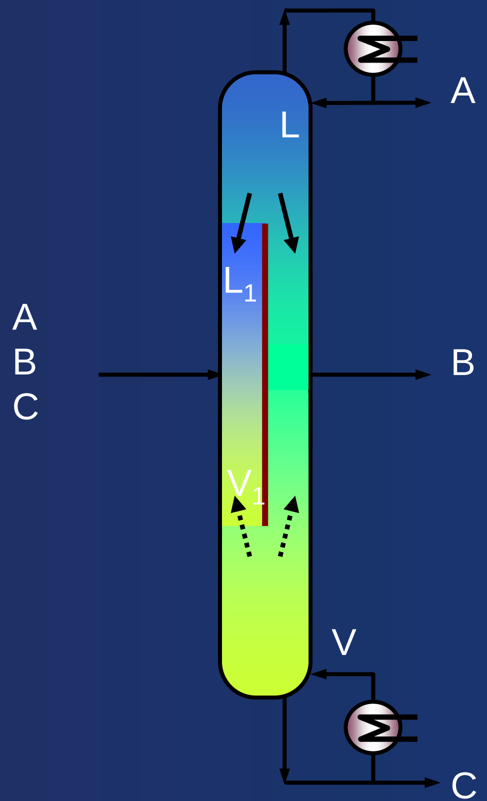
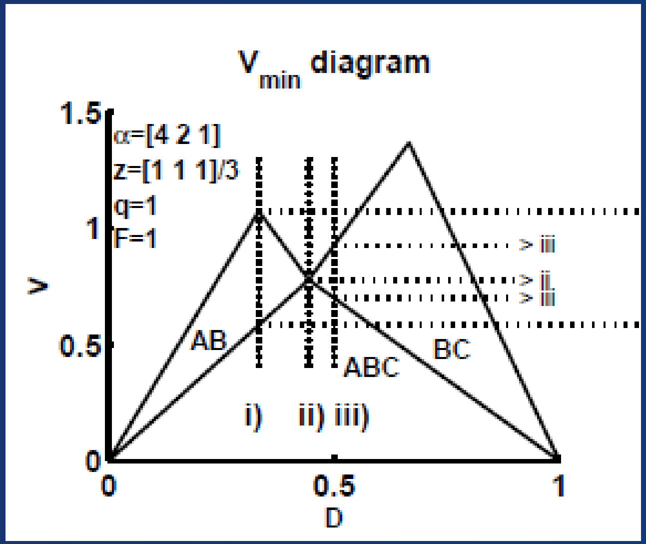
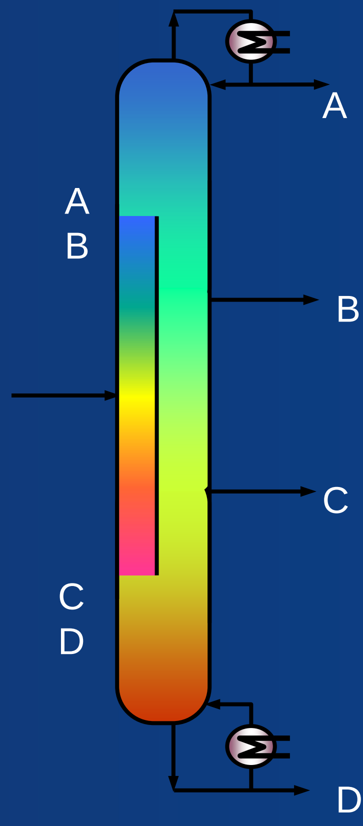
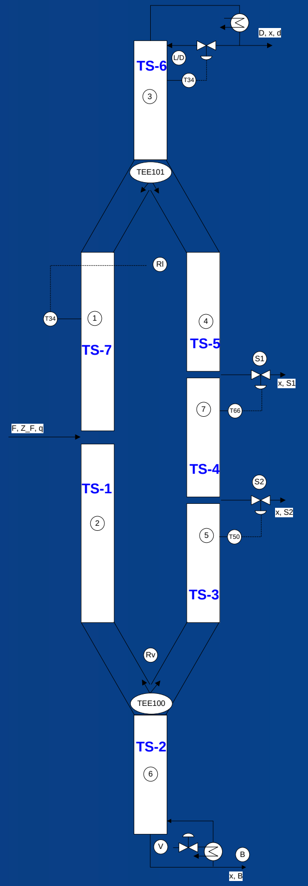








DWC Workshop – NTNU Trondheim – 5-6. October 2023

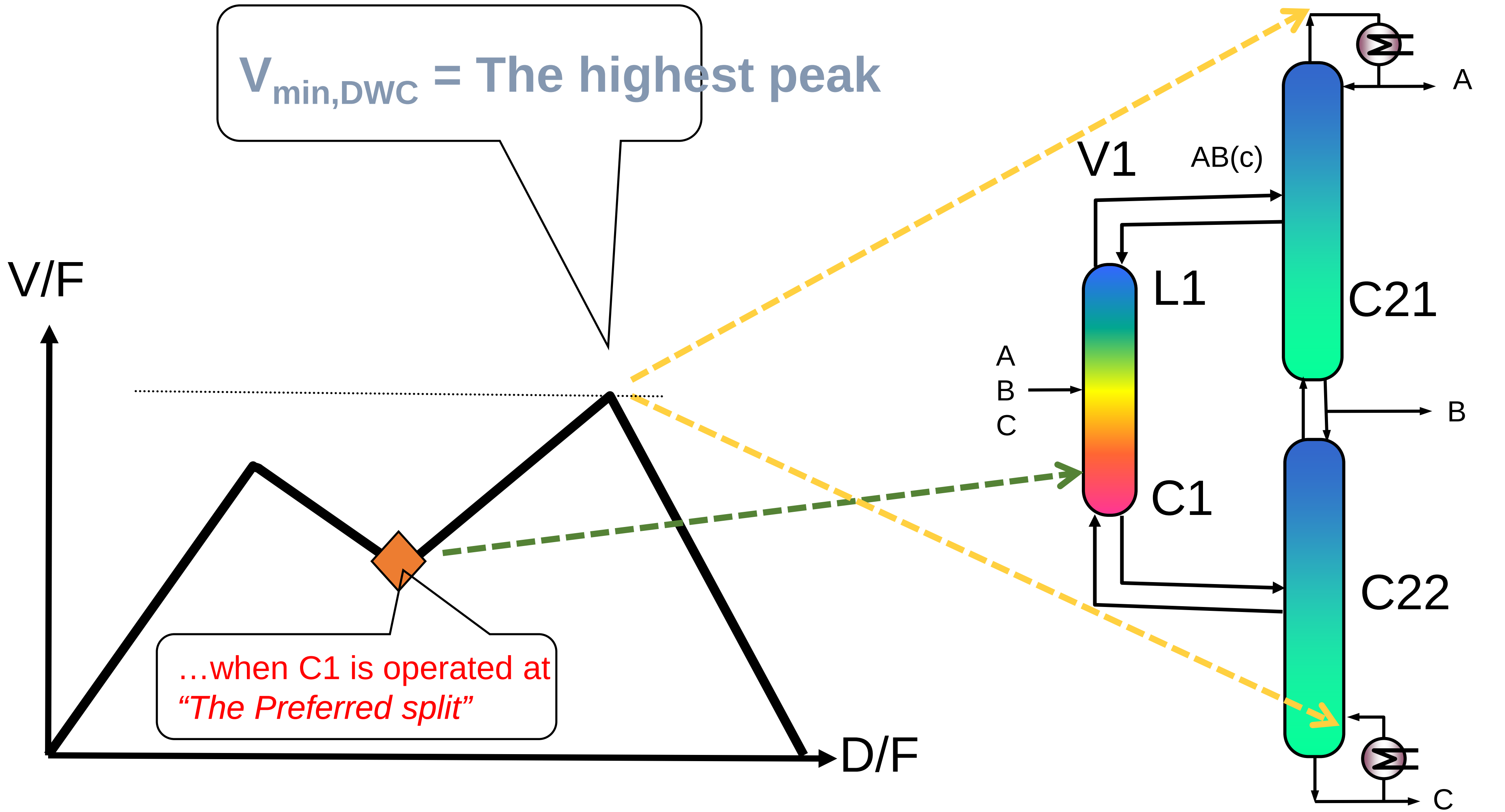
New (or at least not well known) results on the Vmin method

Ivar J. Halvorsen

Content

- Non-sharp split specifications
- Explaining Vmin by pinches – connect the theory to real column behavior – McCabe-Thiele-King
- Reversible DWC columns
- What happens when operating prefractionator outside the V-shaped region (Lena)

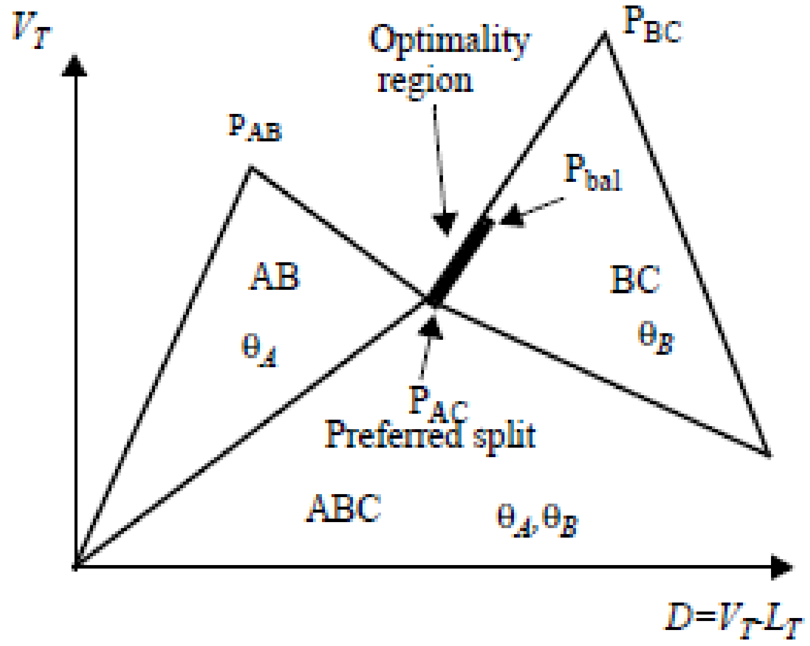
The V_{min}-diagram contains – optimal DWC flow rates



Minimum energy (Vapor flow rate V)

$$V_{min} = f(Splits, Feed, Specs)$$

- Sharp splits: Flat optimum at a line segment (optimality region)
- Optimality region depends on feed properties
- Rapid increased vapor flow outside optimality region



Minimum energy-
Definitions and assumptions

- Vapour flow rate (V) generated from all reboilers is used as the energy measure
- Ideal Assumptions
  - Infinite number of stages
  - Constant relative volatility
  - Constant molar flow
  - Constant pressure
  - No internal heat exchange
- Then, exact analytic solution can be obtained

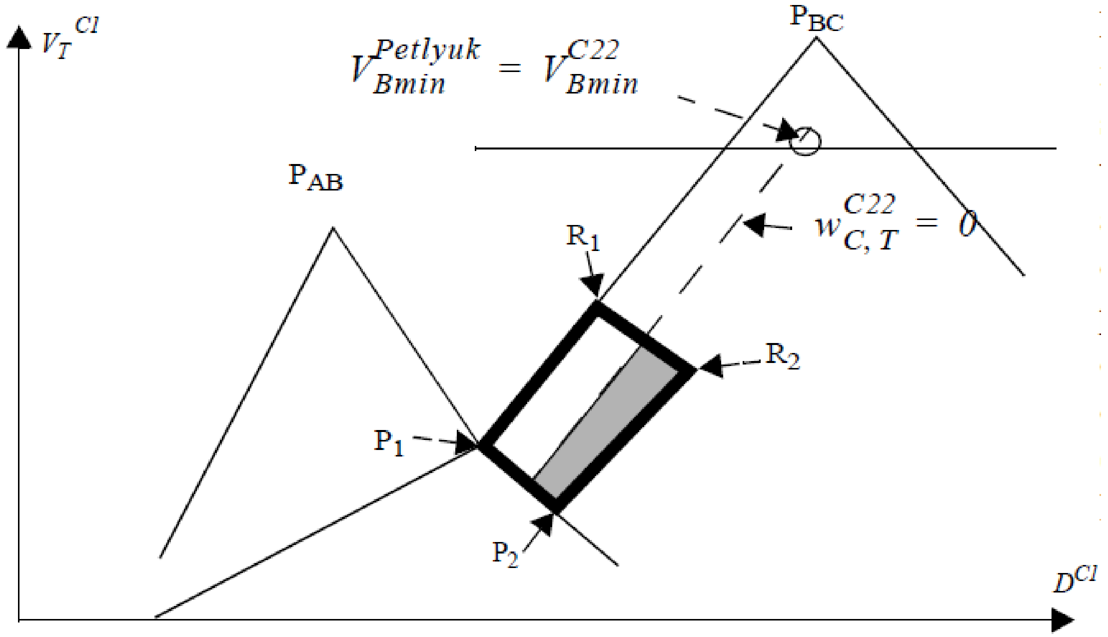
Nonsharp splits

- Sometimes the purity requirements are relaxed
- Sometimes high purity is difficult to obtain

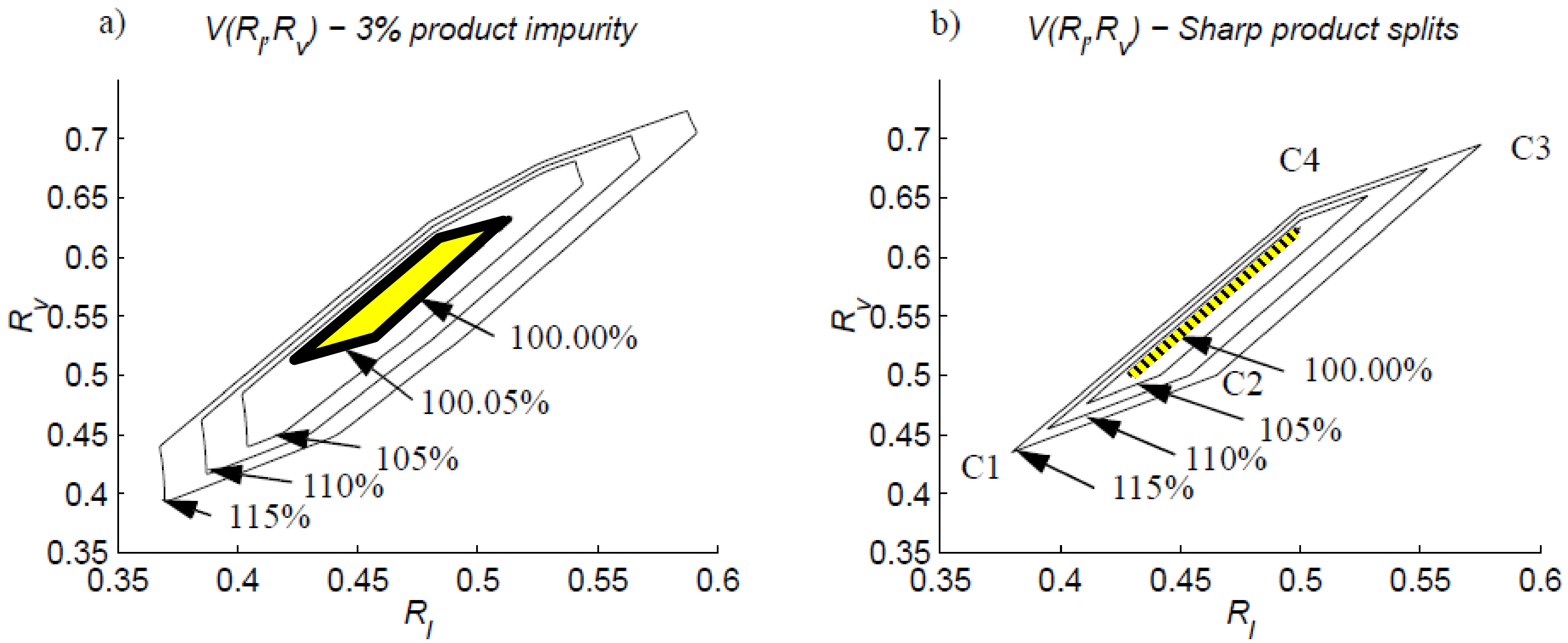
- How does the Petlyuk column behave

Optimality region – nonsharp splits

- The line segment (PR) opens up to become a quadradangle



Impure sidestream spec results in a wider optimality region



Actual simulations on a stage-by-stage model

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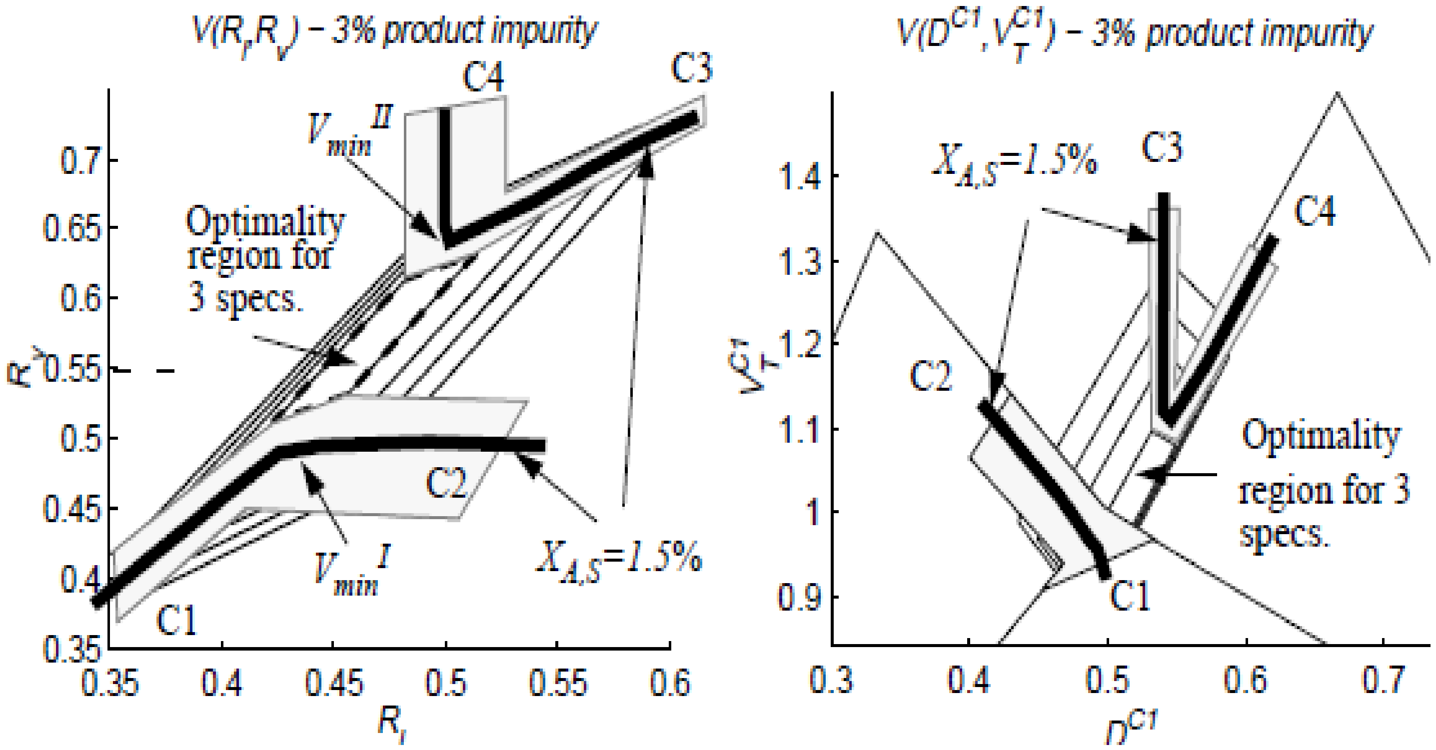
Explanation of the "holes" in the operating region with two side impurities

- Two side-impurities can only occur in the corners of the optimality region
- This is always outside the optimality region with one spec.
- And, the possible soluions will be curves on the 3D solution surfave.
- E.g. No solution for Rv=0.5-0.65 in the figure



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Nonsharp split - details

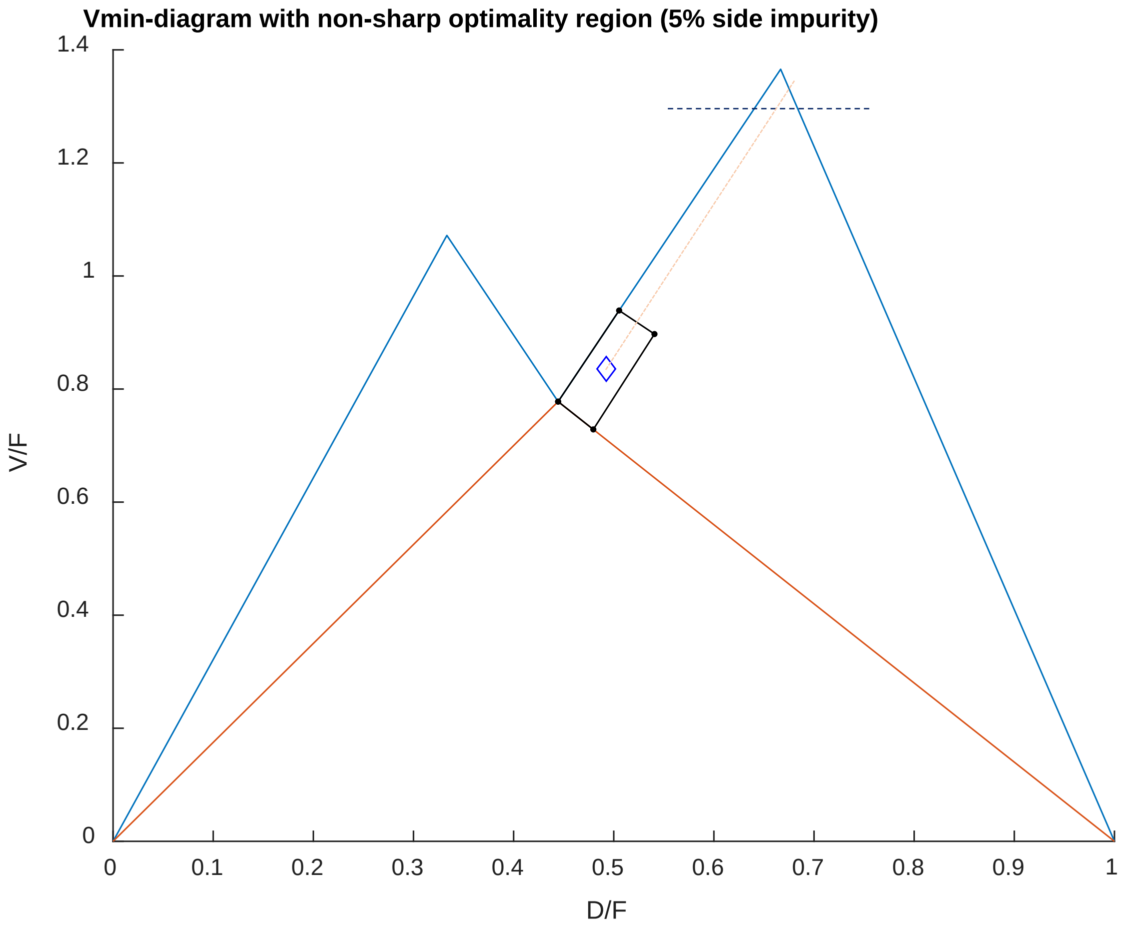
- Only the sidestream impurity opens the otptimality region from a line segment to a quadradangle.
  - Inpurity in top and bottom just moves the line segment a bit
- The impurity component of the side-stream is determined by the highest Vmin-peak:
  - Case 1: Only heavy C (when the B/C split determines Vmin)
  - Case 3: Only light A (when the A/B split detemines Vmin)
  - Case 2: When A/B split is similar to B/C, optimum is found for a given ratio of A- and C impurity in the side-stream
- Warning: Do not specify a give A/C ratio in the sidestream! There are two solutions, and for wrong splits, there may be no solution at all.

Nonsharp split – details 2

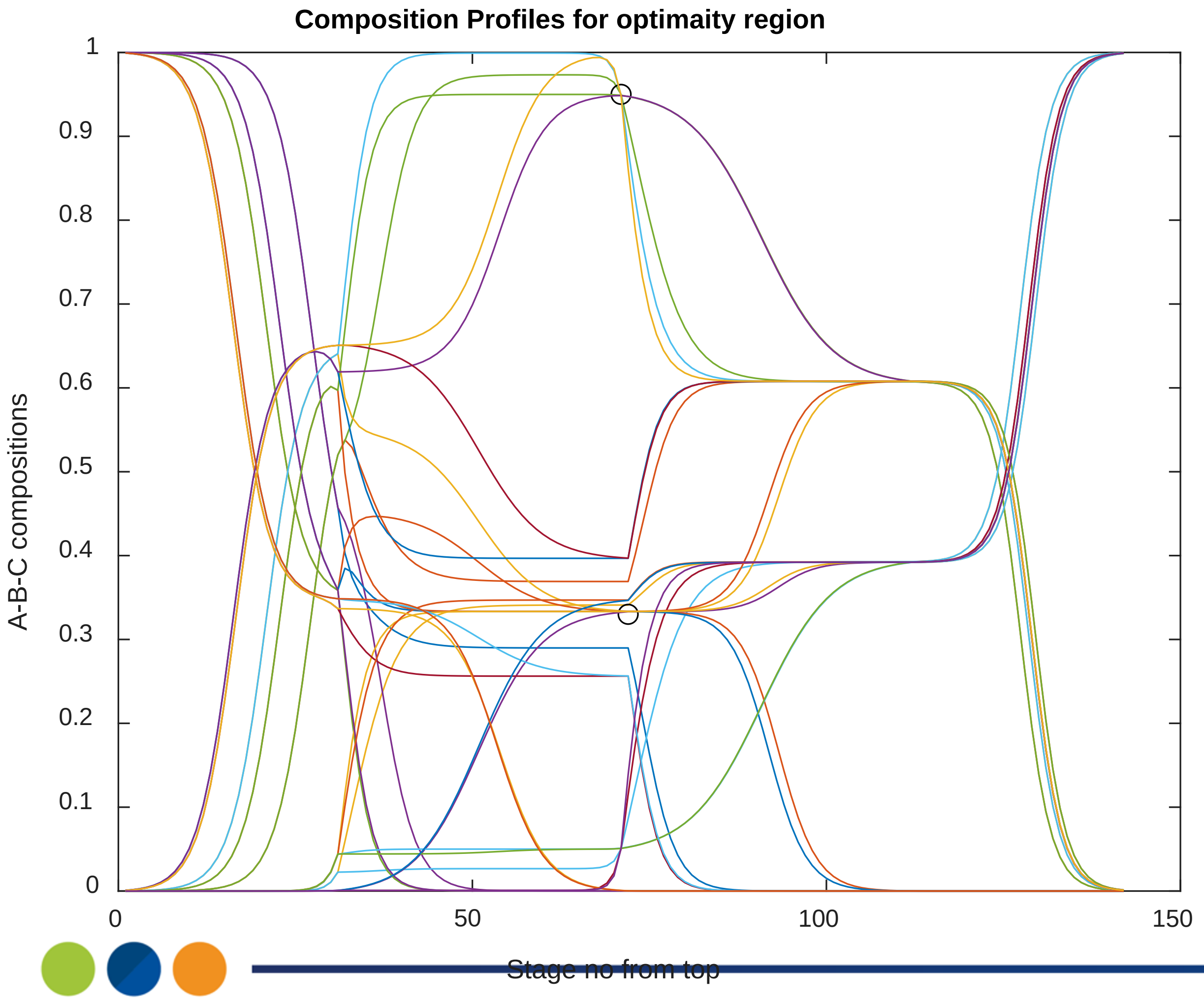
- In normal colunms, all components must travel from the feed stage to either of the product ends.
- In fully thermally coupled sections, a component may also travel in the reverse direction
- Normally - reverse component flow is suboptimal, but the impurity component may travel in reverse direction from the side-stram stage. This occurs in a part of the optimality region.

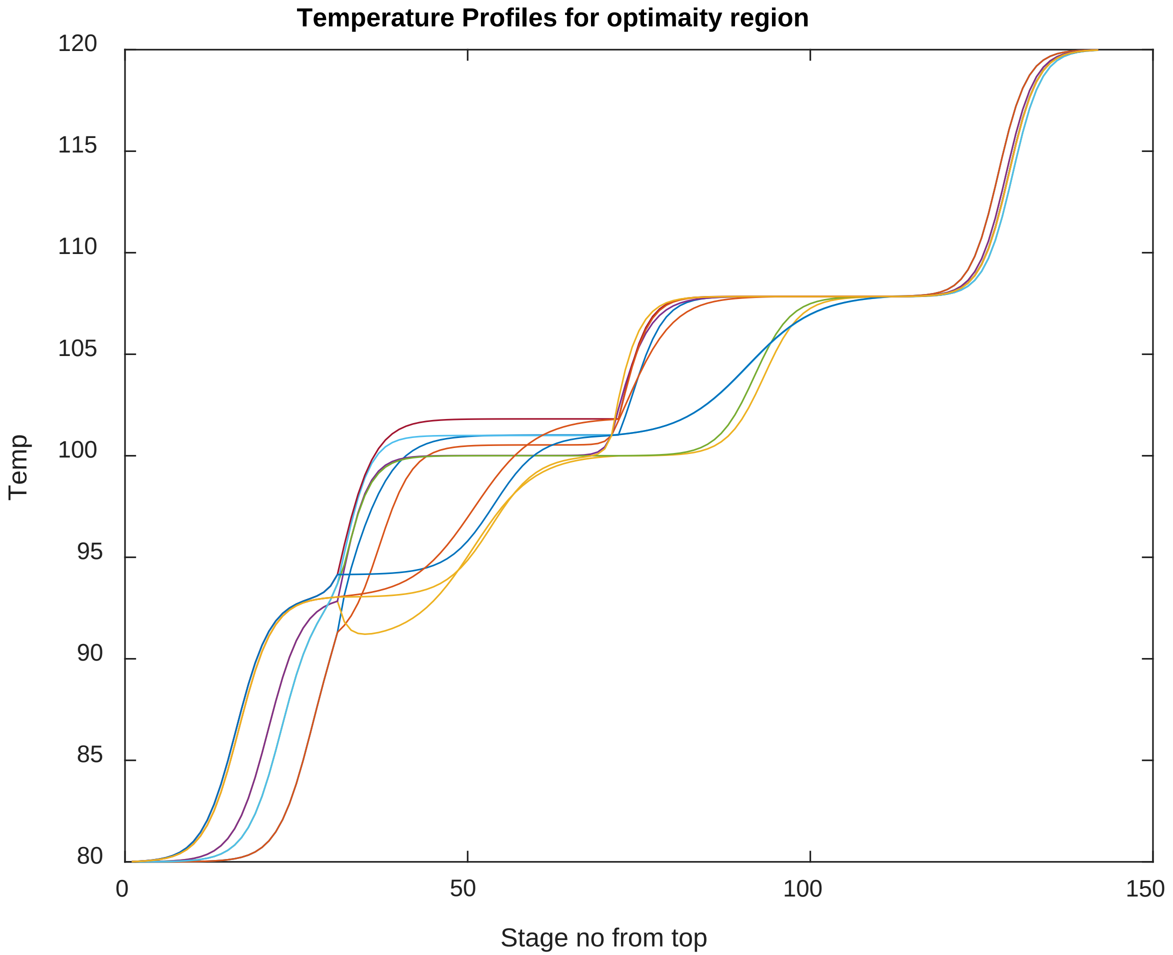
Ex: Optimality region with 5% impurity

- Next:
- Plotting column profiles for all four corners + the central average point
- Pure top & bottom product



All these column profiles has the same reboiler duty and product purities





Consequences

- Characterisitcs:
  - Sharp split: The optimality region is a line segment
  - Nonsharp sidestream: The optimality region opens up to a become a quadrangle

- If high purity sidestream is not required, a relaxed purity spec can be maintained with simpler control (wider margins)

- **If high purity is required, but cannot be obtained:**
  Then this is a symptom of sub-optimal settings of the splits

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Pinches & Underwood roots

- Pinch zones are closely related to Underwoods minimum vapor results.
- Underwood showed that there are asymptotic pinches for each actual underwood root above and below the feed!
  6 in total for a 3-component feed.
- For 3 distributing components the feed zones are connected
- Pinches may be infeasible (negative compositions), but still plays a role as assymtotes for the profile – before nature limits composition to positive numbers

The key pinces in a DWC prefractionator

- Top:
- When C is removed, A/B goes towards a given pinch zone composition.
- When in the zone in (or at) the distribution region under the A/BC peak , this pinch zone is CONSTANT
- Bottom:
- When A is removed, B,C goes towards a given pinch comp. When in the zone in (or at) the distribution region under the B/C peak , this pinch zone is CONSTANT

Multicomponent Pinches. King 1980

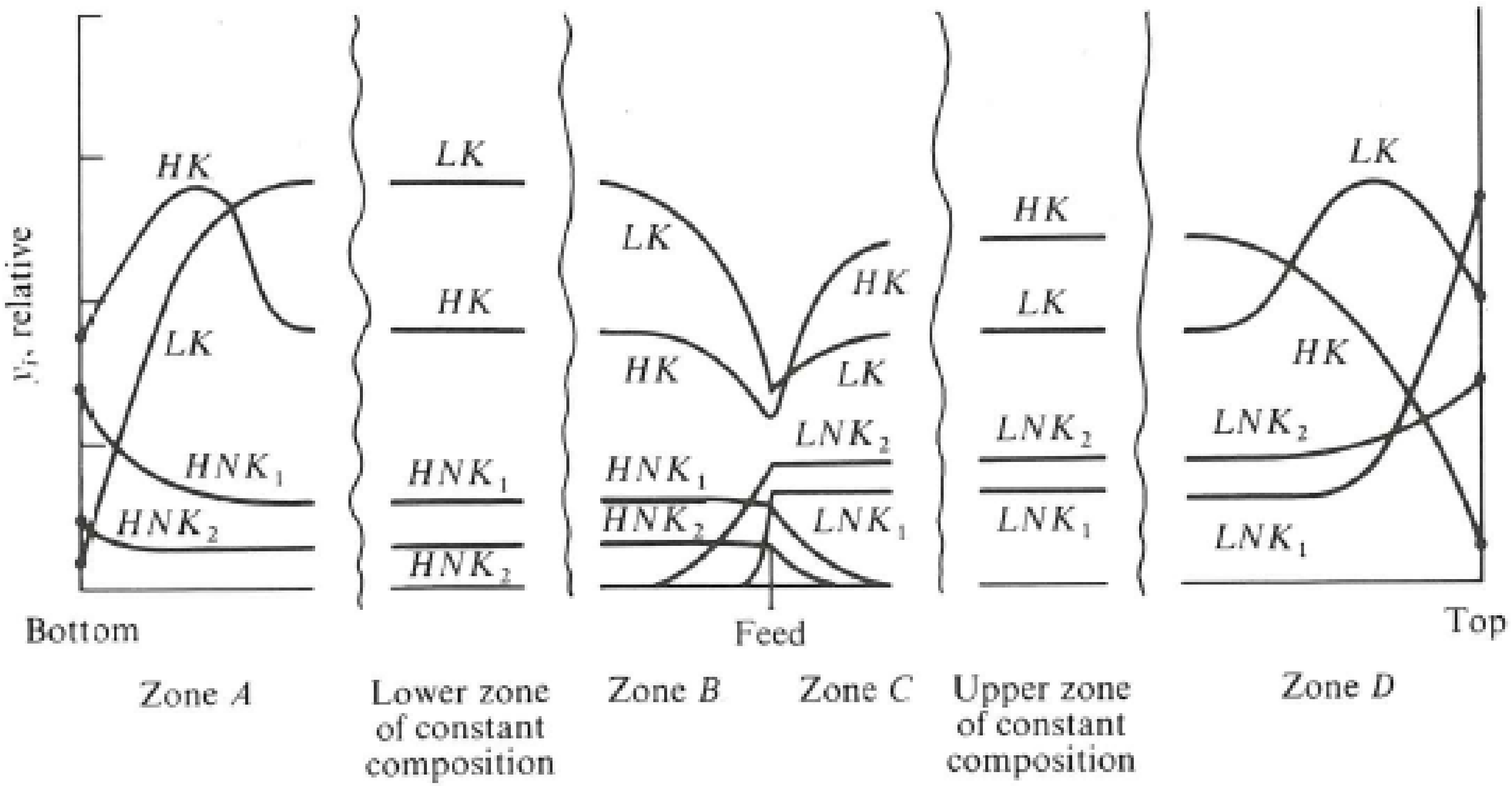

Figure 7-16 Typical vapor-composition profile for multicomponent distillation at minimum reflux.

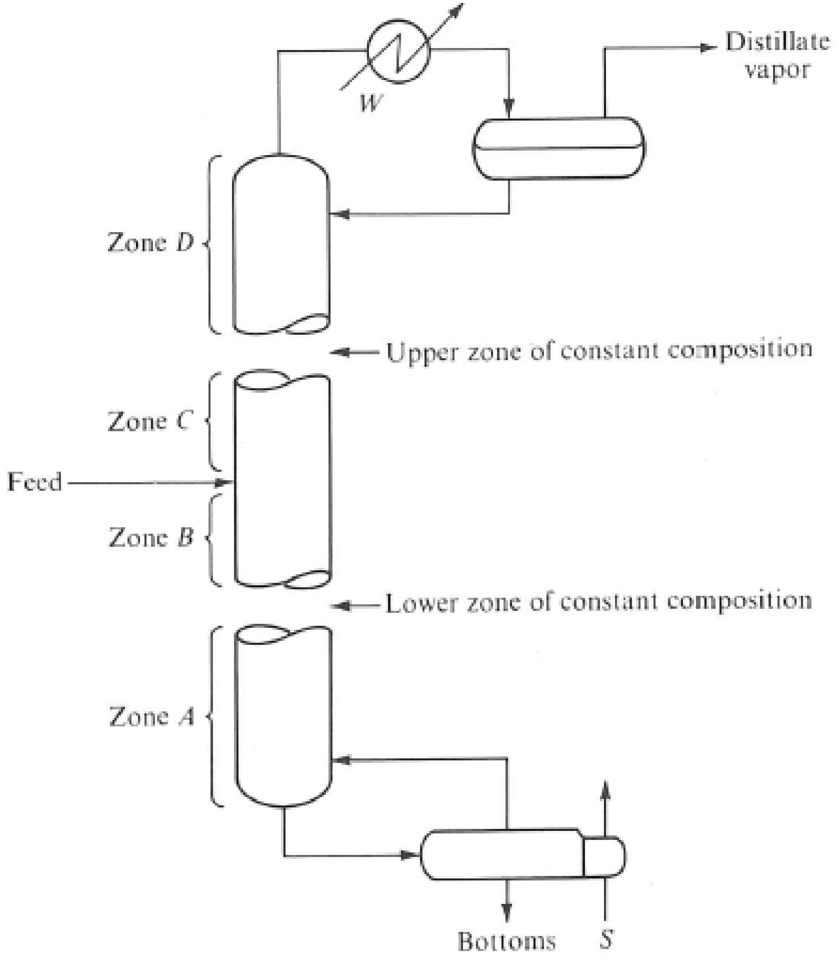

Figure 7-17 Operation of multicomponent distillation at minimum reflux.

Pinch expressions

- Underwood's expression

$$x_{i,PT}^{\phi_k} = \frac{x_{i,D}D}{L_T}\frac{\phi_k}{(\alpha_i - \phi_k)} = \frac{w_{i,T}}{L_T}\frac{\phi_k}{(\alpha_i - \phi_k)} \qquad (3.39)$$

- It can be shown that by calculating net flows and reflux, this value is determined by the Underwood root only.

$$x_{A,PT} = \frac{\alpha_B(\alpha_A - \theta_A)}{\theta_A(\alpha_A - \alpha_B)},\ x_{B,PT} = \frac{\alpha_A(\theta_A - \alpha_B)}{\theta_A(\alpha_A - \alpha_B)} = 1 - x_{A,PT} \qquad (3.41)$$

Surprisingly, from (3.41), which is valid for any operating point within region AB, we observe that the pinch-zone composition in the top section will be independent of the operating point (V,D) since θ_A is a constant. This issue was not pointed out by Underwood, and it is not at all obvious from (3.40) since all variables in (3.40), except α, are varying in region AB.

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- From this follows: Pinch composition is constant if UW-root is!

Value of UW-roots for A/B split and B/C

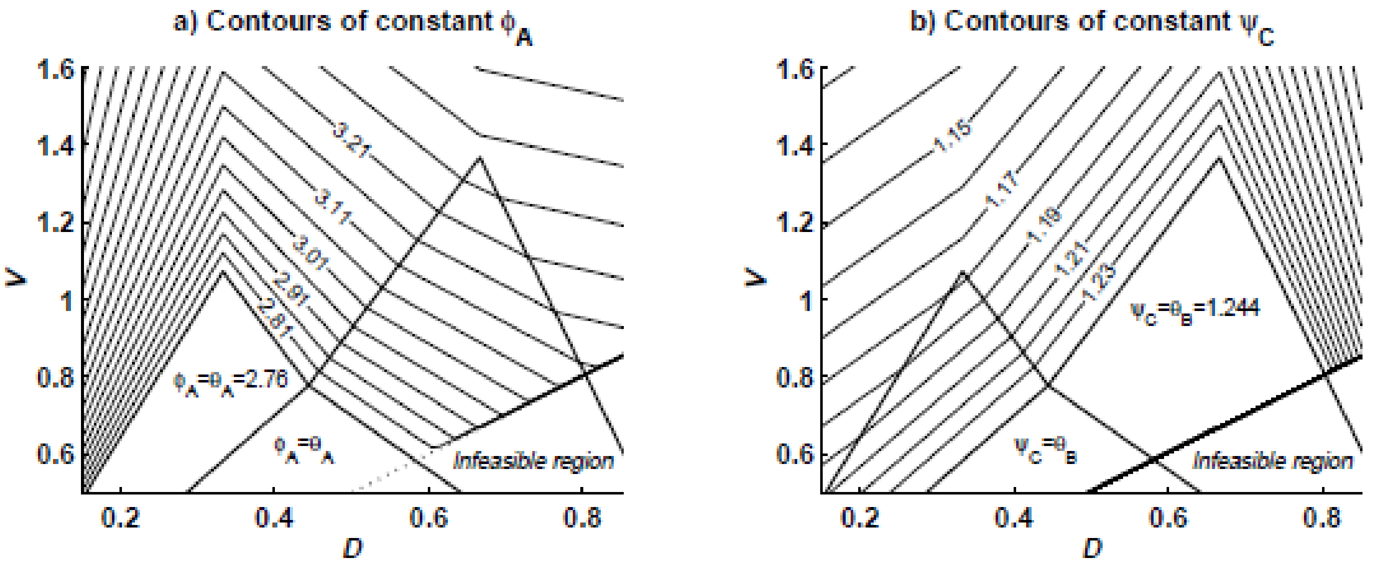

Figure 3.9: Contour plot of the most important roots a) in the top- and b) in the bottom sections outside the region when these roots are active. Same feed as in Figure 3.8

- E.g. at the optimality region the B/C pinc in the bottom is constant. This explains the illustrated profiles above,

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Using pinch to explain Vmin for DWC

- Can be shown by McCabe-Thiele!
- The key is that in the A/B pinch , this asymptotic value is the highest composition A can raise to in the prefractionator
- By conneting the succeeding column by liquid and vapor in equilibrium. That pinch becomes the succeeding feed pinch
- In top: Minimum energy is obtained by highest possible A at the feed stage (connection point)
- In bottom: Minimum energy is for the highest possible C in the connection point

Example

- Note:
- The pinch of A&B in top is the same in all cases since all are under the A/BC peak!
- Pinch goes through feed stage for region ABC/ABC

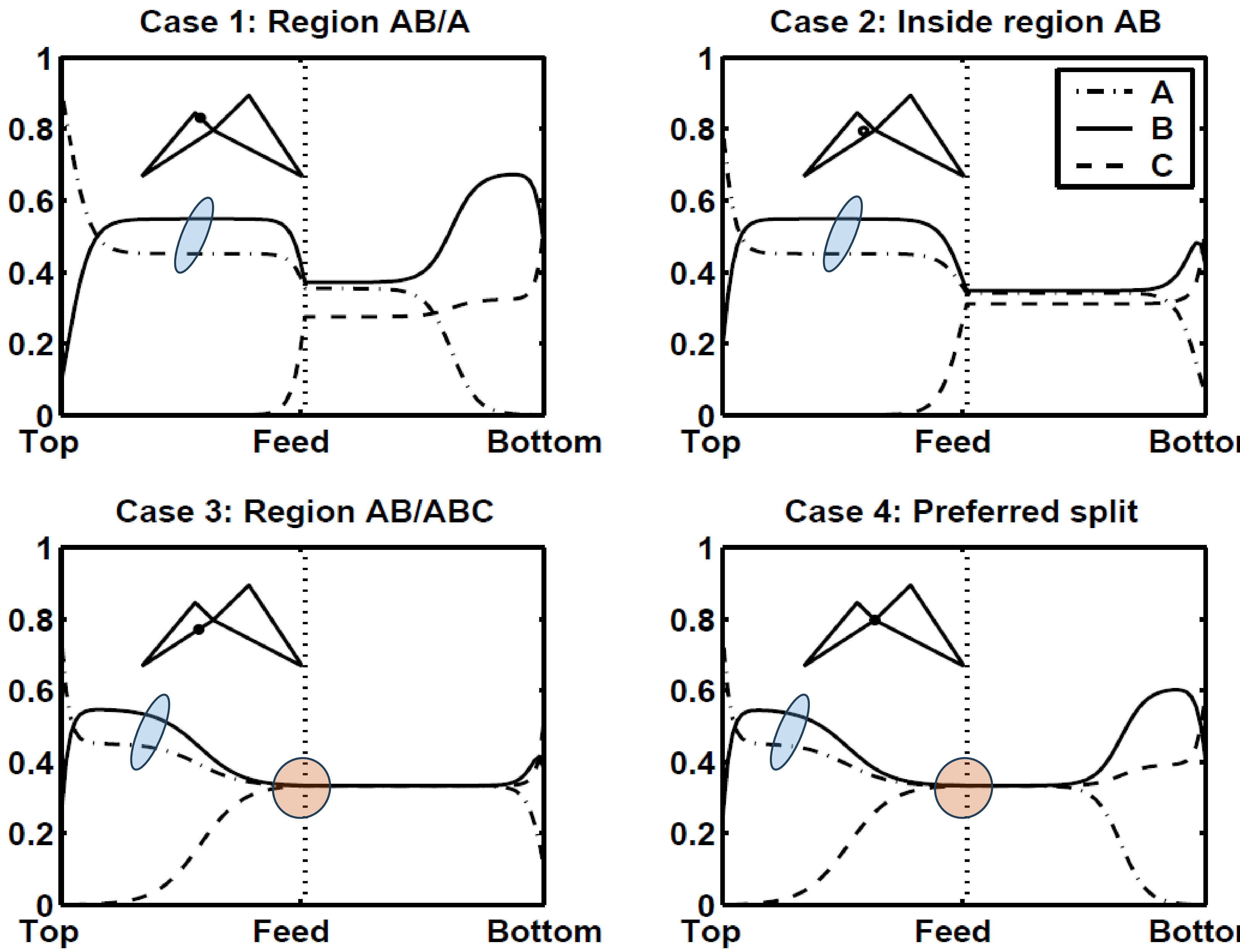
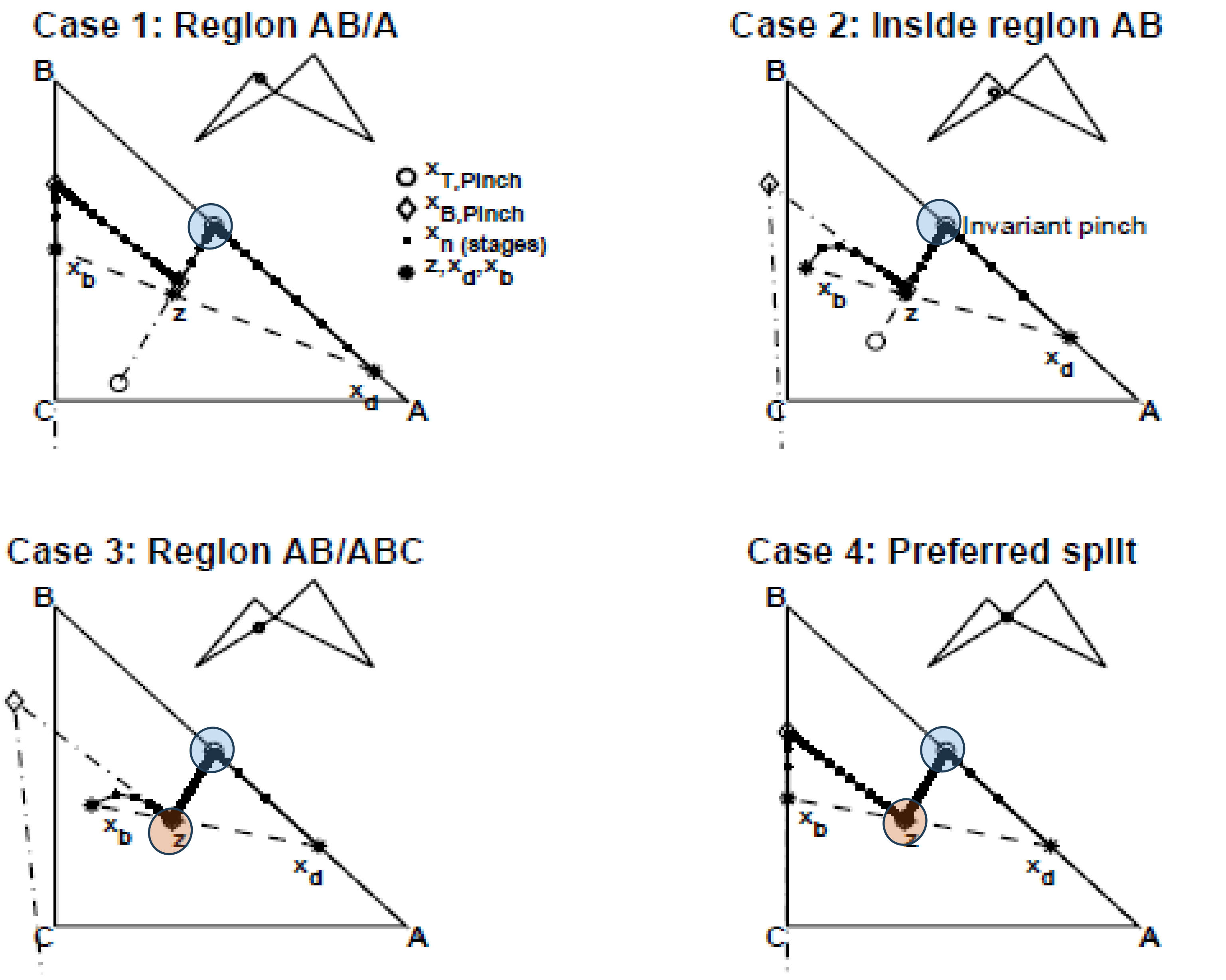


Figure 3.11: Composition profiles by stage number for the four cases given in table 3
Note the constant pinch zone in the top section

Ex. Cont.

- Same cases shown in ternary diagrams
- Curiosity: See how infeasible pinches are asymptotes for profile developments



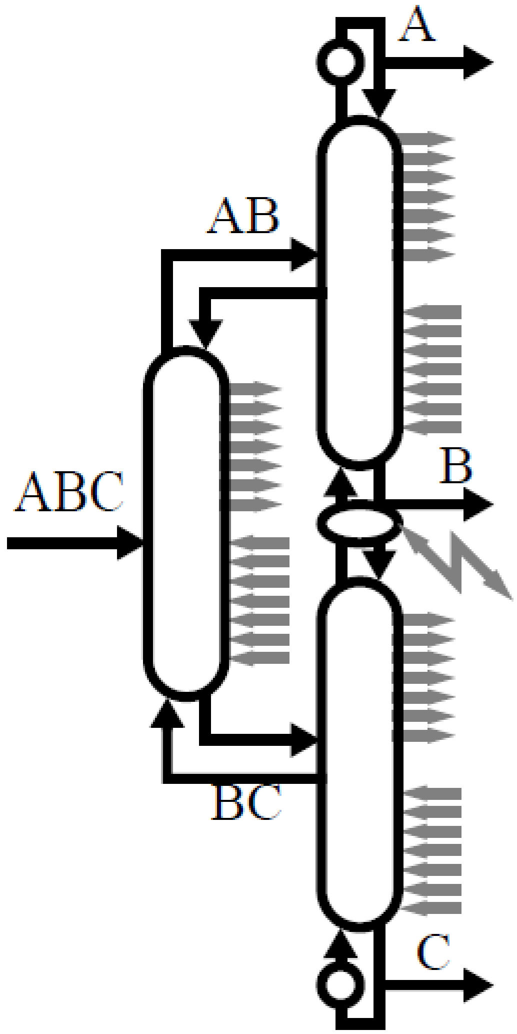
3.10: The composition profiles attempt to reach the theoretical pinch points.

Conclusion on pinches

- The calculation if minimum energy by Underwood is exact (for infinite (or 4x Nmin) stages. It only needs the K-values at the feed stage. This is true for all real zeotropic mixtures!
- The existence of pinches at the ends (when removing C and A, respectively, must be calculated for the local relative volatilities at the junction. In ideal mixures these are the same, but may be somewhat different with real flows. But the concept is the same: There will be a pinch zone, and the two-way equilibrium conection in this pinch zone enables minimisation of energy demand in the succeeding column.
- It all depends on proper prefractionator operation!

Reversible DWC columns

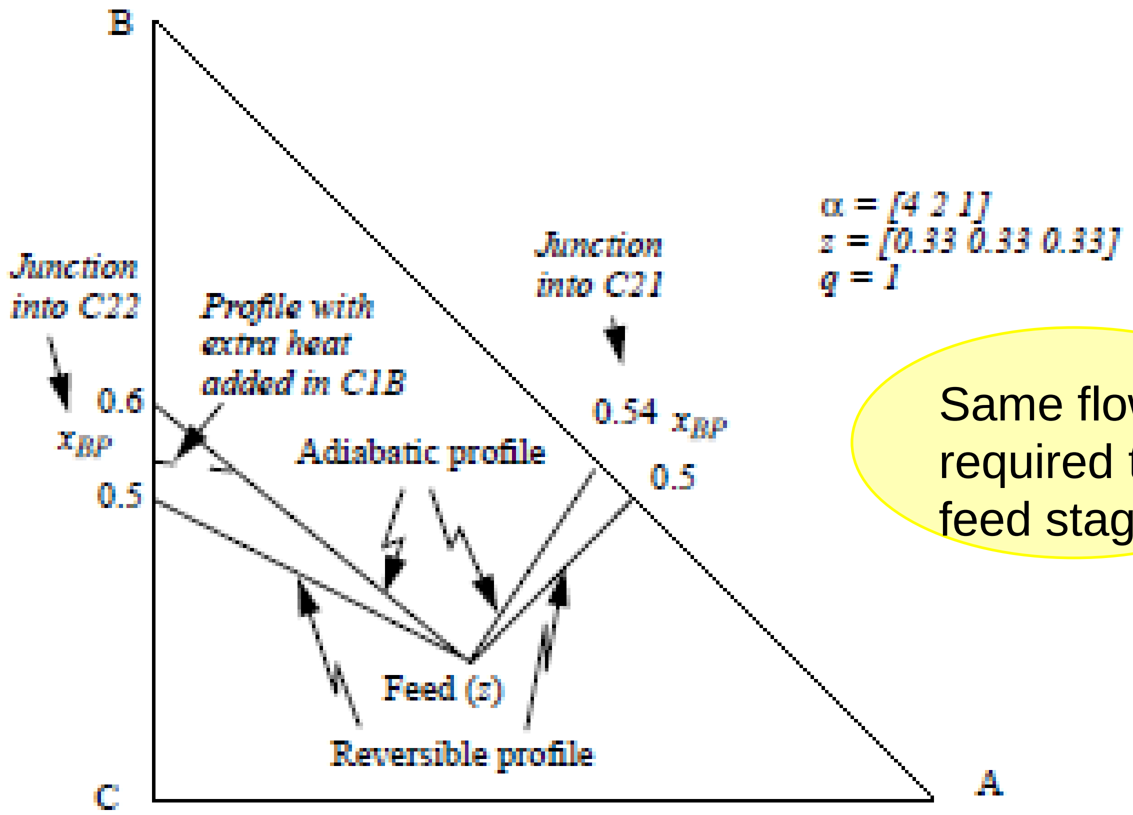
- Reversible DWC as presented by Petlyuk & Fonyo are the only concept that works for multicomponent
- E.g. A direct sequence of (ideal) HiDIC column is NOT reversible, since remixing is inevitable without vapor&liquid in equilibrium across the connection
- A reversible DWC section may also remove irreversible tray-tray mixing just like in a single HiDiC.



V_{min} = 1.667

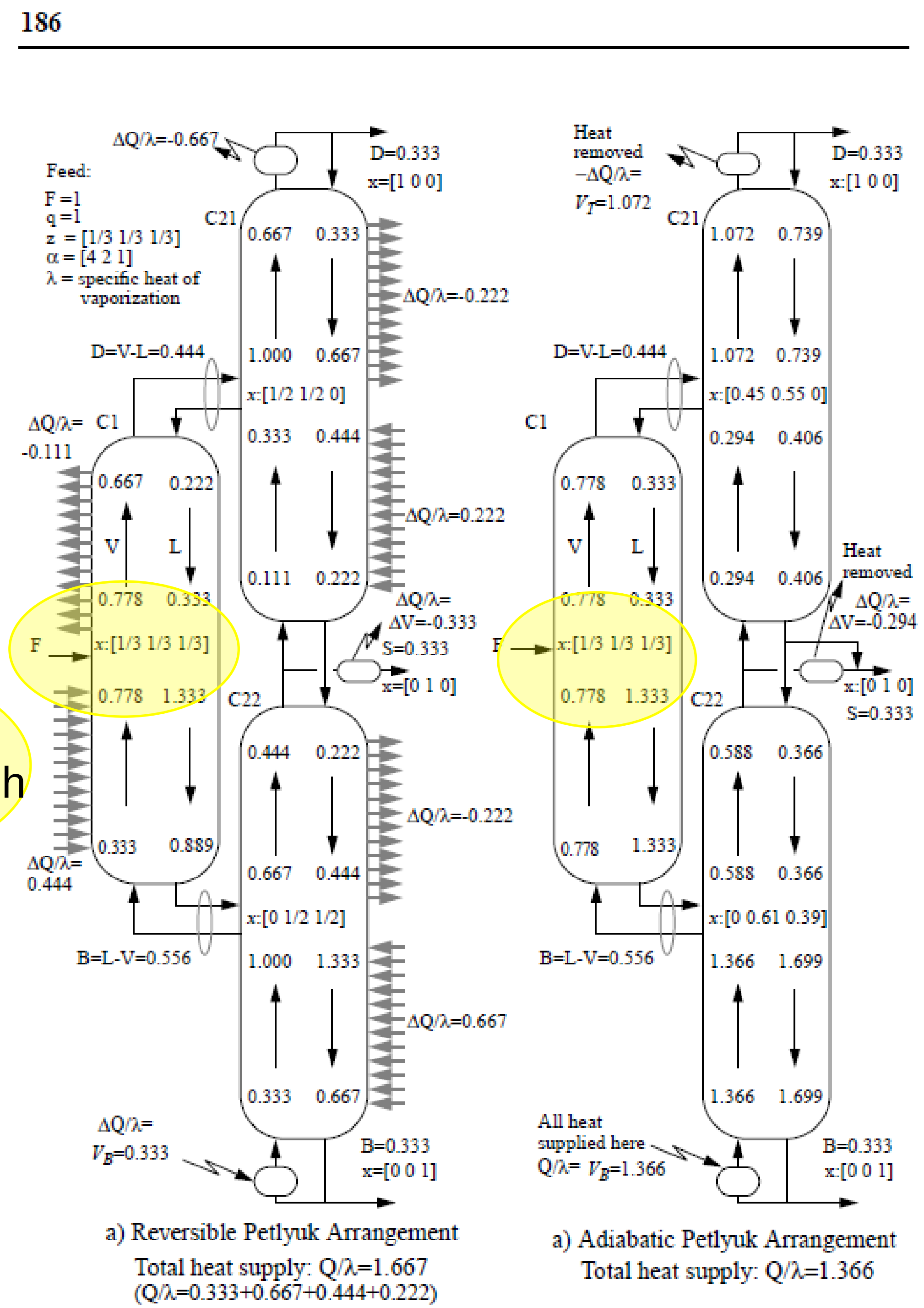
S_r = 0.00

Calculation example



Composition profiles in the prefractionators (C1) for the :

Same flows required through feed stages!



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Operation outside the V-shape

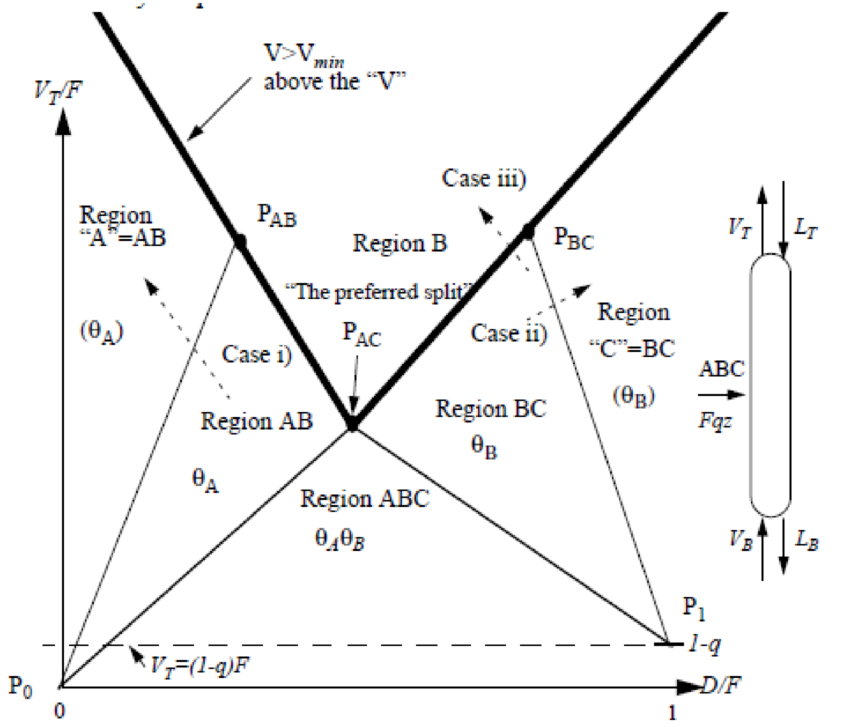

Figure 4.5: The V_{min}-diagram for the Petlyuk column prefractionator is identical to the diagram for the conventional diagram in region ABC and also in AB when C is not present in the top-feed, and in BC when A is not present in the bottom-feed. However, the V-shaped V_{min}-boundary for sharp A/C split (bold) is extended when B is present in the end-feeds (V_B or L_T)

- Feasible operation for sharp product splits require prefractionator operation above the V-shape
- For operation to the left of P_{AB} the B-component will "rotate" down under the wall, upwards in main column and back into prefractionator top!
- Negative net distillate flow (D<0) is also feasible

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