $2\to 34$, $2\to 134$, $2\to 1$, $2\to 3$, $2\to 4$ 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 initial points of the trajectories on face 2–3–4 in Fig. 3 and on face 1–3–4 in Fig. 8);

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

common terminal: the point, in which the pinch branches of two sections finishes;

intersection point: the point, in which 1D bundle of one section intersects the bundle of another section (see, for example, Figs. 3 and 8).

Reflux

minimal reflux: the least reflux, at which the distillation is possible;

minimal active reflux: the reflux in the branching point of first pinch branch or ingrowing pinch branch away from the pinch trunk (see, for example, the initial point of the pinch branch into vertex 1 in Fig. 3);

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 initial point of the pinch branch into azeotrope 13 in Fig. 3);

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

reflux of intersection: the refluxes of two sections dependent on each other by means of the heat balance, at which their bundles intersect each other regardless of whether their vertexes are active or inactive.

Regions

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

distillation region: the region, in which all trajectories have the same unstable and stable nodes (see, for example, two regions, which are divided by means of the curved surface 13–2–4 in Fig. 3);

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

interactive product simplex: the simplex on the product region of one section containing its product point, which is the bounding bundle of another section at the infinite reflux (see, for example, the triangle 134–34–4 in Fig. 7);

inactive product simplex: the simplex on the product region of one section not containing its product point, which is the bounding bundle of another section at the infinite reflux (see, for example, the triangles on face 1–3–4 without the triangle 134–34–4 in Fig. 7);

Split: lists of components of products of each section (For example, 1,3:2,4 where 1 and 3 are the components of the top product, and 2 and 4 are the components of 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, the indirect split 1,3,4:2 in Fig. 7);

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

split with distributed components: the split, products of two sections which contain common components (see, for example, 1,2,3:2,4 in Fig. 4);

infinitely sharp split: the split, at which each of the two products of the simple column contains only the part of components of the feed (see, for examples, the ones in Figs. 1–3 and 6–8);

half-sharp split: the split, at which one product of the simple column contains the part of components of the feed, and other contains all components of the feed (see, for example, the one in Fig. 9);
maximal split: the half-sharp split, at which product points of two sections are maximally far apart (see, for example, the one in Fig. 9);
potentially possible split: the split, the product points of two sections of which are located in their product regions (see, for examples, the ones in Figs. 1–9);
potentially possible half-sharp splits: the split, the product point of one section of which is located in its product region (see, for examples, the ones in Figs. 1–9).

Trajectory

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. 3 and 8);
interactive trajectory: the trajectory of a section, which intersects a trajectory of another section.