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Liquid-only transfer in dividing wall columns – Analytical minimum vapor expressions

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ABSTRACT

Standard dividing wall columns (DWC) are state-of-the-art integrated fully thermally coupled (FTC) (or Petlyuk) distillation arrangements performing several separation tasks within one unit and with a lower energy consumption and capital costs than conventional column sequences. This may require careful design and control of the internal flow rates to achieve the potential energy savings, which typically are about 30%. In particular adjusting the internal vapor split is regarded to be challenging. The Liquid-only transfer (LOT) arrangements offer alternative internal flow rate adjustments that may mitigate this challenge. In addition, its use in retrofit may enable practical cost-effective solutions. The key result in this paper is to provide analytical minimum energy expressions for the LOT arrangement which are shown to be identical to the ones for the standard DWC. Furthermore, the optimal operating region and flexibility for the internal sub-columns in the arrangements are explored and are also found to be equivalent and the available adjustment margines for the LOT draw rates and other operational variables are clarified. The results give valuable insight in the characteristics of optimal operation and can also be used to provide good initialisation values for rigorous simulations.

1. Introduction

Distillation is the most widespread method of separation of liquid components and is responsible for a large amount of the energy consumption in the process industry in form of heating and cooling in reboilers and condensers. The research for developing more energy efficient and realizable practical process arrangements is important to enable the industries to improve the environmental footprint by reduced energy consumption and emissions related to distillation [1]. The dividing wall column (DWC) is a technology for integrated multicomponent separation that saves both energy and capital cost compared to conventional sequences [2]. This is because the integration with the internal full thermal coupling leads to reduced required minimum vapor flow rates for the desired separation, which in in turn require less heating and cooling, smaller width, and footprint. Several hundred DWCs have been built and are in operation worldwide [3,4].

Care must be taken to realize the full energy saving potential. In addition to having enough effective separation stages and well-designed internals, it is very important that the internal flow rates are set correctly. This is done by correctly setting the liquid split above the dividing wall and the vapor split below [5]. Devices for on-line adjustment of the liquid split are available but it is not common in industrial practice to implement devices for on-line adjustments of the vapor split [6]. Luckily, the optimal settings for the vapor and liquid split ratio are usually not at a single point, but rather in a segment in the operating region such that it may be sufficient to fix the vapor split by design and only adjust the liquid split on-line. The optimality region is determined by the feed properties and product specifications. In some cases, there are quite tight margins in setting the vapor split and it is desirable with on-line adjustable vapor split. This is because inevitable variations and uncertainties in feed conditions makes it impossible to obtain minimum energy operation with a fixed vapor split [7]. Offoptimal operation leads to rapid increase in energy consumption and/ or the inability to produce pure products, especially for the side-stream [8] (Ch. 9).

Agrawal and coworkers have made significant contributions in exploring a large number of possible column section configurations and interconnections that can be identified for a multicomponent separation task. An important issue in DWC operation is the practical realisation of on-line adjustment of the vapor split. Agrawal has presented several alternative configurations to get around this challenge e.g. [9,10]. One alternative design is the so-called liquid-only transfer (LOT) arrangement [10–12]. Agrawal [11] shows for a certain LOT configuration that

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Nomenclature	y Molar fraction in vapor phase		
	α Relative volatility		
Symbols	Θ, φ, ψ Underwood roots		
B Molar bottom product flow rate D Molar top product (distillate) flow rate F,z,q Molar feed flow, composition, liquid fraction L Molar liquid flow rate R Split ratio at dividing wall (molar flow to prefractionator divided by total flow) S Molar side draw flow	Subscripts B, bot, balanced (sub)column bottom, balanced split <i>T</i> , <i>t</i> , top (sub)column top p, pref, pinch (sub)column at preferred split, pinch (for composition) 1, 1x, 1y, 2x, 2y, 21, 22 Sub-Column numbering i, (A,B,C) Component i, A, B, C		
I lemperature V Molar vapor flow rate	s Side draw		
wi Net flow of a component (if signed, positive upwards) x Molar fraction in liquid phase	min lower limit		

the liquid/vapor flows in the upper parts can be made equal to optimal flows in the top part of the corresponding optimally operated DWC. This proves that the minimum reboiler duty for the LOT is the same as for the conventional DWC. Simulations studies and comprehensive reviews of a wide range of LOT arrangements are given by Agrawals group [13], Sørensen et. al [14] and Horsch e.t al. [15]. The main advantage is that the liquid-only transfer is simpler to realize in industrial practice than internal devices for vapor split. It must here be mentioned that some papers have discussed on-line vapor split and shown their practical use in pilot plant experiments [6]. Nevertheless, industry remains reluctant to the reliability of internal vapor split adjustment devices. We do not discuss the vapor split option further but focus on the opportunities with LOT arrangements.

For the standard DWC (Petlyuk arrangement), analytical minimum vapor expressions are available for the case of ideal mixtures with constant relative volatility, constant molar flows and constant pressure. The underlying methods used to develop these analytical expressions are the Underwood equations [16]. Fidkowski et al. [17] applied the Underwood equations to derive minimum energy expressions for a standard DWC separating a saturated ternary mixture. Halvorsen et. al. [8,18–21] extended these results to multicomponent feeds and more complex Petlyuk arrangements and introduced the Vmin-diagram as a visualisation and working tool.

In this paper we extend the analytical Underwood expressions and the Vmin-diagram to include LOT DWC arrangements. We explore the characteristics of minimum energy operation, and show for which conditions the LOT-DWC may realise the minimum vapor flow rate. A new result, is to show that there usually is an adjustment margin for one of the LOT draw rates, which implies that one may obtain optimal operation (minimum reboiler duty) with liquid/vapor flows in the top which are *different* from that in the standard DWC.

The paper is organized as follows. The basis for the standard DWC [18–20] is given in section 2, primarily for new readers. The extension of the Underwood equations to LOT DWC is given in section 3. The results are further discussed in Sections 4 and 5. A simulation based on separation of the BTX (Benzene, Toluene, Xylene) feed mixture, found in several DWC publications, is included as an illustrating example in section 5.

1.1. Notation

A short comment on notation and assumptions is helpful for reading the paper.

By the standard dividing-wall column (denoted standard DWC or FTC-DWC) we mean the three-product fully thermally coupled (FTC) arrangement in Fig. 2(b) with a single vapor split and a single liquid split. This is thermodynamically equivalent to the "Petlyuk-arrangement" in 2(a) and both terms may appear in the text. Minimum energy



Fig. 1. Two-product distillation column (a) and generalization to two-product FTC-section with fully thermal coupling potential (b).

operation or "minimum demand" is equivalent to minimum vapor (V_{min}) operation and is achieved with an infinite number of stages. The use of an infinite number of stages is of course unrealistic, but it turns out that the actual energy approaches this minimum for a reasonable number of stages. The vapor flow V in this paper refers to the top of the column (unless stated), that is $V = V_T$. All results in this paper assume steady-state operation and the analytical expression use the standard assumptions of constant relative volatility for the vapor–liquid equilibrium, constant molar flows for the energy balance and constant pressure.

The following subscripts are used; i for the i'th component, n for the n'th stage (counted from the top), p for preferred, b for balanced, and P for pinch. Finally, subscripts A, B, C denotes components A, B and C, where A is the light key, B is the intermediate key, and C is the heavy key. We may denote splits in a single binary column as A/BC or AB/C for sharp splits and AB/BC or just A/C for a sharp split between A and C while the intermediate B distributes to both ends. For example; $V_{minA/BC}$



Fig. 2. Realization of fully thermally coupled (FTC) arrangement as Petlyuk column (a) and thermodynamically equivalent standard Dividing Wall Column (FTC-DWC) (b).

denotes minimum for sharp split between A and BC. Products are denoted D for distillate (containing mainly A), S for side draw (mainly component B), and stream B (mainly C) for bottoms. The context should tell if 'B' is the intermediate key or bottom product.

2. Theoretical background

Fig. 1 shows the conventional two-product column (a) and its generalization to a subsection that allows for thermal coupling (b). Fig. 2 shows how subsections may be used in a fully thermally coupled (FTC) arrangement which may be realized in a Petlyuk column as in Fig. 2 (a) or in a dividing-wall (DWC) arrangement, Fig. 2 (b).

In the following we give a brief overview of the analytic equations leading to the minimum vapor expression for the Petlyuk arrangement and the equivalent standard (FTC) DWC. Most of this is based on [8,18–20] which again is based on Underwoods papers from the 1940's [16]. The expressions will be presented in some detail herein since it is the basis for analysis the liquid-only transfer arrangements in section 3.

2.1. The standard DWC

The expression for the minimum vapor (V_{min}) for the Petlyuk arrangement is amazingly simple [19]. Consider an ideal ternary feed mixture (ABC) with constant relative volatility, constant molar flows and constant pressure. The minimum overhead vapor rate ($V_{T,min}$) for the full Petlyuk and DWC arrangement in is then equal to V_{min} for the most difficult binary separation of either A/BC or AB/C in a two-product column Fig. 1(a).

$$\frac{V_{C217,\min}}{F} = \frac{\max(V_{\min,A/BC}, V_{\min,AB/C})}{F} = \max(\frac{\alpha_A z_A}{\alpha_A - \theta_A}, \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B}{\alpha_B - \theta_B})$$
(1)

This is equivalent to the highest peak in the Vmin-diagram (Fig. 3). This simple insight makes it obvious that the DWC outperforms the conventional direct or indirect split arrangements in term of total vapor requirements (at constant pressure). Equation (1) was derived by Fidkowski and Krolikowski (1986) [17] for a ternary saturated feed, and extended to any number of components, any liquid fraction and any number of products by Halvorsen and Skogestad (2003) [19]. In equation (1), the molar feed rate is F, the liquid feed fraction is q, the molar feed fractions are z_A , z_B , z_C and the relative volatilities α_A , α_B refer to the least volatile component (which for the ternary case implies $\alpha_C = 1$). The "common" Underwood roots θ_A , θ_B are the solution of the so-called Underwood's feed equation:

$$\frac{\alpha_A z_A}{\alpha_A - \theta} + \frac{\alpha_B z_B}{\alpha_B - \theta} + \frac{\alpha_C z_C}{\alpha_C - \theta} = 1 - q \tag{2}$$

The solution fulfills: $\alpha_A > \theta_A > \alpha_B > \theta_B > \alpha_C$. See Appendix A and references for more details.

When working with Underwood equations we also need the definition of the net flow of component *i* in a column section:

$$w_i = V_{n+1} y_{i,n+1} - L_n x_{i,n} \tag{3}$$

Here it is assumed that stage numbers (*n*) are counted from the top in any sub-column. On any stage (n) in a section the composition of a component (*i*) is $x_{i,n}$ in the liquid phase, $y_{i,n}$ in the vapor phase and V and L are the molar vapor and liquid rates. From the mass balance, the net flow rates are constant through any column section between any feeds or draws. This also holds for non-ideal cases where the molar flow rates are not necessarily constant along the section. We trivially have $\sum w_i = V_{n+1} - L_n$ and if, for example, all of the light A component from the feed is transported upwards in a section then $w_A = z_A F$. The following total balance also applies for the top of the column:

$$D = V_T - L_T = \sum w_i \tag{4}$$

The flow rates in the bottom (stripping section) are trivially given by the mass balance around the feed stage.

2.2. The Vmin diagram

In a typical two-product column as in Fig. 1(a), operating with a given pressure and feed, there are only two degrees of freedom in operation. This implies, for example, that if the vapor rate and liquid rate (V, L) or alternatively (V, D) is set at an intersection of the column, the distribution of components, including the product compositions, are uniquely determined. For the thermally coupled section in Fig. 1(b), the product composition may also depend on the in-flow compositions in the ends. Fortunately, when the liquid and vapor rates through the feed stage is set, the actual composition of the in-flows at the ends does not matter to the net material rates unless a component that otherwise not would not be present in a conventional end, is introduced [8]. This key result lets us do calculations for thermally coupled sections like in Fig. 1 (b) just as for the conventional in Fig. 1(a).

The Vmin diagram [18] in Fig. 3 is excellent for visualization. The abscissa is the net distillate flow rate $D = V_T - L_T$ and the ordinate is the top vapor flow rate $V = V_T$ such that each coordinate pair (*V*,*D*) defines a unique operating point. At each boundary line a component in one end is at the limit of appearing/disappearing for a slight change in flow rates. All points below the "mountain-like" top boundary are minimum vapor solutions for a particular component distribution. All points above the "mountain" imply energy waste. For the ternary case we point out three particularly important points. The leftmost peak (P_{AB}) represents



Fig. 3. Vmin diagram for separating a ternary mixture in a two-product column (Fig. 1a). The lines show Vmin for sharp binary separations. [8].

minimum vapor solution (V_{min}) for sharp A/BC split. The rightmost peak (P_{BC}) is a V_{min} operating point for sharp AB/C split, and then we have the very interesting, preferred split (P_{BC}) whin is the minimum vapor solution for sharp A/C split while the intermediate B distributes to both ends (really AB/BC).

The minimum vapor expressions in equation (1) are analytical expressions for the height of the peaks $(V_{\min,A/BC}, V_{\min,A/BC})$ at point P_{AB} and $\ensuremath{P_{BC}}$ in the Vmin diagram, thus, the highest peak determines the minimum requirement in a standard-DWC in Fig. 2. The height of the peaks is determined by both relative volatilities and feed composition. This minimum can only be obtained when the prefractionator (C1) is operated correctly. In short: Operation exactly at the preferred split is always optimal. In addition, when the peaks are of different heights, operation along the V-shape made of PAB-PAC-PBC from PAC on a certain line segment towards the highest peak would also enable the same overall minimum vapor rate for the whole FTC-DWC arrangement. This segment comprises the optimal operation region and is visualised in Fig. 4. The "balance point" or more specifically "balanced main column point" is when the actual minimum vapor above and below the side draw stage in a DWC becomes equal. Because at the preferred split the minimum vapor in C21 is at PAB and, increases when moving up on the V-shape, while the demand in C22 remains constant, until the balance point is reached. Further moving upwards will require increase in overall reboiler vapor production. If the leftmost peak is highest, the argumentation flips to the other side of the V-shape, and also the behaviour of C21 and C22 is interchanged. This may happen by changes in feed composition and liquid fraction and of course for different sets of components with different relative volatilities.

In the following, in most discussion we assume the class of feed where the rightmost peak being highest as illustrated in Fig. 4.

2.3. Underwood roots

We present here in more detail the key equations that represent operation along "V-shape" (from the peak $V_{\min}^{A/BC}$ down to the preferred

split point and up the peak at $V_{\min}^{AB/C}$) in Fig. 3 since those are to be used when comparing to the LOT arrangements.

Along the V-line, all the light A is recovered, so the difference in net distillate flow is caused by a difference in the net flow of the intermediate B to the top. Thus, in Fig. 3, the net distillate flow at the preferred split is $D_{pref} = z_A F + w_{B,p}$ and at the balance point is $D_{bal} = z_A F + w_{B,b}$ and we will show in the following how to compute the values of $w_{B,p}$ and $w_{B,b}$ using Underwood roots.

In this respect, Fig. 5 is quite informative and will be used in the coming sections. Note here that the "actual Underwood root" ϕ_A characterise the A/B split and the "actual root" ψ_C characterise the B/C split. At minimum vapor conditions these roots coincide with the common Underwood roots from the feed equation (2), that is, $\phi_A \rightarrow \theta_A, \psi_C \rightarrow \theta_B$ respectively. An actual root becomes active (equals a common root) when the operation point is crossing a distribution boundary from above. The most important operating point is on the V-shape above the preferred split where one root is active on each branch. At, and below the preferred split, both are active.

2.4. Carry over roots in fully thermally coupled sections

Underwood's definition equation (39) (in Appendix) gives the relation between the Vapor rate, the net material flows and the actual Underwood roots. Consider operating section C1 in the standard Petlyuk-DWC such that the recovery of heavy C in the top is zero (implying $w_C = 0$), that is, above the boundary line origo-preferred split-rightmost peak (which is only partly the same as the "V-shape"). The operating point can then be expressed by Underwood's definition equation (39) to find the two "actual roots" ϕ_A and ϕ_B by solving:

$$V_{T,C1} = \frac{\alpha_A w_A}{\alpha_A - \phi} + \frac{\alpha_B w_B}{\alpha_B - \phi} D_{T,C1} = w_A + w_B \tag{5}$$

Note the discrimination between "actual" roots (ϕ) in (5) and "common" roots (θ) in (2). The latter are only active at a minimum vapor operating point and depends only on the feed properties [Ref. Appendix A]. Using



Fig. 4. The optimality region between the preferred and balanced split for the prefractionator (C1) for a Petlyuk/DWC arrangement is illustrated in the Vmin diagram. Operating outside this regions leads to rapid increase of the overall vapor rate requirement illustrated by the upper curve $V_{\min}^{Petlyuk}(D^{C1})$. [8].



Fig. 5. Illustration of the key Underwood roots in the Vmin Above the upper boundary (origo-P_{AB} + P_{AC}-P_{BC}-end), there are no active common roots[8].

the actual roots covers all possible operating points but requires some care in calculations since the actual roots change with the operating condition. In an fully thermally coupled (FTC) connection it can be shown that the Underwood feed equation for the succeeding column is identical to the definition equation of the preceding column section [19,22];

$$\underbrace{V_{T,C21} - V_{B,C21}}_{\text{Feed equation for C21}} = \frac{\alpha_A w_A}{\alpha_A - \theta_{C21}} + \frac{\alpha_B w_B}{\alpha_B - \theta_{C21}}$$

$$\underbrace{V_{T,C1}}_{\text{Feed equation for C21}} = \underbrace{V_{T,C1}}_{\text{Definition equation for C1 ton section}} + \frac{\alpha_B w_B}{\alpha_B - \phi_{C1}}$$
(6)

 ${\Rightarrow}\theta_{C21}\equiv\phi_{C1}$

This implies that the "common" roots that characterise minimum vapor solutions in C21 is identical to the "actual" roots representing an arbitrary operating point in C1; $\theta_{C21} \equiv \phi_{C1}$. Note the subscript on the roots denoting the relevant section. In some places, where the subscript is omitted, the roots are related to the feed F into column C1 in the arrangements.

Thus, we may say that the "actual roots" in C1 "carry over" and becomes the "common roots" in C21 via the FTC connection. Note that this is valid also for any number of components in the FTC connection, not just only for the A and B components as in the example above. But we will limit the analysis here to the ternary mixture and only A and portion of B leaving the top of C1 in the equations presented here. There is an equivalent relation for the lower connection from C1 bottom to C22, but we do not detail this any further.

The minimum vapor for recovering all the light A as a pure product in top of C21, implying that $w_{A,C21} = z_A F$ and $w_{B,C21} = 0$, can be expressed as:

$$V_{T,\min,C21} = f(\phi_{A,C1}) = \frac{\alpha_A z_A}{\alpha_A - \phi_{A,C1}} F \ge \frac{\alpha_A z_A}{\alpha_A - \theta_{A,C1}} F \text{ since } \alpha_A > \phi_{A,C1}$$
$$\ge \theta_{A,C1} > \alpha_B \dots$$
(7)

The implication of this is that the minimum vapor in C21 depends on how C1 is operated, indicated by the actual root ($\phi_{A,C1}$) in C1. The minimum of $V_{T,C21}$ is only obtained when the prefractionator (C1) is operated exactly at minimum vapor conditions, which is characterised by operating points where $\phi_{A,C1} = \theta_{A,C1} = \theta_A$. That is, at the left branch on the "V shape" for a sharp A/C split in the Vmin diagram.

2.5. The optimality region - Preferred split to balanced split

We are now in the position to narrow the operating region of the prefractionator to obtain overall optimality for the standard Petyuk-DWC arrangement. First, we must operate on or above the V-shape between the peaks to get a sharp A/C split. To get minimum energy, operation must be <u>on</u> the V-boundary. We take a closer look at where exactly this is. The left part of the "V-shape" (boundary line between the left peak in the Vmin diagram and the preferred split) is given by using the first common root (θ_A) from the feed equation (2) which is active under the left peak. At the boundary, all light A from the feed is recovered in the top such that $w_A = z_A F$. Thus, the vapor rate varies linearly with the net flow w_B of intermediate component B.

$$V_{T,\min,C1} = \frac{\alpha_A z_A F}{\alpha_A - \theta_{A,C1}} + \frac{\alpha_B w_B}{\alpha_B - \theta_{A,C1}} \text{ for } w_B \text{ in } [0, w_{B,P}]$$
(8)

It is easy to see that the slope is negative for this line since the denominator is $\alpha_B - \theta_A < 0$ (see Appendix). Similarly, the other side of the V-shape, along the boundary line from the preferred split to the rightmost peak, the second Underwood root is active, and we have:

$$V_{T,\min,C1} = \frac{\alpha_A z_A F}{\alpha_A - \theta_{B,C1}} + \frac{\alpha_B w_B}{\alpha_B - \theta_{B,C1}} \text{ for } w_B \text{ in } [w_{B,p}, z_B F]$$
(9)

How to find w_{B_p} at the preferred split: The preferred split is at the point where the lines in (8) and (9) cross. Thus w_{B_p} is found by setting equation (8)=(9) and solving for w_B . With this value we can obtain the preferred split vapor rate $V_{T,\min}^{AB/BC}$ The corresponding net distillate rate is $D_P = z_A F + w_{B_p}$.

How to find $w_{B,b}$ at the balanced split: Above the upper Vmin boundary, none of the common roots are active. But, then the equation for the net distillate is also quite simple since above the V-shape, between the peaks, only the amount of the intermediate B is varying. The actual root can simply be found from the point right over the leftmost peak, for an arbitrary V, and given $D = z_A F$ (all of the A only, in the top product),

$$V_{T,C1\,peak} = \frac{\alpha_A z_A F}{\alpha_A - \phi_{A,C1}} \tag{10}$$

From this we can solve for $\phi_{A,C1}$, and the solutions for how an arbitrary operating point above the V-shape depends on this root (or indirectly the elevated peak sharp A/BC split) are illustrated in Fig. 5. When solving this for the vapor value equal to the rightmost peak ($V_{T,C1,peak} = V_{\min}^{AB/C}$ in Fig. 4), we may find the actual root associated with balanced vapor requirement for the A/BC split and the AB/C split $\phi_{A,C1,b}$. This root gives us the equation for right part of the dashed line in Fig. 4 (from the dashed peak above P_{AB} to the balance point):

$$V_{T,C1} = \frac{\alpha_A z_A F}{\alpha_A - \phi_{A,C1,b}} + \frac{\alpha_B w_B}{\alpha_B - \phi_{A,C1,b}} \text{ for } w_B \text{ in } [0, w_{B,b}]$$
(11)

So, by setting (11)=(9) we may solve for $w_{B,b}$ which is the crossing between the lines these equations represent.

Thus, the optimality region for prefractionator operation for this standard DWC case is characterised by equation (9) for w_B in $[w_{B,p}, w_{B,b}]$ as illustrated in Fig. 4.

In a case where the A/BC split is more demanding than the AB/C split, the optimality region will be mirrored to the other side of the preferred split point.

2.6. Pinch compositions in prefractionator ends

The minimum vapor expressions are closely related to pinch zone behaviour in the column sections of the arrangement. At the preferred split there will be a continuous pinch zone across the feed stage. For operation along the V-shape, there will be a one-sided pinch at the feed stage. In addition, there will be pinch zones towards the ends where the composition profile of the component to be removed is approaching zero. Pinch zones in multicomponent separation are described qualitatively by King [1] and for DWC by Ränger et.al [7]. Underwood [16] presented an expression for pinch compositions dependent on actual roots and net flow rates.

$$\mathbf{x}_{i,pinch,T}^{\phi_k} = \frac{\mathbf{w}_{i,T}}{L_T} \frac{\phi_k}{\alpha_i - \phi_k} \tag{12}$$

From this it can be deduced that the number of theoretical pinch zones equals the number of roots, and thereby the number of components, in each section. Not all are feasible as they may correspond to roots values outside the allowed region from 0 to 1. It is shown by Halvorsen [18] that this pinch composition can be expressed just in terms of the actual Underwood roots and the relative volatilities. In the upper part of the ternary prefractionator herein there will be a pinch zone where only components A and B appear. For this AB pinch composition, we obtain [8,16]:

$$\mathbf{x}_{AP} = \frac{\alpha_B(\alpha_A - \phi_A)}{\phi_A(\alpha_A - \alpha_B)}, \quad \mathbf{x}_{BP} = 1 - \mathbf{x}_{AP} = \frac{\alpha_A(\phi_A - \alpha_B)}{\phi_A(\alpha_A - \alpha_B)}$$
(13)

This relation is quite interesting and implies that this pinch composition varies with the operating condition in the same way as how the actual root varies with the operating condition. That relation is illustrated in Fig. 5, and any contour of constant actual root could be replaced with a contour of a corresponding pinch composition. At minimum vapor conditions, that is under the left-hand peak, in particular on the left branch of the V-shape we have $\phi_A = \theta_A$ and the pinch composition will then be constant (for a given feed) everywhere where this root is active.

$$\mathbf{x}_{AP} = \frac{\alpha_B(\alpha_A - \theta_A)}{\theta_A(\alpha_A - \alpha_B)}, \quad \mathbf{x}_{BP} = 1 - \mathbf{x}_{AP} = \frac{\alpha_A(\theta_A - \alpha_B)}{\theta_A(\alpha_A - \alpha_B)}$$
(14)

In an FTC-DWC operated with both C1 and C21 at minimum vapor



Fig. 6. Equivalent FTC arrangement where the main column is configured as two binary columns.

condition, the pinch zone in top of the prefractionator continues to form the pinch zone at around the connection inside C21 too. As we will show in the following, this composition expression is vital for minimum vapor operation of the LOT configuration too.

3. Minimum vapor rates for liquid-only transfer arrangements

Based on the presented equations for the standard DWC (Petlyuk), we now are in position to check the equivalent minimum vapor performance and operating regions for the liquid only transfer. For simplicity, we compare it to the DWC (Petlyuk) arrangement in Fig. 6 where the main columns (C21 and C22) are assumed to be separate binary columns with pure B-component C21 bottom and C22 top and separate "virtual" C21 reboiler and C22 condenser. This structure also easily identifies the different minimum vapor rates in the upper and lower parts of the main column "rack" when these are specified to run at their local minimum vapor conditions. This arrangement is equivalent to the FTC connection of these two columns using the same vapor rate in the bottom of C21 as in top of C22. In the full LOT-DWC (as shown in the upcoming Fig. 13) the same treatment of the LOT main "rack" columns C2x and C2y can be done (as in the simulation configuration in Fig. 14). This approach allows for detailed treatment of the upper (C1 + C21) and lower parts (C1 + C22) of the DWC arrangements separately. This also becomes handy for the combined FTC and LOT arrangement in Fig. 11.

The prefractionator (C1) conditions are the same and when working with the top conditions of C1, the bottom conditions are trivially given by the mass balance at the feed stage.

3.1. Comparing FTC and LOT in upper part of a DWC

In the following we will deduce the minimum vapor requirement for the liquid-only transfer arrangement in Fig. 7 (b) and compare it to the corresponding fully thermally coupled (FTC) arrangement in Fig. 7 (a). This represents the upper part of the equivalent FTC arrangement in Fig. 6. The lower part will not be treated in detail, but the procedure will be equivalent.

For simplicity we still assume ideal mixtures with constant relative volatility, constant pressure, and constant molar flow rates through sections and infinite number of stages just as in the FTC expressions above. In this limited arrangement we only consider the full recovery of the light A-component in the top product. The prefractionator subcolumn C1 in (b) is assumed to be operated with full recovery of the heavy C in the bottom such that its net flow rate $w_{C,T} = 0$ in the top. The intermediate B is assumed to be distributed to both ends. The prefractionators in the two arrangements are both denoted C1 and are be operated with the same internal flow rates (V_T, L_T), resulting in the same net component flow rates.

The analytical expression for minimum vapor molar flow rate for sharp split of all the light A-component from the feed in the top product of the fully thermally coupled arrangement (Column C21) in Fig. 7(a) is given by the first term in equation (1) as shown in [19]:

$$V_{T,C21,\min} = V_{\min,A/BC} = \frac{\alpha_A z_A}{\alpha_A - \theta_A} F$$
(15)

In the following, we will show the steps in deducing the corresponding minimum vapor expression for the liquid-only transfer configuration in Fig. 7 (b) through the intersection I1 and compare to this expression.

In this process, we will do a tiny adjustment to the drawing of the connection between C1 and C1x as illustrated in Fig. 8.

Imagine for a moment that section C1x is fully thermally coupled on the top of C1. But with the tiny twist that the vapor rate from below the feed stage for this column is zero. Anyway, we can regard this as an FTC connection and use the "carry over Underwood roots" concept. Thus, the "feed" equation for Cx1 is identical to the equation for the actual roots in the top of C1 just as shown in equation (6).



Fig. 7. Upper part of FTC arrangement in Fig. 6 with thermally coupled indirect split columns (with two reboilers and vapor transfer, but no vapor split) (a) and equivalent liquid-only transfer connected columns (with two reboilers, two condensers and no vapor transfer) (b).

$$\underbrace{V_{T,C1} = \sum \frac{\alpha_i w_i}{\alpha_i - \phi_{C1}} = V_{T,Cx} - \underbrace{V_{B,Cx}}_{=0} = \sum \frac{\alpha_i w_i}{\alpha_i - \theta_{C1x}}}_{\text{Feed equation for C1x}}$$
(16)

 $\Rightarrow \theta_{C1x} = \phi_{C1}$

This implies the common roots in C1x, that characterize minimum vapor operation of C1x is the same as the actual roots on the top of C1: $\theta_{C1x} = \phi_{C1}$. This implies further that any suboptimal operation of C1 limits the ability for minimum vapor operation of C1x since $\phi_{i,C1x} \ge \theta_{i,C1} = \phi_{i,C1} \ge \theta_{i,C1}$. Note that this is general, and valid for any number of components. This relation is basic for deduction of minimum vapor expression and form the important first step in obtaining the analytic minimum vapor expression for LOT connections.

For simplicity let us return to the ternary feed mixture. Some basic material balance equations based on the LOT configuration in Fig. 7 can be defined: The vapor flow from C1 is constant all the way to the top since the side draw in C1x (L_s) is saturated liquid.

$$V_{1xT} = V_{1T}$$
 (17)

$$L_{1xT} = L_{1T} + L_{Sx}$$
(18)

The net product flow from C1x is:

$$D_{1x} = V_{1x} - L_{1x} \tag{19}$$

The net flow rates in the top are $D_{1x} = w_{Ax} + w_{Bx}$ and the net flow rates in the LOT stream is $L_{sx} = w_{As} + w_{Bs}$

We use the fact that the set of net flow rates in sub-column C1 is completely determined by the flow rates through the feed stage [18], both for the LOT arrangement and FTC arrangement. Assume here that the operating point of the pre-fractionator has been selected such that no heavy component (C) is appearing in the top of column C1. The vapor rate can be described by Underwood's definition equation (omitting the subscript C1 for these variables).

$$V_{1T} = \frac{\alpha_A w_A}{\alpha_A - \phi_A} + \frac{\alpha_B w_B}{\alpha_B - \phi_A}$$
(20)

The vapor rate through C1x can also be described by Underwoods definition equation expressed via the net component flow rates through the top. And still, it equals the rate from below.

$$V_{1xT} = \frac{\alpha_A w_{Ax}}{\alpha_A - \phi_{A,C1x}} + \frac{\alpha_B w_{Bx}}{\alpha_B - \phi_{A,C1x}} = V_{1T}$$
(21)

From (15), we know something vital about the roots in these two columns, so we have $\phi_{i,C1x} \ge \theta_{i,C1} = \phi_{i,C1} \ge \theta_{i,C1}$, and for minimum energy operation for both we must have equalities such that $\phi_{A,C1x} = \theta_{A,C1x} = \phi_{A,C1} = \theta_{A,C1} = \theta_{A,C1} = \theta_{A,C1} = \theta_{A,C1}$

The liquid side-stream is simply the sum of net flow rates of A and B in the draw:

$$L_{sx} = w_{A,S} + w_{B,S} = w_A - w_{A,x} + w_B - w_{B,x}$$
(22)

These two equations can be solved for the net flow rates to the top as function of L_{sx} . (All the others are given by the fixed operation of C1). There is a particular limiting value of the draw, namely when all the B-component is removed in the draw, and as such does not appear in top of C1x: $w_{B,x} = 0$.

Then, from (21) and using $\phi_{A,C1x} = \theta_A$, the amount of A component out from the top of C1x can be calculated knowing the vapor rate being the same as in the prefractionator C1.

$$V_{1xT,\min} = \frac{\alpha_A w_{A,x}^0}{\alpha_A - \theta_A} = V_{1T,\min} \Rightarrow w_{A,x}^0 = \frac{\alpha_A - \theta_A}{\alpha_A} V_{1T,\min}$$
(23)

The corresponding minimum draw rate for removing all B from the top is determined by:

$$L_{\text{sxmin}} = L_{1xT} - L_{1T} = V_{1T} - w_{A,x}^0 - L_{1T} = w_A - w_{A,x}^0 + w_B$$
(24)

The A-composition of the side stream is then given by looking at the net flow rates in the LOT stream. By substituting the minimum vapor Un-



Fig. 8. Conceptual drawing of connection between C1 and C1x as a full thermal coupling.

derwood expressions, a very interesting relation appears.

$$x_{As} = \frac{w_A - w_{A,x}^0}{w_A - w_{A,x}^0 + w_B} = \frac{w_A - \frac{\alpha_A - \theta_A}{\alpha_A} V_{1T}}{w_A - \frac{\alpha_A - \theta_A}{\alpha_A} V_{1T} + w_B}$$

$$x_{As} = \frac{w_A - \frac{\alpha_A - \theta_A}{\alpha_A} \left(\frac{\alpha_A w_A}{\alpha_A - \theta_A} + \frac{\alpha_B w_B}{\alpha_B - \theta_A}\right)}{w_A - \frac{\alpha_A - \theta_A}{\alpha_A} \left(\frac{\alpha_A w_A}{\alpha_A - \theta_A} + \frac{\alpha_B w_B}{\alpha_B - \theta_A}\right) + w_B}$$

$$x_{As} = \frac{-\alpha_B (\alpha_A - \theta_A)}{\alpha_A (\alpha_B - \theta_A) - \alpha_B (\alpha_A - \theta_A)}$$

$$x_{As} = \frac{\alpha_B (\alpha_A - \theta_A)}{\theta_A (\alpha_A - \alpha_B)}$$
(25)

We recognise this as the pinch composition in top of the prefractionator (C1) in a standard DWC arrangement as shown in (14). This is very interesting and also very natural. It is very important for this deduction that C1 and C1x is operated such that the same root is active in both subcolumns. We will discuss the cases when this is not so in section 3.2.

Here we continue to deduce the overall minimum vapor rates. So step 2 of the LOT minimum vapor expression is to state that at minimum vapor conditions, the composition in the side stream (L_{sx}), which constitutes the saturated liquid feed to the succeeding column C2x, is the same pinch zone composition as in the top of the prefractionator column of the FTC-DWC when operated optimally. Note that this occurs for a particular value of the side draw rate given by equations (23) and (24).

The process to show the minimum vapor of column C2x is now trivial. For a binary split A/B the minimum reflux for a saturated liquid feed is given by the simple King's formula:

$$\frac{L_{\min}}{F} = \frac{1}{\frac{a_A}{a_B} - 1} \quad \Rightarrow \quad \frac{V_{\min}}{F} = \frac{1}{\frac{a_A}{a_B} - 1} + z \tag{26}$$

However, being in the Underwood world we may continue to use his methods and find the common Underwood root from the feed equation to C2x expressed with the compositions in the LOT transfer stream as feed. Assume that this stream is saturated liquid, implying liquid fraction q = 1.

$$\frac{\alpha_A \mathbf{x}_{A,S}}{\alpha_A - \theta_{C2x}} + \frac{\alpha_B \mathbf{x}_{B,S}}{\alpha_B - \theta_{C2x}} = 1 - q = 0$$
(27)

The single common root for this binary system solved from (27) is then found as:

$$\theta_{C2x} = \frac{\alpha_A \alpha_B}{\alpha_A \mathbf{x}_{A,s} + \alpha_B \mathbf{x}_{B,s}} \tag{28}$$

The interesting part is that when inserting the LOT compositions which is found as the A/B pinch sone composition from C1 we get this amazing result when simplifying the expression:

$$\theta_{C2x} = \frac{\alpha_A \alpha_B}{\alpha_A \frac{\alpha_B (\alpha_A - \alpha_B)}{\theta_A (\alpha_A - \alpha_B)} + \alpha_B \frac{\alpha_A (\theta_A - \alpha_B)}{\theta_A (\alpha_A - \alpha_B)}} = \theta_A$$
(29)

This tells us, that for this saturated liquid connection, the Underwood root characterizing the A/B split carry over from the feed to C1, into C1x and further into C2x provided that both C1 and C1x are operated such that the common root θ_A is active. For C21, this implies operating at the left V-branch in the Vmin-diagram and for C1x, that the LOT stream is set at exactly the correct value to remove all B from the top of C1x. This relation can be regarded as the third step in the minimum vapor deduction for LOT arrangements, and since the key Underwood root (θ_A) is active in all of C1, C1x and C2x the calculation of the overall minimum vapor rate becomes straightforward.

Going back to C2x, the minimum vapor for pure A in the top product in C2x can then be written directly by applying the common root and then net flow of the light A component in the LOT stream.

$$V_{T,2x,\min} = \frac{\alpha_A w_{A,S}}{\alpha_A - \theta_A}$$
(30)

When all light A is to be recovered ($w_{A,x} + w_{A,s} = w_A = z_A F$). The minimum total vapor rate through intersection I2 in Fig. 7 is the sum of vapor rates int tops of columns C1x and C2x. Since the active Underwood roots in both sub-columns are the same, this sum becomes very easy to calculate:

$$V_{\min,LOT} = V_{1xTm} + V_{2T\min} = \frac{\alpha_A w_{A,x}}{\alpha_A - \theta_{A,C1x}} + \frac{\alpha_A w_{A,S}}{\alpha_A - \theta_{A,C2x}} = \frac{\alpha_A w_{A,x}}{\alpha_A - \theta_A} + \frac{\alpha_A w_{A,S}}{\alpha_A - \theta_{A,S}}$$
(31)

$$V_{\min,T,LOT} = V_{\min,T,1x} + V_{T2xmin} = \frac{\alpha_A z_A F}{\alpha_A - \theta_A} = V_{\min,T,C21,\min}$$
(32)

Or stated directly as:

By comparing (31) (for the liquid-only transfer arrangement in Fig. 5b) with the corresponding FTC expression in (15) (for the arrangement in

Fig. 5a) we conclude that the minimum vapor expressions for the FTC and LOT arrangements in Fig. 7 are indeed identical. This also imply that the LOT DWC cannot perform with a lower vapor supply than the standard DWC.

A similar procedure can be applied for the lower part of the DWC as illustrated in Fig. 9 where the focus is on the B/C split and recovery of all heavy C from feed into pure bottom products.

The results are equivalent to the upper part, and we find that the minimum vapor expression for the AB/C split equals the height of the rightmost peak in the Vmin diagram.

Similarly, as in the top of C1x, it can be shown that the optimal product rate for pure C in the bottom of column C1y can be calculated, and from that the liquid rates and LOT side-draw at minimum vapor conditions.

$$w_{b1y} = \frac{\theta_B - \alpha_C}{\alpha_C} V_{b1y} \quad , \quad L_{b1y} = V_{b1y} - w_{b1y} , \quad L_{sy} = L_{t1} + F - L_{b1y}$$
(33)

We summarise the steps in this proof:

Step 1:

The common Underwood roots in the section above the LOT draw, (C1x) equals the actual roots in the prefractionator (C1), provided that the draw is set exactly at the limit required to produce pure A in the top of C1x.

Step 2:

The composition in the upper LOT side stream then equals the A/B pinch in top of C1 at the same value as the pinch in the top of C1 in an FTC-DWC operated with the same flow rates in the prefractionator. This pinch can be expressed by the Underwood roots. When the prefractionator is operated such that the common roots are active, this pinch is given by the appropriate common roots.

Step3:

Provided that C1 and C1x are operated such that the common roots are active, the same root will then become the common root in the succeeding LOT connected column (C2x), and thereby the expression for pure A in top of column C1x + C2x will be ruled by the same Underwood roots and the flow rate expressions in these two sections

are easily added up to become the same Underwood expression as in the corresponding FTC-DWC.

3.2. Discussion of the LOT-side stream characteristics

Note that the optimal solution occurs at a particular single operating point for the partial arrangement in Fig. 7, given by the operating point of C1 being at the left branch of the V-shape, <u>and</u> the LOT side draw has to be set exactly at the minimum required for pure light A-component in the top of C1x.

If the side draw is reduced it will imply that the top of C1x is no longer pure, so it does not help that the vapor in top of C2x is reduced too. The purity spec cannot be fulfilled. The extreme limit is reduction to zero and then the top product composition will be given by the net flow rates from the prefractionator and not the above-mentioned pinchcomposition. The maximum value for the side draw is when it equals the vapor from C1. Then C1x will operate on total reflux with zero product. The side stream composition will then also be given by the net flow rates from the prefractionator. This is equivalent with a conventional top condenser on the prefractionator. This may still work in a LOT-DWC if the heavy B/C split (right peak) is significantly more demanding than the A/B split (left peak) [8] (page 124). The lower part may still be FTC or LOT. (E.g. Fig. 4 V and VI in [15]).

What happens if the side draw is increased? Note that we consider the same operating point in C1, so this implies that the top reflux must be increased with the same amount as the LOT side draw. such that the flow rates in C1 remain unchanged. This will also lead to over-purification in the top of C1x, which is another indication of operation above minimum reflux in C1x.

Then two things will happen: This increases the feed to C2s since more of the light A-component is going in the side stream. Further the light A-composition is increased and both these changes are easily seen to increase the load in C2x, e.g. by entering the changes into Kings' formula (26).

The common Underwood root will no longer be active, and the actual root can be found from (23)



Fig. 9. Lower part of FTC arrangement in Fig. 6. Thermally coupled columns (a) and equivalent liquid transfer configuration (b) for the intermediate/heavy split.

$$\phi_{A,C1x} = \alpha_A (1 - \frac{w_{A,x}}{V_{1T,\min}}), \text{ for } w_{Ax} < w_{A,x}^0$$
(34)

Note that this implies that the actual Underwood root in column C1x is different from that in C1. This implies that the LOT composition found to be in the natural A/B pinch in equation (25) is not valid for the suboptimal case with larger than the optimal LOT side stream flow rate. (Note that this is because some of the terms in (25) are from C1 and some from C1x, so the result is only valid when the actual roots in C1x and C1 are equal.)

3.3. The optimality region for LOT-DWC

Compared to the optimality region expressions for a full ternary FTC-DWC, with a Vmin-diagram where the rightmost peak is highest, it is allowed to operate the top of the arrangement somewhat suboptimal until the vapor requirement int the top (related to the A/BC split) is balanced with the minimum requirement for the intermediate/heavy coming from the lower part.

It is clear that if C1 is operated up to the balance point in the Vmindiagram in Fig. 4, given by the actual root in C1 $\phi_A = \phi_{A,b}$ the limiting minimum vapor for full recovery of pure A in the top can be expressed by the same set of equations above, just by replacing θ_A with $\theta_A \leq \phi_A \leq \phi_{A,b}$.

$$w_{A,x}^{0}(\phi_{A}) = \frac{\alpha_{A} - \phi_{A}}{\alpha_{A}} V_{1T}$$
(35)

This value, used in the equation for minimum side draw gives:

$$L_{\rm sx,min}(\phi_A) = w_A - w_{A,x}^0(\phi_A) + w_B$$
(36)

Thus, when C1 is operated such that $\theta_A < \phi_A < \phi_{A,b}$ and the LOT side draw is set by the expression in equations (35) and (36) the actual root ϕ_A will carry over to C1x and also to C2x, and the pinch composition will be given by (13), and the total vapor will be as described by equation (10). This is simply done by replacing the common root θ_A with the actual root ϕ_A in the overall minimum vapor expression.

Thus, the optimality region will in this way be identical to the FTC-DWC as illustrated in Fig. 4. We repeat that the prefractionator must be operated within the optimality region all the time, which for the illustrated case in on the right branch in the Vmin diagram and given by equation (9). In this region, note how the actual root ϕ_A varies as illustrated in Fig. 5. This actual root varies monotonically with the amount of net flow of the intermediate component (B) from the preferred split to the balance point as used in (9). Thus, the range of the optimality region can equivalently be expressed by the range for the actual root: $\theta_A < \phi_A < \phi_{A,b}$.

However, in the LOT arrangement there is another option for "suboptimal" operation of the upper parts of the arrangement by playing with the LOT side stream. Let us look at the two extremes and one intermediate way of operation.

- 1. Operate C1 in Fig. 13 at its preferred split: Then a minimum value for the LOT side draw is given by the common root θ_A . The LOT side stream rate can then be increased until the increased minimum vapor requirement in the upper succeeding column (C2x) equals the lower part.
- 2. Operate column C1 in Fig. 13 at its balance point such that $\phi_A = \phi_{A,b}$. Then there is no further adjustment possibility on the LOT side stream, and it must be set exactly such that $L_{\text{sx,min}}(\phi_A) = L_{\text{sx,min}}(\phi_{A,b})$
- 3. Operate C1 in Fig. 13 within the optimality region, such that $\theta_A < \phi_A < \phi_{A,b}$. Then there will be a remaining adjustment margin for the LOT side draw from $L_{\text{sx,min}}(\phi_A)$ to $L_{\text{sx,min}}(\phi_{A,b})$.

In sum, the flexibility along the optimality region can be shared by

adjustment of the operating point of C1 and, for the remaining margin to the balance point, the LOT side-draw may be increased somewhat above the minimum which depends on the selected C1 operating point.

But these two adjustments policies cannot be used independently since both "share" the same optimality region. We may conclude that with properly set liquid draw rates, operating the prefractionator at the optimality region for an FTC-DWC will enable the same minimum energy consumption in an FTC-DWC and a corresponding LOT-DWC.

In an LOT-DWC the flexibility can in a way be distributed as suboptimal operation of C1x by using an adjustment margin for the LOTstream or use an equivalent adjustment margin for possible suboptimal operation of the prefractionator. But still, it is essential that the prefractionator is operated within the same optimality region as for the FTC-DWC. Otherwise, higher overall energy demand will follow or infeasibility in producing pure products.

3.4. Relation to Agrawal's proof of equivalence between LOT and standard DWC

Agrawal [10,11] shows that by applying the optimal L/V ratio for the upper section of the standard DWC (C21T) to both upper sections of the LOT configuration (C1x, C2x), the column sections will perform the same separation tasks and have identical internal profiles. Thus, the minimum energy is the same as for standard DWC. This is a quite elegant deduction since it also covers not only the case when the DWC is operated at its minimum vapor conditions, but also sub-optimal operating points, e.g. with some heavy C from the top of the prefractionator and other sub-optimal operation of the prefractionator like using higher vapor rate than at the optimality region, and also multicomponent mixtures since the proof only consider bulk net flow rates and not individual components net flow rates. Thus, starting with an optimal DWC operating point, the equivalent LOT-arrangement with the same L/V ratio in each end can be calculated and will of course reach the same overall optimum.

It is straightforward to find the actual L/V ratio by the Underwood equations. When considering sharp A/C (AB/BC) split in the pre-fractionator and pure A the L/V ratio simply becomes:

$$\left(\frac{L}{V}\right)_{C1x} = \left(\frac{L}{V}\right)_{C2x} = \left(\frac{L}{V}\right)_{C21T} = \frac{\frac{\phi_A w_A}{\alpha_A - \phi_A}}{\frac{\alpha_A - \phi_A}{\alpha_A - \phi_A}} = \frac{\phi_{A,C1}}{\alpha_A} > \frac{\theta_A}{\alpha_A}$$
(37)

This implies that having the same L/V ratios implies having the same actual underwood roots. The minimum ratio is obtained when operating the prefractionator at the preferred split such that θ_A is active. For lower C1x L/V ratios, the intermediate B will start to appear in the top. For C1x, it is straightforward to show that this requires the actual root in C1x being: $\phi_{A,C1x} = \phi_{A,C1}$. For this condition there will be a pinch condition around the draw stage, and the draw rate has to be the minimum rate given by equation (36) which has to be the same as deduced by Agrawal for the particular separation an prefractionator operation point. Thus, it all fits together.

As described in the above sub-section, there is an adjustment margin for the upper LOT draw in a LOT-DWC for the illustrated feed case where the AB/C split sets the overall minimum vapor requirement to the DWC. We expressed this by the Underwood roots in the previous section but, by the simple relation by Underwood roots and L/V ratio in (37) it can alternatively be expressed by the L/V ratio. Then we can show that it is not necessary to operate C1x and C2x with the same L/V ratio and the adjustment margins can be described. The adjustment margin starts with the minimum value giving the equal L/V ratio and may be increased until the balance point.

For the given feed case, note that the lower LOT draw rate needs to be set accurately to obtain equal L/V ratio in C1y and bottom of C2y to reach the full savings potential.

The conventional McCabe-Thiele diagram in Fig. 10 can be used to illustrate how the L/V ratio can be found in the upper part of the



Fig. 10. McCabe Thiele diagram for the upper parts where only A and B is present.

standard DWC subsection C21 and also C1x and C2x in the LOT DWC.

The minimum slope of the operating line for all of C21 in a standard DWC or C1x and C2x in a LOT DWC, is determined by the maximum Acomponent pinch composition in the top of the prefractionator. This occurs at the preferred split point (or generally whenever the Underwood root θ_A is active.). Further decrease, e.g. by reducing Lsx in C1x will lead to impure top. The operating line can be seen as using the pinch point as a "hinge" and will rotate downwards reducing the slope as illustrated by the dashed line. An increase in L/V would lead to the operating line rotating downwards around the point [1,1] as a "hinge", and the L/V-line (dash-dot) will not hit the pinch, thus, there will be no pinch around the side draw anymore, even if the C1 is still operated at the preferred split. See case IV in the simulation example in section 5.

For any operating point of C1 from the preferred split to the balance point, the maximum amount of A in the pinch zone in the prefractionator will be reduced until the illustrated balance point. The two operating lines represent the limiting slopes for the operating line for a DWC for the upper parts of the column for the example case presented above in this chapter.

For the LOT DWC, the L/V range gives additional adjustment margins for the LOT transfer rate. This follows since even if the standard DWC is operated at the preferred split, C1x is not required to operate exactly at the minimum L/V ratio but can increase it by extracting some more LOT rate until the L/V in C1x reaches the L/V limit for a balanced main column. This additional adjustment margin for the top column C1 in the prefractionator for our example case can be expressed by

$$\frac{\phi_{Ab}}{\alpha_A} > \left(\frac{L}{V}\right)_{C1x} > \frac{\phi_{A,C1}}{\alpha_A} > \frac{\theta_A}{\alpha_A} \tag{38}$$

This equation states that the L/V ratio in C1x, which is directly deter-

mined by the LOT draw rate, must be between the ratio given by the balance point in the DWC prefractionator (C1), and the ratio given by the actual C1 operation (that determines $\phi_{A,C1}$). Thus, the additional range is largest if C1 is operated at the preferred split but reduces to a single value when it is operated at the balance point.

We repeat that this margin only applies to the upper sections for our feed case in Fig. 4. The lower must be set exact to obtain the same L/V ratios in all bottom sections of both standard and LOT DWC.

3.5. Comparing entropy losses

The expressions for energy savings in a DWC do usually not involve entropy, but rather direct expressions for minimum vapor rate in adiabatic distillation sections, e.g. by using the Underwood equations. However, the potential savings are directly related to reduction of internal entropy losses in the different sections and interconnections.

So where are the losses? First, we have the stage-to-stage mixing losses within so-called adiabatic sections (insulated sections without any heat transfer other than via streams in & out at interconnection points). Then we have the interconnections. E.g. in a direct split arrangement, there is a mixing loss in the reboiler itself since vaporisation of a fluid with compositions x leads to a vapor with the same composition x, while on the equilibrium stage, the equilibrium vapor composition is y = f(x). Thus, we are mixing vapor with composition x into the equilibrium stage with composition y, so there will be a mixing entropy loss. Only for pure components, the vapor and liquid will be in equilibrium with the same composition. In addition, neighbouring stages will also be affected, such that there will be a so-called remixing zone penetrating several stages. This will occur in the bottom of the first column in a direct split arrangement. In addition, the flow rates and profiles are different, so the

total stage-to-stage entropy loss will be different too.

In an optimally operated FTC-DWC, and similarly optimally operated LOT-DWC, it is ensured that there are no mixing losses in the interconnections. For FTC – the interconnecting vapor and liquid streams are in equilibrium and are "mixed" into the same phase state with the same composition. Thus, there will be no entropy loss in mixing flows with different compositions since we "mix" vapor with composition y into a stage with equilibrium vapor composition y, and liquid with composition x into a stage with equilibrium composition x. Similarly, the LOT extracts a liquid in a pinch zone, and the same pinch composition will be present at the succeeding column (mixing saturated liquid stream with composition x with liquid equilibrium stage composition x).

Note that this is not completely true unless C21 + C22 and C2x + C2y are separate columns (see Fig. 14), or there is a heat exchanger at the side draw stage that supplies/removes heat corresponding to vaporisation or condensation of the difference in vapor rate of the two peaks. Normally, in a standard DWC and LOT DWC it is sufficient to ensure equilibrium in the critical connection, that is in the connection between C1 and C21 for the illustrating case where the rightmost peak is the highest. Thus, there is some remixing loss in a standard DWC and a LOT that reduces the 2nd law efficiency slightly, compared to a configuration with the above-mentioned side heat exchanger.

Then, by looking closer at the column profiles, the profiles and total flow rates (again at optimal conditions) are found to be the same, e.g. in column C1, in the top of column C21 in the FTC-DWC and in both C1x and top of C2x in the LOT-DWC. This implies that the inevitable entropy losses from stage-to-stage mixing in the corresponding adiabatic sections will be equal.

The conclusion is simply that when comparing LOT-DWC, and FTC-DWC the internal entropy losses (at optimal operation) are equal and only relates to inevitable adiabatic stage-to-stage losses between pure product end and the same internal pinch composition zones at the interconnections. And, that the LOT transfer streams are set such that the corresponding L/V ratios are the same. Thus, the energy requirement for separation will also be the same for otherwise identical feed and operating conditions.

4. Discussion on some LOT and FTC arrangements

There are several cases where LOT arrangements are applicable. We will not elaborate much in this direction and refer to the comprehensive review papers, where Agrawals group [11] in particular shows a large number of different energy equivalent configurations. Some examples are included here.

Based on the presented results for the arrangement in Fig. 7 we observe that at minimum energy conditions, the composition profiles along column C1x and the top of C2x are identical. So why not join them in the same shell, and join the condensers too? Devising a liquid split in an FTC-DWC is not more complex than with a LOT connection. Thus, a possible combined FTC/LOT-DWC can be arranged as shown in Fig. 11. This requires single pressure operation, while LOT configuration allow for different pressures in C1x and C2x, e.g. in refitting to existing column



Fig. 11. Ternary separation with combined thermal coupling and liquid-only transfer (a) and its DWC equivalent (b).

shells.

The vapor split below the dividing wall is a key to maintain optimal operation of an FTC-DWC. However, in many applications there will be a certain range of split ratio values that ensures that the minimum energy operation is feasible. For some feed mixtures, this range will be small, and the range itself is influenced by changes in feed composition and liquid fraction. Thus, there may be a need to adjust the vapor split ratio for some changed feed conditions, otherwise some of the potential energy savings may be lost, or the column may be unable to produce the designed side stream purity.

There is some reluctance in the industry to implement internal devices for on-line vapor split adjustments. The liquid-only transfer offers a possibility to do additional vapor split adjustments outside the column, directly from the reboiler. Together with adjustment of the LOT stream this gives the same flexibility of operation as adjustable vapor split in an FTC-DWC. Thus, the arrangement in Fig. 11 is a LOT alternative to a FTC arrangement with on-line vapor split adjustment.

The combined full thermal coupling and liquid-only transfer DWC illustrated in Fig. 11 (b) enables total control of the vapor to each side of the dividing wall by the two external reboilers. The number of manipulators allows for sufficient flexibility to ensure that the prefractionator is operated within the optimality region and at the same time control the products to their purity specifications.

It is also possible to combine the two reboilers into a single reboiler with a split vapor outlet equipped with a device to adjust the vapor split to each side of the wall as indicated in Fig. 12. There may even be an opening under the dividing wall such that the liquids from each side can become mixed. This should work fine since the composition profiles along the sections C1y and C2y-bottom should be quite similar when the column separation operation is properly controlled, at least towards the bottom. Note that some care must be taken to ensure individual control of the profiles on each side since there is a mixing effect in the bottom if the liquids in the bottoms are connected.

The key to this is that this can be done with external devices.

The liquid-only transfer can also be used also for cases where the pressures in the succeeding columns are different from the prefractionator. That may be an advantage in special applications where this is found beneficial. That kind of options is not discussed further herein, but in such cases the mechanical design and precautions for larger pressure differences and correspondingly larger temperature differences must be taken into consideration for a possible DWC design or alternative column arrangements. Note that the balance point in the optimality region should be calculated more directly by looking at the minimum vapor rates in the main column rack, C2x and C2y, but the main concept of the optimality region remains the same.

An interesting option is to use two LOT connections as illustrated in Fig. 13. In the DWC realisation (b) the wall goes all the way from the bottom to the top. This may seem a bit peculiar but will have the same



Fig. 12. The two separate reboilers (a) can be replaced by a single reboiler with external vapor split control devices (b).

optimal operation characteristics as for a "classical" DWC. But operation in two parallel shells may be an option, for example in retrofit/revamp of existing units.

Also, for this double LOT-DWC configuration the prefractionator column (C1) must be operated in the same optimality region as for the FTC-DWC.

5. Discussion and simulation

5.1. How to get the minimum solution for real columns

The analytic results are valid for a set of ideal assumptions. However, the key characteristic of the optimal solution is quite general and valid for many zeotropic or even some azeotropic feed mixtures. The key is so look at the basic 3-column system and analyse the first the sloppy AB/BC split for the prefractionator, and then the remaining A/B- and B/C-split can be analysed individually. The system flexibility depends on how different the demands in these two separations are.

Note the importance of the optimality region, and by that the importance of being able to set independently the vapor and liquid rates through the feed stage of the prefractionator. It is crucial that the operation point can be realised within the optimality region. Even in an FTC-DWC with fixed vapor split, it must be selected (by design) such that is possible to get to the optimality region by adjustment of the liquid split. If not, e.g. if the feed composition has changed significantly, minimum energy operation with high purity products is simply not feasible.

Also, for LOT arrangements, feasibility is an issue. If e.g. the reboiler duty below the prefractionator is too low or too high for the actual feed properties, pure products or minimum energy operation is not feasible.

The optimality region may not be straight line segment as for the presented results for an ideal case, but its characteristics is still well defined. The preferred split point is the minimum for separating the light A from the heavy C. The optimality region is from the preferred split and along the branch of the Vmin diagram that represents the boundary when the heavy C is at the limit to appear in the top of the prefractionator. By increasing the prefractionator vapor rate from the preferred split value and adjust the liquid rate to maintain the boundary line condition, the operation moves along the optimality region. The balance point is found when the load in the upper part of the main column leads to the same minimum vapor requirement as in the lower part.

Note that the text above relates to the illustrated cases in the paper where the rightmost peak is highest. For the other cases the argumentation is similar but kind of mirrored in the Vmin-diagram.

The more complicated cases occur when the peaks are similar, because then the optimality region collapse form a line to a point, which is simply to operate the prefractionator exactly at its preferred split.

5.2. Simulator specifications from Vmin-diagram characteristic points

For ideal mixtures, as used in this paper, it is possible to calculate all internal flow rates from the given equations and the mass balances. For a real mixture with a finite number of stages this may still be used as initialisation, but it is obvious that some tweaking of real streams is required.

However, it is not so difficult to specify operation close to the real boundary lines in the Vmin diagrams by specifying the impurity of a component that is about to be removed in a product stream or stage to a "reasonable small value" and use large ("infinite") number of stages [23]. The trick is that "infinite" stages in a typical adiabatic column section does not need to be so "infinite" as the mathematical definition indicates. It is well known in distillation that from specifying a certain separation factor that gives a design product impurity, it is possible to calculate a corresponding minimum number of stages (Nmin). In practice, a real number of stages for an industrial application can be in the



Fig. 13. Double liquid-only transfer connections that can be realised in two separate shells (a) or a single shell with a dividing wall all the way from top to bottom.

ballpark from 2 to 2.5 times Nmin, dependent on balancing the capital and operating costs. Then, "infinite" is simply N = 4-5 times Nmin, when considering the similar impurity specs [24]. Another, more practical way is to ensure the expected pinch regions are clearly observable, and also that adding more stages has little effect on the overall vapor rate (provided that the same product purity and prefractionator operation is applied).

Assume now that we have implemented the LOT-DWC as in Fig. 13 in a simulator, and that the stage numbers are "large" or "infinite" according to the discussion above.

Consider first the "prefractionator rack" consisting of the prefractionator (C1) plus the top and bottom sections (C1x & C1y). This can be regarded as a standard column with the two LOT streams as sidedraws. At constant pressure and given feed there are then four degrees of freedom in operation. We chose the two LOT draw rates (L_{sx} and L_{sy}) and the vapor rates at an intersection immediately above the feed stage (V1T and L1T) to be able to set the prefractionator rates directly. Feasible setting of these variables (such that all internal liquid and vapor rates are positive) will uniquely determine the column operating point. From a control point of view, the vapor rate from the reboiler in C1y and the condenser in C1x are more natural choices and can of course be interchanged with our choice here for the simulations.

The following specifications will give operation at the preferred split and minimum side stream rates:

- 1. Specify composition of component C in top of C1 to a small value Note that this is the composition in the upper LOT side-stream L_{sx} . Ensures operation along the boundary $0-P_{AC}-P_{BC}$ in the Vmindiagram
- 2. Specify composition of A in bottom of C1 to a small value Note that this is the composition in the lower LOT side-stream L_{sy} . Ensures operation along the boundary P_{AB} - P_{AC} - 0^*) in the Vmindiagram
 - The combined solution will determine V1T and L1T exactly at the preferred split P_{AB} .

Further, the LOT-rates is determined to the desired minimum values by:

- 3. Specify top B impurity of C1x to a small value obtains C1x distillate product to be close to pure. This determines the exact L_{sx} rate that gives equal L/V ratios in top section.
- 4. Specify bottom B impurity of C1y to a small value obtains C1y bottom product to be close to pure. This determines the exact L_{sy} rate that gives equal L/V ratios in bottom sections-

Note that specifying the impurities in this way ensures the desired operation point in the Vmin-diagram even for real systems where the boundary lines are not completely straight, and it can be done without calculating any Underwood equations.

Simulation of the main column is even simpler, but a practical trick is to use two separate binary columns for C2x and C2y with two degrees of freedom each. The binary column impurity specs can be:

- 1. Specify composition of B in top of C2x to a small value
- 2. Specify composition of A in bottom of C2x to a small value
- 3. Specify composition of C in top of C2y to a small value
- 4. Specify composition of B in bottom of C2y to a small value

These specifications determine the minimum vapor and liquid rates in each binary column for the actual LOT streams as feeds. This way we clearly observe which part with the highest vapor requirement, and if the LOT rates are changed, when the columns become balanced.

To simulate a single main column, ensure to set the same vapor rate in the bottom of C2x as in the top of C2y. Then one or both ends of the column that get an increased vapor rate will be over-purified in at least one end.

Going back to the prefractionator arrangement consisting of C1y, C1, and C1x. For operation along the optimality region, to the right of the preferred split, simply omit the specification of A impurity in bottom of C1, because that end should now be over purified according to the Vmindiagram concept. This may be obtained simply by specifying prefractionaor vapor rate (V1T) to a value higher than at the preferred split. The LOT streams will also be altered, but with clearly different behaviour. The lower (for our type of case) will be adjusted to maintain the same L/V ratio in C1y, and unchanged composition. The upper will need to be adjusted to maintain operation at the top B-impurity, the the LOT composition will change, as the pinch composition tin the top of the prefractionator will change. Observe also how this mode affects the main column(s). At a specific value of the vapor rate in the prefractionator, the main columns become "balanced" which can be seen directly when the duty in the virtual condenser of C2y equals the virtual reboiler of C2x. For real systems, this is a more direct way of finding the balance point, than calculating via Underwood roots from C1.

The other mode of sub-optimal operation is to increase the upper LOT side stream, which implies that the top of C1x is over purified. (Just remove that spec, and replace with LOT flow rate specification which is higher than the minimum to keep the exact B-impurity specification.) This also implies that the L/V ratios of C1x and C2x top will become different and there will not be pinch zone around the draw stage.

The interesting thing is that similar adjustment *cannot* be done for the bottom LOT-stream for our case (when the rightmost peak is highest in Vmin diagram). The reason is that then the optimality in the lower connection will be violated, and the total vapor rate from both reboilers will have to increase to fulfil product purity specifications.

Thus, for the given case characteristic, there are only two manipulative variables that may be adjusted while still being in the optimality region and, that is the prefractionator vapor rate, and the upper LOT rate.

Note that we only discuss (close to) infinite number of stages here. Methods for more detailed design and optimisation can be added, but the above-described scenarios are the keys to understanding optimal operation of this plain ternary LOT-DWC arrangement.

5.3. Rigorous simulation example

A very common DWC case study is separation of Benzene, Toluene and p-Xylene (BTX). The equimolar feed case at 1 bar and saturated liquid is used as the illustrating example in [7,25]. An Aspen Hysys V14 process flow sheet is shown in Fig. 14. It has the same energy requirement as a standard DWC (and also the equivalent standard DWC with virtual reboiler and condenser in C21 and C22 respectively as in Fig. 6). The NTRL thermodynamic package is used.

In a LOT-DWC implementation, the main column is joined, removing condenser in top of C2y and reboiler in C2x. In this case study there are 88 stages in the prefractionator rack C1xy (ref to C1 + C1x and C1y in Fig. 13), and 44 in each of C2x and C2y. The number of stages from top to bottom in each"rack" is chosen as 88 which is approximately as 4 times Nmin(=22), obtained for product impurity specification at 1 % and the relative volatilities at the feed stage. Then this simulation setup will be close to the infinite stage case for purity specifications in the simulation in that ballpark. The LOT streams are drawn from stage 22 and 66 respectively. The state in the figure above is for the preferred split operation, and minimum LOT-streams, thus representing an overall minimum vapor condition for the arrangement.

The relative volatility from the K-values at the feed stage is used to calculate the Vmin-diagram shown in Fig. 15 using the Underwood equation described in the theory section above. Note the important preferred split point and the balance point that is found along the V-shape when the power demand in the reboiler of C2x equals the condenser duty of C2y.

The three marked points ($\langle \rangle + o \rangle$) are the result of the simulator solution with the appropriate combination of impurity and flow specifications for the prefractionator. This shows in practice that this BTX case behaves very close to the ideal mixture with constant relative volatilities and constant molar flows. We present a set of five simulation cases as shown in Table 1.

First, the composition profiles for the prefractionator rack are shown in Fig. 16 for cases I, II and III. For each case the prefractionator is operated at the three pints on the optimality region (\Diamond), (+), (o). The LOT streams are set to achieve the specified small (here 0.5 %) Toluene impurity specification in C1x top, determining L_{sx}, and bottom of C1y, determining L_{sy}. This leads implicitly to exact LOT-values that ensure that the B-component is at the limit of being removed in top and bottom and result in equal L/V ratios in the tops of C1x and C2x and similarly in C1y and bottom of C2y. The rates will of course be different in each case, but the values are calculated to the actual minimum for each case. We might use the analytical expressions from section 3 for this, but the use of impurity specification in the simulator ensures correct values also for real (fairly ideal) mixtures.

The preferred split operation can be recognised by the pinch zone extending across the feed stage in case (I) (solid curves).

Note that all profiles approach nicely to zero and one at each outlet stage, that is both in top and bottom and to the LOT-draws. The LOT draws are from clearly visible pinch zones, as described theoretically above. The clear extent of the pinch zones also indicates that the number of stages is reasonable for getting close to infinite stage results in the simulation [25].

A key indicator of optimal operation is the behaviour in the lower part since the profiles overlap, also in the top of the prefractionator, the heavy C is just at the limit of appearing (no waste of vapor for overpurification). This is so for all cases where the intermediate/heavy peak in the Vmin-diagram is highest. Note that for all cases the composition profile from the lower LOT pass through the same molar fraction, indicating the same feed composition to the lower main column C2y. Although the LOT rate will vary since the boilup is varying along the V-shape in these three cases, the sum of vapor in the prefractionator rack (C1y) and the main column bottom (C2y) will remain the same!

For these three cases, a standard-DWC prefractionator will have exactly equal profiles for column C1 (between the LOT draws, stage

SPRDSHT-1		
Sum condensers	22,06	kW
Sum reboilers	35,63	kW
Inbalance Main Bottom-Top	11,86	kW

Fig. 14. Hysys PFD for LOT configuration. The main column is represented as two separate conventional columns to visualize the differences in load demand in C2x and C2y.

Fig. 15. Vmin diagram for equimolar BTX feed at 3 kmol/h, 1 bar, saturated liquid. Relative volatilities are 5.79, 2.31, 1 referred to the heavy p-Xylene key (X). The preferred split point is calculated as V = 1.901, D = 1.274. Preferred split used in simulation is marked with "diamond" (\Diamond) at V = 1.888. Note also the balance point (circle) at V = 2.83 and the intermediate (+) at V = 2.30. The optimality region is on the V-shape between the preferred split and the balance point.

22-66).

In the upper part (left) it can be observe that the composition of the draw stage will change. This change will lead to increased demand in the upper part of the main rack, column C2x, up to the balance point. Any further increase would lead to operation outside the optimality region which leads to increased overall duty requirements. But a very important observation is that for all cases, the upper LOT draw is in a pinch zone, also as described in the theory above.

The next examples are cases IV and V and the prefractionator profiles is illustrated in Fig. 17.

Table 1

Overall	description	of	simulation	cases	– all	within	optimality	region	for	C1
(Fig. 15).									

Case	C1 – operation/ specifications	Lsx operation/ specification	Lsy operation/ specification	Overall DWC Duty
Ι	Preferred split (\Diamond)	Minimal at (\Diamond)	Minimal at (\diamondsuit)	Minimal
	L_{sx} -C-imp = 0.5 % L_{sy} -A-imp = 0.5 %	Top-B-imp = 0.5 %	Bot-B-imp = 0.5 %	
II	Prefbalanced (+)	Minimal at (+)	Minimal (same as ◊)	Minimal
	$L_{sx}-C-imp = 0.5$ % V1T - 2.30	Top-B-imp = 0.5 %	Bot-B-imp = 0.5 %	
III	Balanced (o)	Minimal at (o)	Minimal (same as ◊)	Minimal
	L_{sx} -C-imp = 0.5 % V1T = 2.83	Top-B-imp = 0.5 %	Bot-B-imp = 0.5 %	
IV	Prefbalanced (+) L_{sx} -C-imp = 0.5 % V1T - 2.30	Fixed > minimal Top-B-imp ≪0.5 %	Minimal (same as \diamond) Bot-B-imp = 0.5 $\%$	Minimal
v	Preferred split (\Diamond)	Minimal at (\diamondsuit)	Fixed > minimal	Higher (not optimal)
	L_{sx} -C-imp = 0.5 % L_{sy} -A-imp = 0.5 %	Top-B-imp = 0.5 %	Bot-B-imp ≪0.5 %	

First case IV. Consider first the prefractionator (C1) operated at the intermediate point between preferred and balanced split as in case II. Then we increase the upper LOT draw to a constant value. We keep the prefractionator rates constant, so this extra draw rate requires the same amount of extra reflux in top of C1x and the same reduction in distillate product in top of C1x. Thus, the top of C1x will be over-refluxed, and thereby over-purified as indicated by the B-composition profile going to zero very early and far from the top. The draw is no longer from a pinch zone as the profile changes rapidly across the draw stage, and the

Fig. 16. Composition profiles for the prefractionator rack for case I (solid), II (dashed) and III (++). The components are intuitive as Benzene is pure in top and goes to zero in bottom (right). It is opposite for the heavy P-Xylene, and the intermediate Toluene does not appear pure, but is removed from both top and bottom. The LOT draw stage points are indicated by 'o' and will become feed composition to C2x and C2y, respectively.

Fig. 17. Composition profiles for case IV (dashed) and case V (dash-dot). Case I (solid) is included as reference.

profiles in C1x and top of C2y are now different and so are also the L/V ratios. However, in the bottom, the profiles coincide with the optimal profile as for cases I, III and III. So, even with this peculiar behaviour in the upper part, the lower part, that is most important for optimal operation remains constant, and the overall vapor demand in the LOT-DWC is still at its minimum.

In case V, we assume starting from the optimal case I. The prefractionator is obviously within the optimality region. But then we increase the lower LOT stream from its optimal value of 1.197 to 1.50. This has dramatic effect since there is an obvious change in the lower LOT draw composition too. This will lead to increased reboiler duty in C2y and the overall DWC operation is not optimal anymore. We can also clearly observe that the bottom of C2y becomes over-purified.

These simulations clearly confirm that the lower LOT side draw must be precisely adjusted on-line such that there is no over-purification in the bottom of the prefractionator rack. While (for this class of Vmindiagram shape) there is a certain adjustment margin for the prefractionator as for the standard DWC and in addition there is a margin for the upper LOT draw rate. The total margin depends on the difference between the peaks in the Vmin-diagram.

For completeness, the profiles for C2x (left) and C2y (right) is shown combined in Fig. 18. Note that the optimal cases (I, II, III, IV) overlap in C2x, indicating the same performance, while in the sub-optimal case V (++) the profile in C2x differ. For all cases the impurity specifications on both ends of C2x and C2y are set to 0.5 %, and the solver then calculates minimum vapor rates and the corresponding profiles.

Note that impurity specifications as described above are used to get the preferred split solution in the simulator.

In the prefractionator rack there are 4 degrees of freedom, and the caption in Fig. 19 shows the active specs for case I and the calculated Actual Values shows the solution for the four manipulated variables. The preferred split in C1 requires "small" impurity specification values of the heavy key (C: p-Xylene) in top of C1 and light key (A: Benzene) in the bottom, which are at the LOT draw-stream positions for the LOT configuration. Here a fraction of 0.005 (0.5 %) is used as the "small" value. Similarly for pure top and bottom, a small value of the

Fig. 18. Composition profiles in the main rack for all cases. I (solid), III(dashed), III(dash-dot), IV(dotted) and, V(++). I-IV has same reboiler duty, V is not optimal and has higher. All products are pure.

Variable	Specified values	Actual values	Deviation	Active	
Lsx Rate	1,146 kgmole/h	0,4768	-0,5839		
Lsy Rate	1,500 kgmole/h	1,197	-0,2017		
V1T	2,300 kgmole/h	1,888	-0,1792		
L1T	0,6172 kgmole/h	0,6172	0,0001		
Top-B-Imp	5,000e-003	5,000e-003	-0,0000	V	
Lsx-C-imp	5,000e-003	5,000e-003	-0,0000	$\mathbf{\nabla}$	
Lsy-A-imp	5,000e-003	4,990e-003	-0,0008	\checkmark	
Bot-B-imp	5,000e-003	5,000e-003	0,0000	\checkmark	

Fig. 19. Caption of Hysys solver specifications for the prefractionator rack.

intermediate (B: Toluene). The solver calculates all streams. V1T and L1T are at the intersection of the feed stage and the stage above.

For case II and III, we may adjust the vapor rate directly but only give up the small value of the light impurity in the bottom of the prefractionator, and this automatically gives the operation points along the V-shape to the balance point. Both LOT streams and L1T are calculated and will vary.

For increasing the LOT streams, the impurity specification of the corresponding end must be turned off. (Alternatively, the same is obtained by specifying these impurities to be "very, very small" and let the solver calculate the streams.).

Note that the simulation with 4*Nmin stages represents close to the "infinite stage" case. For real columns the factor is the ballpark of 2–2.5 times Nmin. As a result, when using more typical design numbers, the extent of the pinch-zones will be reduced, and not so obvious observable as in the presented simulation. But the same methods of analysis may be applied, although by some tweaking of how to define "a small impurity value". More advanced sizing calculations using costing of equipment and utilities will give more precise numbers, but that is not considered here.

5.4. Control structure issues

Control of a DWC may look somewhat overwhelming but the key task is to control the product purities to the required specifications, and in addition maintain operation close to minimum energy conditions. The latter implies keeping the prefractionator operation within the optimality region, and, not to forget, not over-purifying any of the final products as it does not help keeping the prefractionator optimal if the main column is supplied with higher vapor rate than required.

In the (double) LOT configuration in Fig. 13 there are the two extra top and bottom products from the LOT prefractionator rack (C1x, C1y), such that there are in total five product outlets as opposed to three for a standard DWC. But there are also an extra reboiler and condenser for control manipulation in the prefractionator rack. Common for both is the requirement to control the prefractionator operating point, and two manipulator variables are required for that. This may be relaxed to one, but then it must be ensured that the vapor rate through C1 is set such that operation within the optimality region is feasible by manipulating the liquid rate (or vice versa). The vapor and liquid splits for a standard DWC is replaced by two side-draws in the LOT-DWC, thus the number of manipulative variables is sufficient for both controlling the vital prefractionator operating point, and the product purities. And importantly, there is no need for internal vapor split manipulation.

The fact that the standard DWC is a 5 by 5 system (5 manipulators by 5 specifications) while the LOT-DWC is a 7 by 7 system, this might indicate higher complexity for LOT-DWC. However, there is no interaction upstream from the main column rack (C2x + C2y) to the pre-fractionator rack (C1x + C1 + C1y) as opposed to the standard DWC where the liquid and vapor splits affects both sides of the dividing wall. Thus, the LOT arrangement may be regarded as a 4 by 4 prefractionator "rack" with a separate downstream 3 by 3 main column "rack", so from this viewpoint, control may become simpler. As mentioned in the steady-state simulation study, it is possible to reduce the LOT prefractionator to a 2 by 2 system by fixing the vapor rate (within a region) and the top side draw (within a region) and still run optimally (but less

prepared for changes in the feed properties). The latter correspond to fixing the vapor split in a standard DWC which reduces that from a 5 by 5 to a 4 by 4 system. For both arrangements it is also possible to fix the overall reboiler duty and thereby reduce the interaction complexity further, but then at a cost of reduction of energy savings since the duty must be set high enough to give sufficient bottom purity for the expected (small) feed property variations that the column must handle.

The steady-state simulation study above clearly shows the type of operation targets to be used to obtain optimal operation. More detailed control studies are needed to evaluate controllability and finding good control structures with respect to dynamic control performance. What kind of measurements that are available also plays an important role. In distillation it is common to use feedback from key temperature measurements for stabilisation and disturbance rejection as described by Skogestad (2007) [24]. This will be applicable for DWC columns too. If composition measurements are available, these may be used to adjust temperature profile points reference values, rather than for direct manipulation of flow rates. The guidelines in [24] can also be applied when looking at how to control each sub-column in the arrangements with respect to the local specifications within each. We will not discuss control in more detail, but just state that to handle variations in feed properties and manipulator uncertainties it is needed to use a feedback control structure that is able to capture the key properties of the profiles.

6. Conclusion

Based on the assumptions of ideal ternary mixtures, it is shown analytically using the Underwood equations that the liquid-only transfer (LOT) structure has the same minimum vapor requirement as the fully thermally coupled structure (FTC). The proof is different from that in Agrawal [12]. In addition, for a ternary mixture the ternary LOT-DWC has the same optimality region for prefractionator operation as for the standard DWC. This is so also for combined LOT and FTC in the same arrangement. The solutions for minimum vapor and the required operation region for the LOT arrangement can be visualised in the Vmin diagram just as for the classical FTC-DWC. A simulation example is used to illustrate the key factors that must be in place for reaching minimum energy operation in practice. The analysis also shows that the LOT-DWC cannot outperform the standard DWC, but it may have exactly the same minimum vapor requirements, not more, not less, for the assumptions and conditions used.

A new result, is that there usually is an adjustment margin for one of the LOT draws, thus, the minimum reboiler duty for a LOT DWC can be reached even if the liquid/vapor ratio is somewhat different from the corresponding optimal ratio in standard DWC. There is also an adjustment margin for the two distillate ends in the LOT-configuration. The results can also be used for precise initialisation of rigorous simulations on many real zeotropic mixtures.

CRediT authorship contribution statement

Ivar J. Halvorsen: Conceptualization, Methodology, Writing – original draft, Writing – review & editing. **Sigurd Skogestad:** Conceptualization, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Underwood's equations basics

A brief description of the use of Underwood equations with the application to fully thermally connected column sections is given herein [16,18]. In the following it is assumed an ideal mixture with constant relative volatilities, constant molar flow rates, constant pressure, and infinite number of stages.

The Underwood roots above (subscript T) and below (subscript B) the feed stage of a two-product column are defined as the solutions of ϕ and ψ , respectively for these so-called definition equations:

$$V_T = \sum_i \frac{\alpha_i w_{i,T}}{\alpha_i - \phi} \quad , \quad V_B = \sum_i \frac{\alpha_i (-w_{i,B})}{\alpha_i - \psi} \tag{39}$$

The section vapor rates V, the net components rates w_i and relative volatilities α_i are given. The relative volatility $\alpha_{i,j} = K_i/K_j$ is the ratio of K-values $(K_i = y_i/x_i)$ for a component (i) relative to component (j). Here we use the heavy key component as common reference and omit the second subscript. The net component flow rate is defined as the net transport of a component through a cross-section between stage n and n + 1 (counted from the top).

$$w_i = V_n y_{i,n} - L_{n-1} x_{i,n-1} \tag{40}$$

The positive direction is defined upwards, and this explains the negative sign in the equation for V_B since the net flow rates below the feed stage are (normally) downwards. Note that the net component flow rate is constant anywhere in an adiabatic column section even without the simplifying assumptions of ideal mixtures and constant molar flow rates. With the assumption of constant molar flow rates, the stage number (n) can be removed from these; $w_i = Vy_{i,n} - Lx_{i,n-1}$ or just use a subscript to define what section it is valid for, e.g.: $w_{i,T} = V_T y_{i,n} - L_T x_{i,n-1}$ where subscript T denotes a top (or rectifying) section.

Note that Underwood's definition equations are valid at any cross-section in a distillation column, thus, the Underwood roots can be calculated for real mixtures in real columns too. But then the roots will vary along the section and some "book-keeping" is required for appropriate use. In the following we apply the simplifying assumptions, and then the roots are also constant in each column section.

The roots solved from the definition equations are denoted "actual" roots. The number of roots depends on the number of components. Underwood showed that at minimum vapor rate, there will be a pinch zone around the feed and pairs of the roots in the top and bottom will coincide to a common root θ that can be solved from the so-called feed equation:

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$$V_T - V_B = \sum_i \frac{\alpha_i(w_{i,T} - w_{i,B})}{\alpha_i - \theta} = \sum_i \frac{\alpha_i z_i F}{\alpha_i - \theta} = (1 - q_f) F$$

$$\tag{41}$$

Here, the mass balance around the feed has been used to introduce the feed composition:

$$w_{i,T} - w_{i,B} = w_{i,F} = z_i F$$
 (42)

The solutions for the common Underwood roots depends only on feed properties and can be solved from (41). The solutions obey:

$$\alpha_A > \phi_A \ge \theta_A \ge \psi_A > \alpha_B > \phi_B \ge \theta_B \ge \psi_B > \alpha_C \dots \tag{43}$$

Note the distinction of the actual roots (ϕ, ψ) in the definition equations (39) and the common roots, (θ) from the feed equation (41). A common root θ_i is said to be active when the corresponding roots in the definition equations coincide to a common root $\phi_i = \theta_i = \psi_i$. This condition is the property of a minimum vapor rate solution and is uniquely related to a certain distribution of the feed components to the product streams. (Strictly, the inequality in (43) require all component flow rates to be positive in the top, which is always fulfilled in a conventional binary column. With fully thermally coupled sections, "reverse" rates may occur thus, care must be taken to ensure correct interpretation and usage of Underwood equations.)

Note that to calculate an operating condition for a binary column two independent (and feasible) specifications are needed. Thus, the term minimum vapor is not a single solution point but is a function of the required operation. However, when specifying for example two key component recoveries in the products, there will be a unique operating point where the product rates, internal flow rates and all component recoveries are determined. If then, e.g. the internal vapor and liquid rates are increased, the original specifications will become "over-fulfilled", indicating waste of energy (heating & cooling utilities).

By using the mass balance for the total flow rates, it is straightforward to express the liquid rates:

$$L_{T} = V_{T} - \sum w_{i,T} = \sum_{i} \frac{\phi w_{i,T}}{\alpha_{i} - \phi} \quad , \quad L_{B} = V_{B} + \sum_{i} (-w_{i,B}) = \sum_{i} \frac{\psi(-w_{i,B})}{\alpha_{i} - \psi}$$
(44)

The usage of the Underwood equations usually starts with finding the common roots (θ) from the feed equation (41). The key to calculate column solutions is to know when these roots can be applied in the definition equations and from that solve for flow rates and net component rates. The Vmindiagram can be used to illustrate this quite directly. In each boundary region, a particular set is active, and at the boundary line a certain root is at the limit of becoming active/inactive and that also corresponds to that a feed component is at the limit of appear/disappear in one of the column ends. More detailed explanations of usage of the Underwood equations for column calculations are given in [8,18] or for the curious reader, in Underwood's original papers from the 1940s. It is amazing what he could do without even the simplest computers.

Data availability

No data was used for the research described in the article.

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