SHORTCUT DESIGN OF EXTRACTIVE DISTILLATION COLUMNS

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ABSTRACT

Extractive distillation is a common process for the separation of homogeneous azeotropic mixtures. In this process entrainer feed flowrate and reflux ratio of the extractive column represent the crucial design degrees of freedom which govern feasibility and operating cost. In this work feasibility and operational stability of the extractive column is related to the analysis of the nonlinear dynamics of the extractive section. A fully-automated shortcut design method for the simultaneous determination of minimum entrainer feed flowrate and minimum reflux ratio is presented. The application of this method to a ternary and a quaternary example is shown.

INTRODUCTION

Extractive distillation is commonly used to separate mixtures which display minimum boiling azeotropes. In the extractive column a heavy boiling entrainer is fed to a tray above the main feed stream. The entrainer facilitates the separation by interacting with the azeotropic mixture and altering the thermodynamic equilibrium in the extractive section of the column. Figure 1 displays the column configuration for a binary process feed. The heavy entrainer E preferably associates to component B and takes it down the column. Therefore a binary mixture of B and E is recovered in the bottom product whereas high purity A is obtained in the distillate product. Separation feasibility and process cost are characterized by two major parameters: entrainer feed flowrate and reflux ratio (or condenser and reboiler heat duties, see shaded degrees of freedom in Figure 1). In addition to minimum reflux, which limits feasibility for all zeotropic and azeotropic separations, there is a maximum reflux above which separation cannot be achieved. These bounds for the reflux ratio depend on the entrainer feed flowrate. The range of feasible choices for the reflux ratio decreases with decreasing entrainer flowrates. Below a minimum entrainer flowrate the extractive effect is no longer sufficient for separation and a feasible reflux policy cannot be found.

DESIGN OF EXTRACTIVE DISTILLATION COLUMNS

The standard approach for process design of such separation processes usually involves the detailed specification of all relevant design parameters: the number of trays, the location of process and entrainer feed trays and the reflux ratio (or either condenser or reboiler heat duty, see Figure 1). This column configuration is analyzed

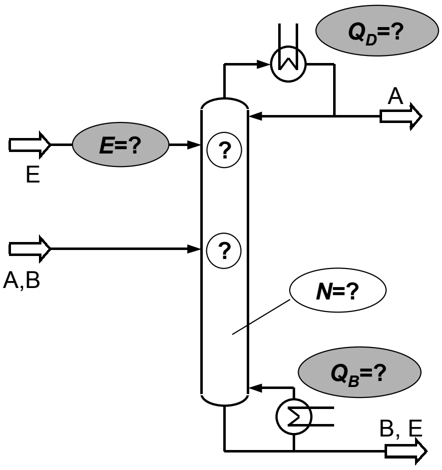

Figure 1: Design degrees of freedom for the extractive column.

using a standard process simulator such as Aspen+ [1] or Hysys [2]. The design engineer is left with the difficult task to iteratively change the design variables and repeat this process until all design constraints like required purities etc. are met and convergence is achieved. Such simulation-based design is a good method to specify all relevant design variables, however it is also a rather tedious and time-consuming undertaking.

In the early stages of process synthesis a large number of different design alternatives can be formulated. A good example is the purification of a binary alcohol-water mixture which can be achieved by heteroazeotropic distillation using a heterogeneous entrainer [3], extractive distillation using a homogeneous entrainer [4] or by using a hybrid membrane-distillation configuration [5]. For both the homogeneous and the heterogeneous azeotropic distillation processes the choice of the entrainer, usually from a list of potential candidates, defines the structure of the process and is crucial to the economic performance. Then the number of structurally different design alternatives easily grows too large to be effectively tackled using simulation tools. Therefore there is a need for simple and fast algorithms that support process screening and provide an estimate of economic potential. Shortcut methods for the determination of the minimum energy demand of distillation are well suited for this task because they allow fast evaluation of the separation without needing detailed unit information and present valuable insight into the thermodynamic limitations of the mixture.

For the separation of ideal mixtures the shortcut method of Underwood [6] has become a standard tool for process design. In the last 20 years several research groups have proposed geometric criteria for the determination of the minimum energy demand of nonideal distillation. Bausa et al. [7] present a critical review of state-of-the-art methods and propose a new, entirely general method for the separation of arbitrary nonideal multicomponent mixtures in single-feed columns. For extractive distillation in columns with multiple feed streams a general design method is missing. In a recent publication [8] the authors present a new design method that is applicable for an arbitrary number of components and can be fully automated. Feasibility and operability of extractive columns are related to the nonlinear analysis of the pinch map of the extractive section. A lower bound for the entrainer feed as well as a lower and an upper bound for the reflux ratio is obtained from a bifurcation analysis of this pinch map. The shortcut method of Bausa et al. [7] is extended for columns with multiple feed streams. This conference article will present the application of this design method for the separation of a ternary and a quaternary mixture in an extractive column.

PROPERTIES OF THE EXTRACTIVE SECTION

In the last 20 years several research groups have investigated the nonlinear dynamics of extractive distillation processes. Most of the publications focus on the analysis of the middle section of the column between the upper extractive and the lower process feed because the manipulation of the thermodynamic equilibrium by injection of the extractive agent overcomes the limitations for the product purities imposed by the azeotrope. This section will show how the feasibility of the distillation process can be inferred from the analysis of the pinch map of the extractive section. A simple illustrative example, the separation of an azeotropic mixture of isopropanol and water using pure ethylene glycol as the heavy entrainer, will be introduced.

Illustrative Separation Example

The thermodynamic behavior of ternary mixtures can be visualized using residue curve maps which represent the composition profiles of a simple batch still or of a column operating at infinite reflux. Doherty et al. [9] have identified all classes of ternary residue curve maps that allow separation using extractive distillation processes. Therefore all feasible entrainers must give rise to one of these residue curve topologies. Foucher et al. [10] simplify this residue curve analysis and present an algorithm for checking the feasibility of an entrainer that can easily be automated.

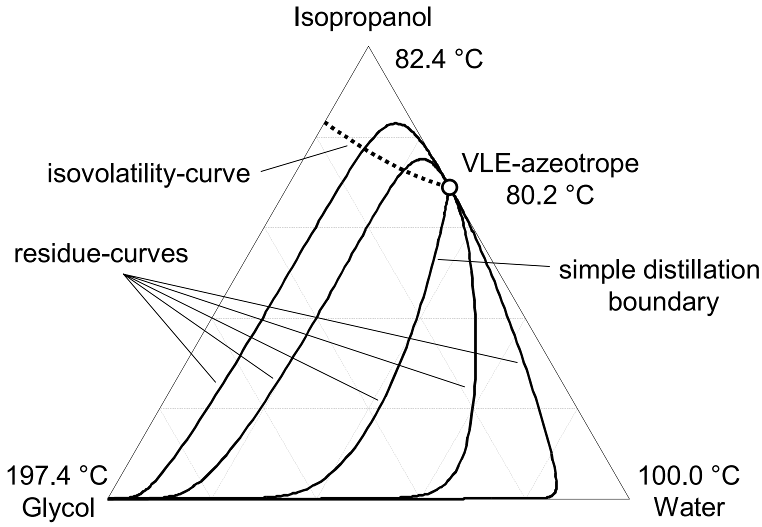

Figure 2: Residue curves, simple distillation boundary and isovolatility curve for the PWG-separation.

Figure 2 shows the residue curve map for the isopropanol-water-ethylene glycol (PWG) example. The topology of this mixture is typical for extractive distillation processes. All profiles originate from the minimum boiling azeotrope which is the unstable node of the residue curve map and end at the pure ethylene glycol vertex which corresponds to the stable node of the residue curve diagram. Profiles running close to the edges of the Gibbs triangle are attracted either by the pure isopropanol or pure water vertices and then repelled towards the stable node. In the context of nonlinear dynamics the isopropanol and water vertices therefore correspond to saddles of the residue curve map. Mathematically all nodes and saddles of the saddles are defined as the fixed points of the thermodynamic equilibrium. It is important to note that these fixed points completely describe the qualitative behavior of all column profiles at infinite reflux.

Another interesting piece of information can be obtained from the isovolatility curve of isopropanol and water (see Figure 2) which can be calculated from

$$\frac{y_P / y_W}{x_P / x_W} = \frac{K_P}{K_W} = 1. \tag{1}$$

Laroche et al. [11] show that the component which can be withdrawn with high purity from the extractive column can be directly determined from an analysis of the isovolatility curve. In the PWG example the distillate will therefore be specified as high purity isopropanol. Using this information and assuming that the bottom product will be essentially free of isopropanol the distillate flowrate can be calculated from the mass balance around the column (see Table 1). In fact, the only information missing to completely specify all input and output streams is the entrainer feed flowrate.

Column Behavior at Finite Reflux

While the fixed points of the residue curve map are sufficient to describe column profiles at infinite reflux they do not represent the course of profiles at finite reflux. Nonlinear analysis can however also be applied to columns with finite reflux by augmenting the thermodynamic equilibrium with the material and heat balances around each tray. Figure 3 shows the corresponding balance envelope.

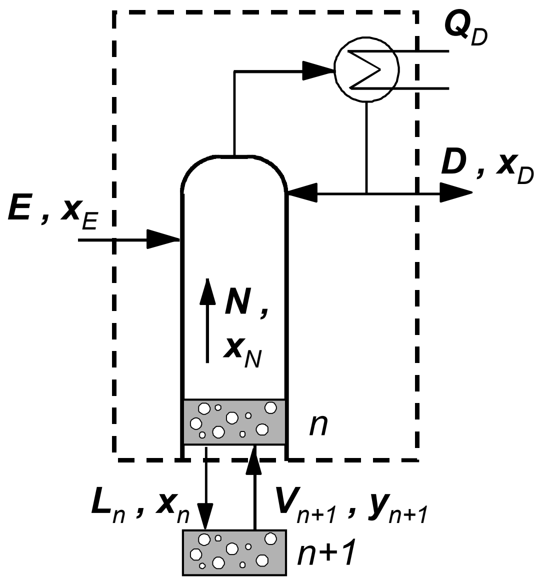

Figure 3: Balance envelope of the extractive section

The occurrence of a fixed point implies that all state variables, i.e. concentrations and internal flowrates, remain constant along the column:

$$V - L - N = 0\,, \tag{2}$$

$$Vy_i - Lx_i - Nx_{N,i} = 0\,, \qquad i = 1 \ldots N_C\,, \tag{3}$$

$$y_i - K_i x_i = 0\,, \qquad i = 1 \ldots N_C\,, \tag{4}$$

$$\sum_{j=1}^{N_C} y_j - x_j = 0\,, \tag{5}$$

$$Vh^V - Lh^L - Nh_N = 0\,, \tag{6}$$

where N, $\mathbf{x}_N$ are the flowrate and the composition of the product of the respective column section. For the extractive middle section of the column these quantities are defined as

$$N = D - E\,, \tag{7}$$

$$N\mathbf{x}_N = D\mathbf{x}_D - E\mathbf{x}_E\,, \tag{8}$$

and the enthalpy h_N can be calculated from

$$Nh_N = Dh_D - Eh_E + (r+1)D\Delta h^{VAP}(\mathbf{x}_D)\,. \tag{9}$$

This set of equations (2)-(6) is commonly known as the pinch equations and their fixed points are commonly referred to as pinch points. Since the distillate composition and flowrate are already specified *N* and $\boldsymbol{x}_N$ are fixed for a given entrainer feed flowrate. The solutions of (2)-(6) are thus one-dimensional functions of the reflux ratio and the loci of these solutions are called pinch branches. These pinch branches can be calculated by homotopy continuation. Refer to Bausa [12] for details.

Figure 4, left, shows the pinch branches for varying reflux at a entrainer to process feed flowrate of *E/F*=0.750. The corresponding pinch points at a reflux ratio of *r*=2.042 and the column profile obtained from an Aspen+ simulation with the same specifications and a large number of trays is also shown. It can be seen that there are two types of pinch branches that connect the azeotrope and all pure component vertices. The type of the pinch branch, node or saddle pinch line, depends on the stability of the pinch points located on it. The stability and the directions from which the profile either approaches the pinch or is repelled from it can be determined using the eigenvalues and eigenvectors at the pinch (see [12] for details). For the given reflux three pinch points, an unstable node on the isopropanol/glycol edge, a stable node close to the glycol vertex and a ternary saddle are found. Comparing the extractive section column profile with the pinch points and their eigendirections it can be seen that the pinch points give a good qualitative approximation of the column profile in this section and obviously the existence of the ternary saddle pinch is an important factor for the connection of the rectifying and stripping section column profiles (dotted lines) by the extractive section column profile (continuous line).

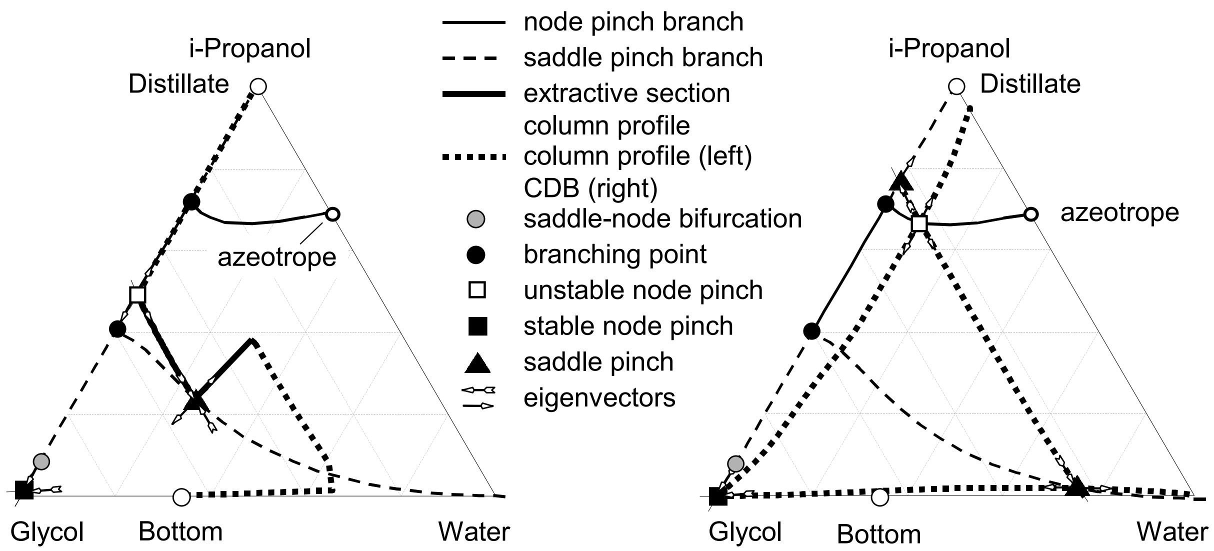

Figure 4: Bifurcation diagrams for the PWG mixture at E/F=0.750 and r=2.042 (left hand side) and r=5.0 (right hand side). All pinch branches and pinch points, saddle-node bifurcation points and branching points are shown.

Figure 4, right, shows the pinch branches and pinch points for the same entrainer feed flowrate but a larger reflux ratio *r*=5.0. Note that the pinch points have moved on their respective branches according to the higher energy supply in the column. The unstable node pinch has moved into the ternary space and a new saddle pinch has appeared on the binary isopropanol/glycol edge. A simulation with Aspen+ shows that the desired product specifications cannot be obtained for this reflux. Careful examination of Figure 4 allows to draw this conclusion directly from the pinch diagram. Due to the occurrence of the unstable node within the ternary region on the pinch branch originating from the azeotrope there can be no extractive section profile that connects the rectifying section to the stripping section profile like in Figure 4, left.

Fidkowski et al. [13] introduce the concept of continuous distillation boundaries (CDB) that easily allows to illustrate this situation. The CDB (dotted lines in Figure 4, right) cannot be crossed by feasible column profiles and therefore confine all feasible profiles into self-contained regions of the composition space. In the PWG example all column profiles starting from the binary isopropanol/glycol edge where the rectifying profile is located will stay close to this binary edge and cannot access the stripping profile which lies in a different region.

Comparing the left and right hand side of Figure 4 it can be concluded that the appearance of the ternary unstable node originating from the azeotrope pinch branch makes the separation infeasible while the existence of a ternary saddle originating from a pure component is a prerequisite for a feasible process. Knapp et al. [14] formulate this criterion and relate separation feasibility to the appearance of saddle-node bifurcation points and branching points. Using this criterion a lower bound for the entrainer feed flowrate and a lower and an upper bound for the reflux ratio can be determined. In a recent publication [8] the authors present an algorithmic formulation for obtaining these bounds.

SPLIT FEASIBILITY AND DETERMINATION OF MINIMUM REFLUX

A feasible separation requires that distillate and bottom product are connected by a continuous concentration profile representing the compositions on each tray of the column. The criteria for obtaining a lower and an upper bound for the reflux ratio and a lower bound for the entrainer feed flowrate that were deduced from topological analysis of pinch maps (see [8]) provide a range of operating conditions for which such a feasible column profile might be obtained. However, they do not guarantee that the separation is feasible for all specifications within those bounds. Therefore a method for guaranteeing feasibility and for the determination of the minimum reflux ratio is necessary.

For this task several methods are proposed in the literature. For example Levy et al. [15] present an algebraic criterion for the determination of minimum reflux of ternary separations in multiple feed columns. It is based on the argument that at minimum reflux one of the feed concentrations and specific pinch points of two column sections must lie on a straight line. This method works reliably and generates quite accurate results. However, for the application of this method the type of split (direct/indirect), the controlling feed and in the case of multiple pinch solutions for one section also the controlling pinch must be known a-priori. Furthermore the method is restricted to ternary mixtures.

Bausa et al. [7] present a new criterion for the determination of the minimum reflux ratio (minimum energy demand) of single-feed columns that is applicable to arbitrary splits and mixtures with an arbitrary number of components. The method is based on the approximation of all column profiles by so-called rectification bodies which are constructed from the pinches of each section. Using some insight from the nonlinear analysis of the pinch equations this rectification body method can be extended to columns with multiple feeds and therefore applied to extractive distillation.

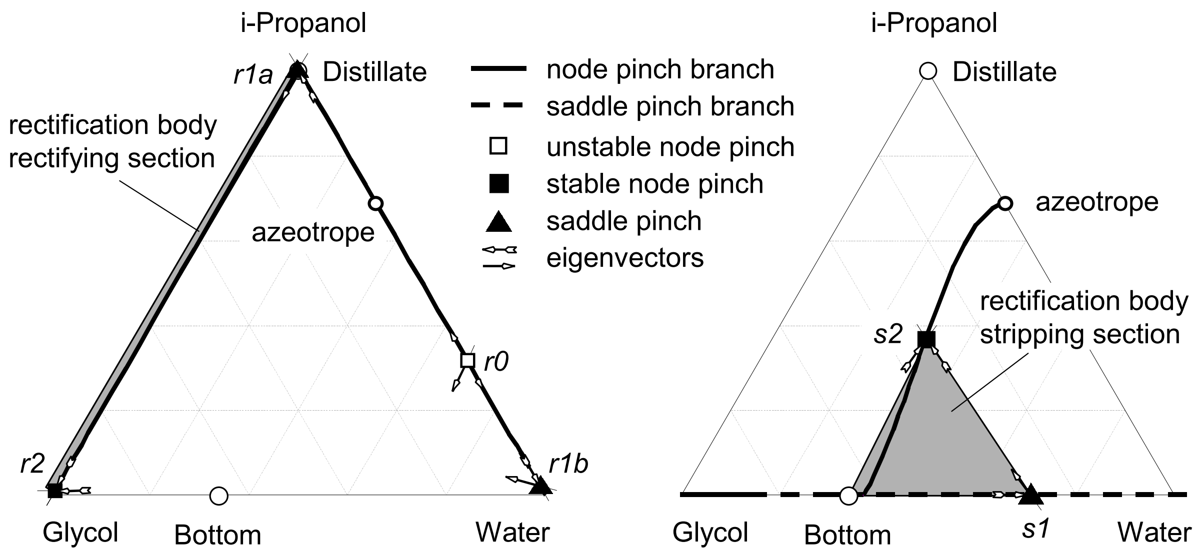

Figure 5: Pinch lines, pinch points and rectification bodies for rectifying (left) and stripping section (right) at E/F=0.750 and r=2.042.

For the rectifying and stripping sections the construction of the rectification bodies can be performed as presented in the original algorithm (see [7]). First, the pinch branches of the respective section are determined. Given some reflux ratio for which the feasibility of the split is to be tested all pinch points on these pinch branches and their stability are calculated. Now all possible paths of the profiles are determined. Some rules for the course of plate-to-plate profiles are exploited. The first rather trivial rule is that all profiles start at the respective product composition. Second, under minimum reflux the profiles will touch one or more pinch points. The number of stable eigenvectors in the pinch points touched by a profile must increase strictly monotonously. Figure 5, left, shows the pinch branches and pinch points of the rectifying section for the PWG separation at an entrainer to process feed ratio of *E/F*=0.750 and a reflux ratio of *r*=2.042. Four pinch points are found, one unstable node *r0*, two saddle pinches *r1a* and *r1b* and one stable node *r2*. Applying the rules for the construction of the rectification body it is found that *r0*, *r1a* and *r1b* can be discarded. Therefore only one potential path *D-r2* for the column profile remains. The corresponding rectification body in the rectifying section is shown in Figure 5, left. It is a straight line on the binary isopropanol-glycol edge. The construction of the rectification bodies for the stripping section is similar. Two pinch solutions, one saddle pinch *s1* and one stable node *s2* are found. They correspond to one path *B-s1-s2* and the corresponding triangular rectification body is shown in Figure 5, right.

The rectification bodies of the extractive middle section cannot be constructed using the same approach as for the rectifying and stripping sections. The overall product composition $\mathbf{x}_N$ of the middle section as determined from (7)-(8) often lies outside the physically attainable composition space. Hence, some of the pinch branches and pinch points also move outside the composition space. Therefore the pinch map of the extractive section is not always complete. As deduced from the nonlinear analysis of an extractive distillation column a saddle pinch must always be present for a feasible ternary separation. For multi-component separations there may be more than one saddle pinch as will be shown in the quaternary example. Levy et al. [15] observe that the eigenvectors of such extractive section saddle pinch points give a very good approximation of the directions in which the profiles approach and leave a saddle pinch. This observation is also supported by examination of the column profile of the PWC separation in Figure 4, left. The profile matches the eigenvectors of the saddle nearly exactly and shows only small curvature. Therefore the course of the middle section profile can be approximated by rectification bodies that obey the following rules as defined in [8]:

1. Calculate all saddle pinch points.
2. Determine all paths of saddle pinches using the rule that the number of stable eigenvectors on a path must increase strictly monotonously.
3. Approximate the starting point of the profile by following the most stable (largest eigenvalue) eigenvector of the first saddle of the path until some edge of the composition space is reached (S_1, S_2 in Figure 6).
4. Approximate the end point of the profile by following the most unstable (smallest eigenvalue) eigenvector of the last saddle of the path until some edge of the composition space is reached (E_1, E_2 in Figure 6).
5. Consider both directions of the eigenvectors in steps 3 and 4. Therefore one path typically corresponds to four middle section rectification bodies.

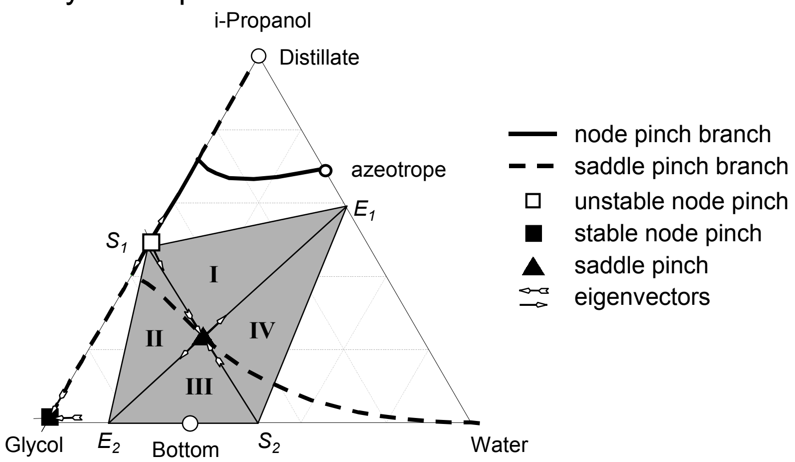

Figure 6: Pinch lines, pinch points and rectification bodies for the extractive section at E/F=0.750 and r=2.042.

Figure 6 shows the application of these rules to the middle section of the PWG separation at *E/F*=0.750 and *r*=2.042. Only one ternary saddle pinch and therefore only one path is obtained. The unstable and stable eigenvectors are extended in both directions resulting in four rectification bodies. The rectification bodies for all three sections of the column are collected in Figure 7. It can be seen that both the rectifying and middle and the middle and stripping sections intersect each other. In the middle section rectification body (I) is active. Since the rectifications bodies are an approximation of column profiles there must therefore exist one profile that continuously connects the distillate with the bottom product. This claim is supported by the column profile obtained from an Aspen+ simulation with the same specifications that is also shown in the figure.

To determine the minimum reflux with the rectification body method means to find the smallest reflux ratio that makes intersection of the bodies possible. If they do not touch at all, the separation is infeasible and below minimum reflux (Figure 8, left). If the bodies penetrate each other the separation is feasible but above minimum reflux (Figure 8, right). Starting with one reflux that is known to be below the minimum

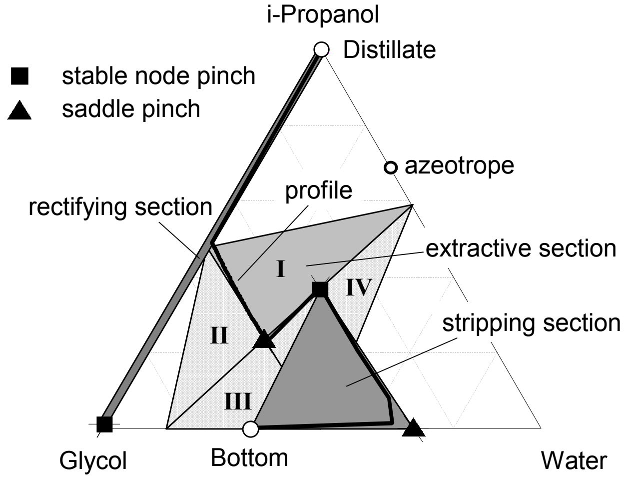

Figure 7: Rectification bodies at E/F=0.750 and minimum reflux r=2.042.

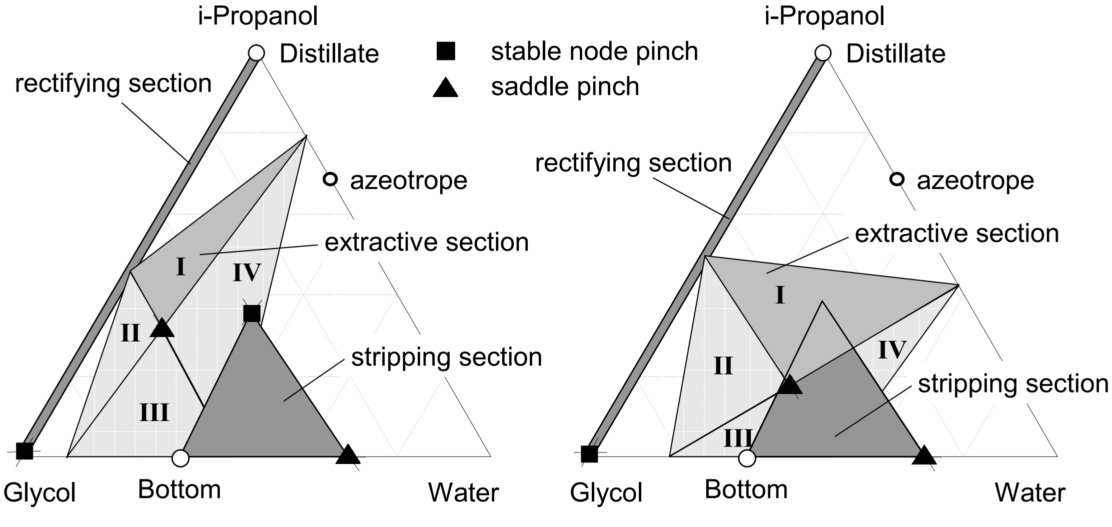

Figure 8: Rectification bodies at r=1.9 below minimum reflux (left) and at r=2.2 above minimum reflux (right). The entrainer to process feed ratio is E/F=0.750 in both cases.

reflux and another one which is known to be above minimum reflux, the minimum reflux that makes the rectification bodies just touch can be determined using a bisection algorithm. The minimum reflux situation is shown in Figure 7.

OPERATIONAL CONSTRAINTS

Operational stability of separation processes is a crucial factor to the economical success of such processes. This is especially true to extractive distillation because extractive distillation columns often show counterintuitive operational properties [16]. Due to the extractive effect and the existence of a maximum reflux the separation is not necessarily improved by increasing the reflux ratio which is a common property of simple distillation. Furthermore the range of feasible reflux ratios may be small. In

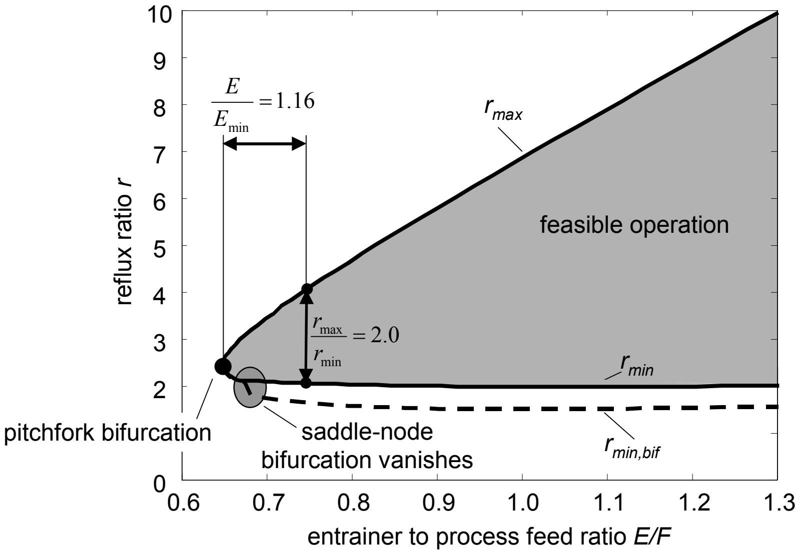

Figure 9: Minimum and maximum reflux ratios for the PWG separation as a function of the entrainer feed flowrate.

this case very elaborate and expensive control mechanisms are required. Therefore it is sometimes useful to sacrifice cost-optimality of a steady-state design in favor of better operational stability.

Andersen et al. [17] and Knight et al. [18] discuss the impact of operational properties on the design of extractive columns. In order to illustrate the tradeoff between cost-optimality and operability they make extensive use of diagrams in which the energy requirement of the column (internal vapor flow in [17], energy cost in [18]) are plotted against the entrainer feed flowrate. Using the design method presented in [8] such a diagram can also be produced for the PWG example and is shown in Figure 9. It can be seen that the feasible region is contained by the minimum and maximum reflux ratios as a function of the entrainer flowrate. The lower bound for the entrainer flowrate which was found from bifurcation analysis is also shown.

The operating cost of the extractive column are essentially specified by the reflux ratio which determines the condenser and reboiler heat duties. In addition to the extractive column an entrainer recovery column is necessary in which the bottom product of the extractive column is further separated into water and the entrainer ethylene glycol. This column is a conventional binary column and its energy demand can readily be analyzed with the conventional rectification body method for simple columns [7]. The operating cost of the solvent recovery column increases with the entrainer feed flowrate to the extractive column because consequently more material must be purified downstream. Therefore a cost-optimal extractive distillation process is operated at low entrainer feed flowrate and low reflux of the extractive column. This corresponds to operation close to the tip of the nose of the tradeoff diagram in Figure 9. However operating the extractive column at these conditions will be difficult since the range of feasible refluxes is quite small. Furthermore the number of trays required to achieve the desired purities will be large because for operation close to the minimum or maximum reflux ratios the separation can only be achieved in a column with an infinite number of trays whereas operation at intermediate refluxes will require fewer trays.

These operational implications for design from above indicate that a good design of the extractive column will be operated at some distance from the feasibility boundaries. This can be ensured by restricting the design variables entrainer feed flowrate and reflux ratio with operational constraints. Some useful formulations of such constraints on the entrainer feed flowrate and the reflux ratio are presented in [8]. For the PWG example the operational constraints have been chosen as $E_{max}/E_{min}>\Pi E_{min}=1.1$ and $r_{max}/r_{min}>\Pi r_{min}=2.0$. The resulting operating conditions, $E/F=0.750$ and $r=2.042$ are indicated in Figure 9. The constraint on the reflux ratio is the driving design constraint. The results for the PWG example problem are summarized in Table 1.

DESIGN PROCEDURE

Using the insights gained from the nonlinear analysis of an extractive column, the extension of the rectification body method to multi-feed columns and by incorporating operational considerations a novel procedure for the design of extractive distillation columns has been formulated in [8]. Using this design procedure the optimum operating entrainer feed flowrate as well as the corresponding minimum and maximum reflux ratios are directly determined. The results are identical to the graphical analysis of the tradeoff curve presented in Figure 9. The minimum feasible entrainer feed flowrate and the corresponding reflux ratio are also determined. This design procedure has been implemented in C. Results for the PWG example and the computational performance of this code can be inferred from Table 1. Results are generally obtained well below 10 seconds of computation and therefore the design procedure can be used interactively.

A QUATERNARY EXAMPLE

A second alcohol, ethanol, is added to the isopropanol-water mixture that has already been discussed. As can already be inferred from the molecular similarity of ethanol and isopropanol, ethanol can also be separated from water by extractive distillation with ethylene glycol as heavy entrainer. A possible straightforward approach to separation process design for the ternary mixture ethanol-isopropanol-water is to first

Table 1: Specifications and results for the example separations. A pressure of p=1.013 bar, saturated liquid feed and product streams and operational constraints of ΠE_{min}=1.1 and Πr_{min}=2.0 are specified. The Wilson activity model was used. Physical property parameters were obtained from Aspen+ [1]. CPU time was determined on a P-III 900 Mhz PC.

Figs.	Components	x_F	X_E	x_D	$(E/F)_{min}$ r_{min} r_{max}	E/F r_{min} r_{max}	CPU [s]
7, 9	isopropanol water ethylene glycol	0.62 0.38 0.0	0.0 0.0 1.0	1.0 0.0 0.0	0.649 2.428 2.428	0.750 2.042 4.084	2.67
10	ethanol isopropanol water ethylene glycol	0.124 0.496 0.38 0.0	0.0 0.0 0.0 1.0	0.2 0.8 0.0 0.0	0.662 2.214 2.214	0.756 1.905 3.810	5.26

split this mixture into the binary mixtures ethanol-water and isopropanol-water and then feed these mixtures to separate extractive distillation trains. This process alternative does not really seem appealing from an economic point of view since needs five columns: pre-separation into two binary mixtures, two extractive columns and two entrainer recovery columns.

Like isopropanol ethanol is recovered at the top of the extractive column. Therefore it seems worthwhile to try the separation of both alcohols from water in one extractive column. The operational constraints, ΠE_{min}=1.1 and Πr_{min}=2.0, were chosen identical to the PWG separation. Using these specifications (cf. Table 1) the design procedure is applied as presented above. The algorithm rates this split feasible and suggests an operating entrainer to process feed ratio of $(E/F)_{op}$=0.756. This is only marginally more than for the PWG example. Minimum and maximum reflux ratios are r_{min}=1.905 and r_{max}=3.810 which is even less than for the PWG example. Figure 10, left, shows the active pinches and rectification bodies at $(E/F)_{op}$ and r_{min}. It can be seen that due to the appearance of the ethanol the number of pinch points and the dimensionality of the rectification bodies has increased. In the rectifying section one saddle pinch and one stable node pinch are found and form a triangular rectification body. In the stripping section two saddle pinches and one stable node pinch are found. This corresponds to a tetrahedral rectification body. The extractive section is characterized by the occurrence of two saddle pinch points. The more unstable one lies on the ternary ethanol-isopropanol-water edge. Two triangular rectification bodies are formed. The results of the design method were confirmed with an Aspen+ simulation for the same specifications. The column profile obtained from this

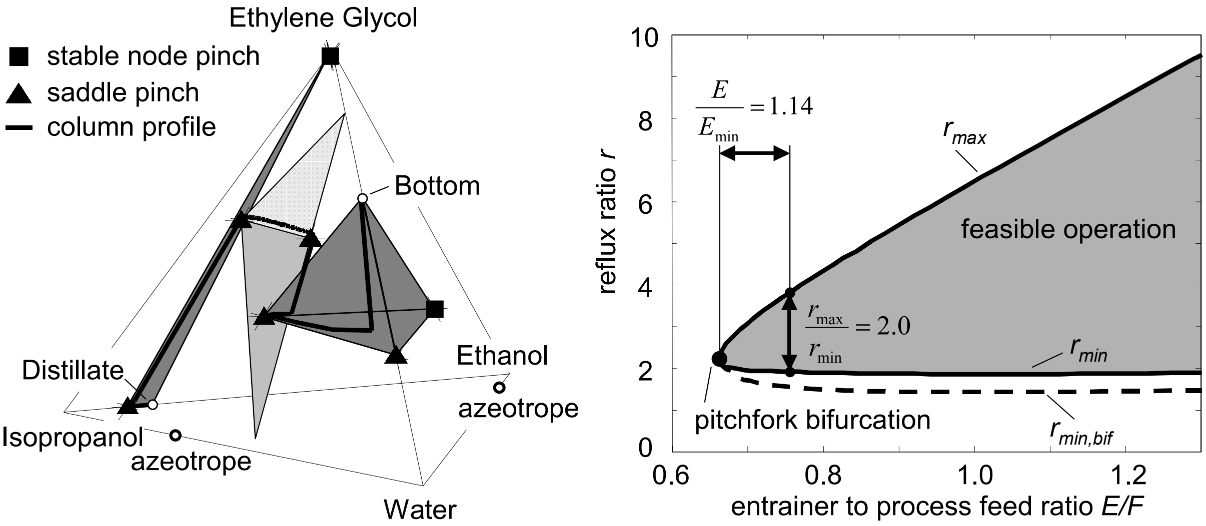

Figure 10: Pinch points, rectification bodies and column profile at E/F=0.756 and rmin=1.905 (left hand side) and feasible operating region (right hand side) for the EPWG mixture.

simulation is also shown. It can be seen that the course of this profile is nearly identical to the path predicted by the rectification bodies.

Figure 10 right hand side shows the feasible operating region as a function of entrainer to process feed ratio and reflux ratio. It is nearly identical to the one obtained for the ternary PWG example (cf. Figure 9).

CONCLUSIONS

The application of a new design method for extractive distillation processes is presented for a ternary and an quaternary example. The design method is based on the nonlinear analysis of pinch maps and an extension of the rectification body method for the determination of the minimum energy demand. It can be applied to arbitrary azeotropic mixtures without limitations regarding the number of components or certain types of splits. It determines the minimum entrainer flowrate and the corresponding feasible reflux ratio as the thermodynamic boundaries of the extractive distillation process. Using the concept of operational constraints the method further aides in finding robust operating conditions. The calculation of the minimum and maximum reflux ratios provides the range of feasible reflux policies and therefore contributes a measurement of process flexibility.

The results of this shortcut design algorithm can be used to directly compare the economic performance of different entrainers and provide good initial values for more rigorous calculations such as mixed-integer nonlinear optimization (MINLP) [19].

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