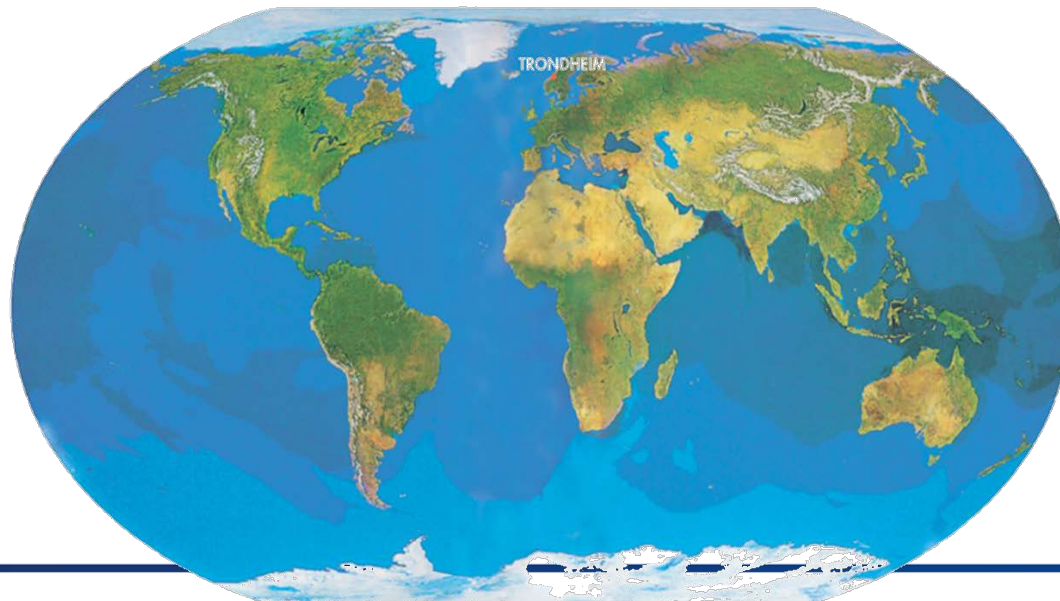


DWC Workshop – NTNU Trondheim – 5-6. October 2023



# The $V_{min}$ -method and the need for vapor split control

Ivar J. Halvorsen



# Distillation consumes energy

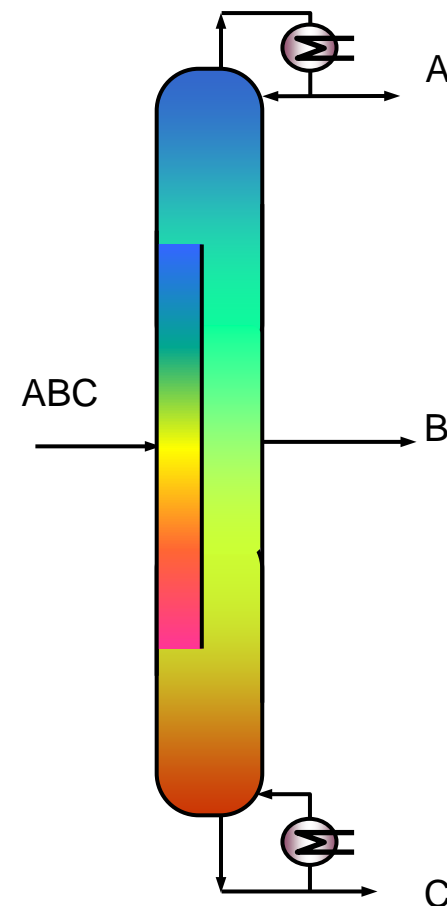
- 2-5% of the world industry heat consumption
- There is a potential for more energy efficient solutions
- Picture: Fractionation columns at the Snøhvit LNG-plant in Hammerfest

Foto: I.Halvorsen 21.09.2005



# The Dividing Wall Column (DWC)

- Here: 3-product arrangement
- Remarkable properties:
  - 3-product DWC saves 10-30% in BOTH energy AND capital cost
  - 4-product DWC has potential for more
- **But, still:**
  - **Challenges in design and operation?**



# Content

- Introduction - minimum energy - operation
- Vmin-diagram basics
- Connecting column sections to make a DWC
- DWC operation and flexibility by the Vmin-diagram
- Importance of correct prefractionator operation
- Impact from feed property variations
- 4-product columns – Kaibel column
- When is active vapor split beneficial



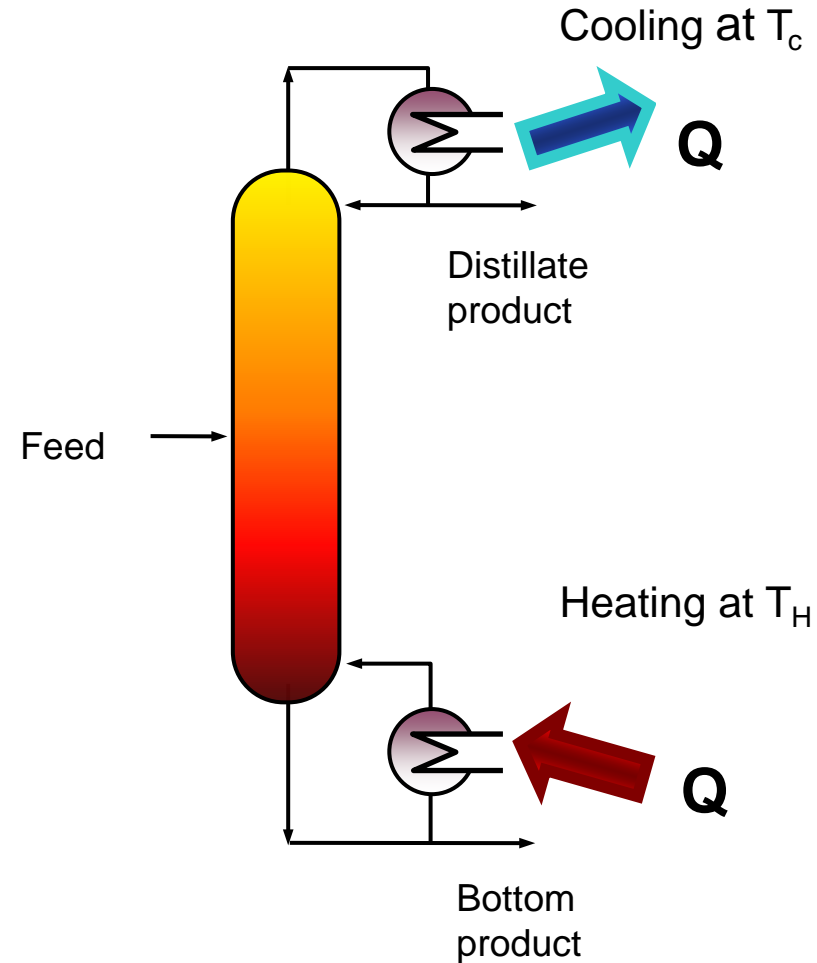
# Theoretical minimum energy

An ideal reversible process requires:

$$Q_{\min} = \frac{\Delta S T_C}{1 - \frac{T_C}{T_H}}$$

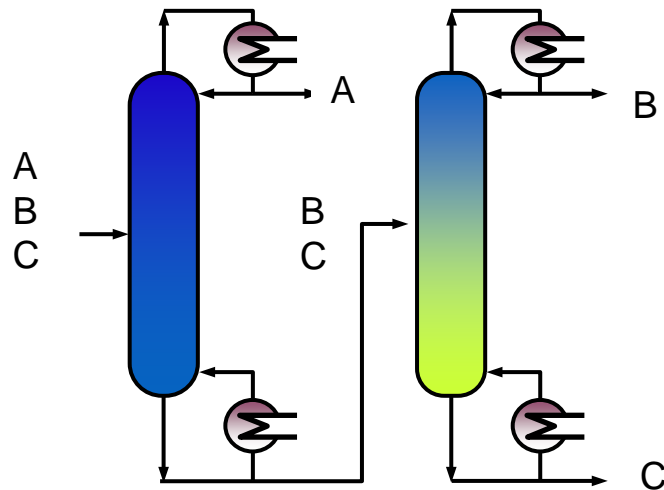
Where entropy of mixing is

$$\Delta S = -\sum_i R x_i \ln(x_i)$$

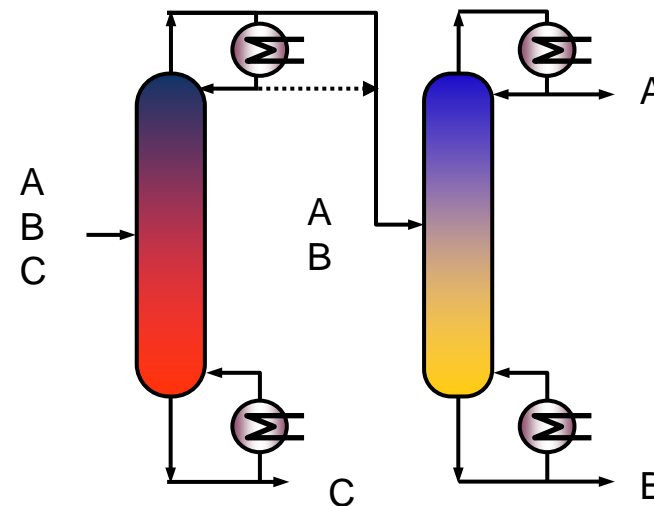


# Conventional alternatives for 3-product separation: Sequence of binary columns

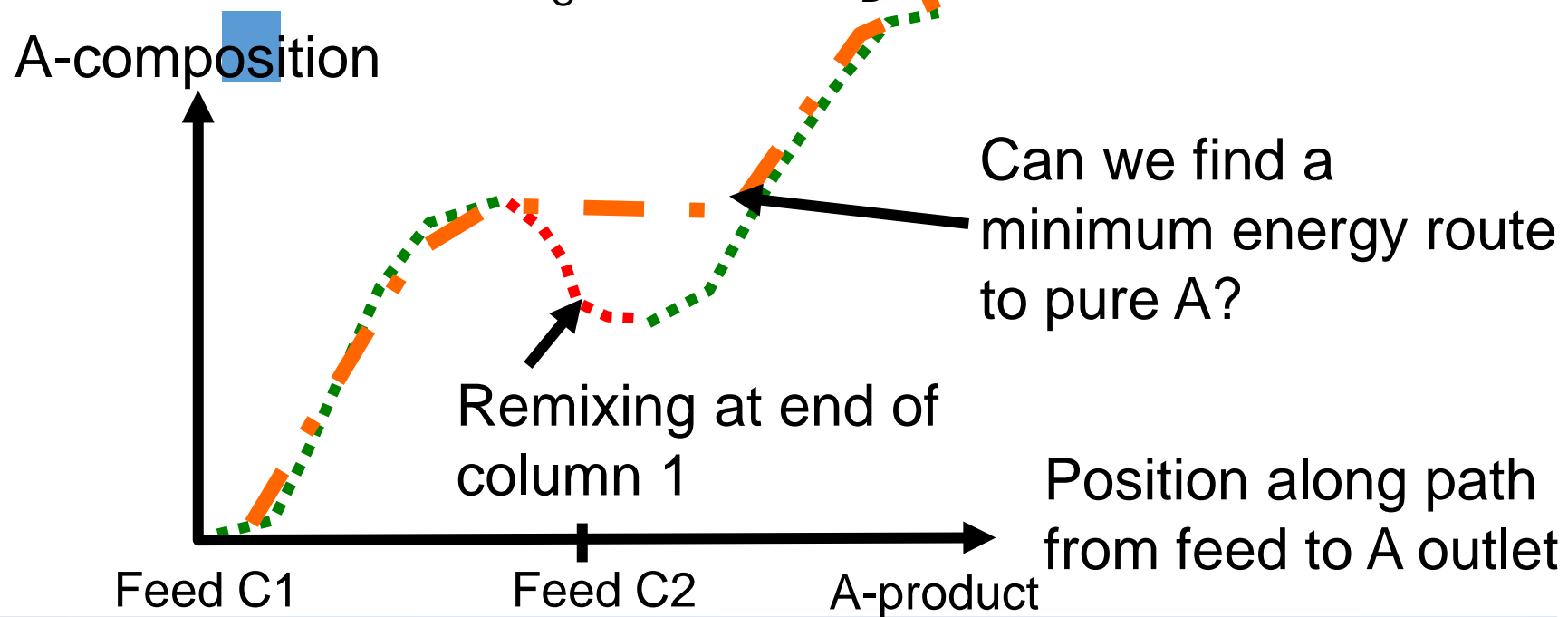
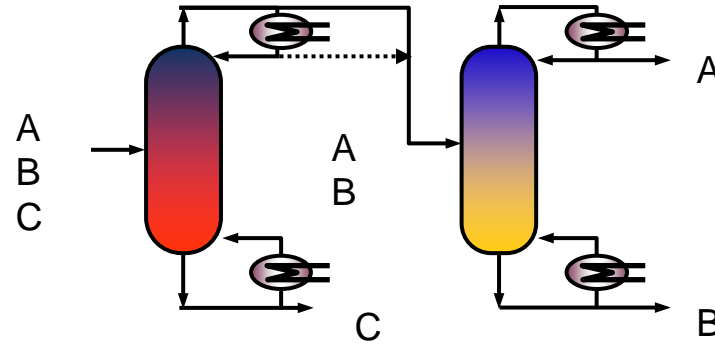
## Direct Split: DS



## Indirect split: IS

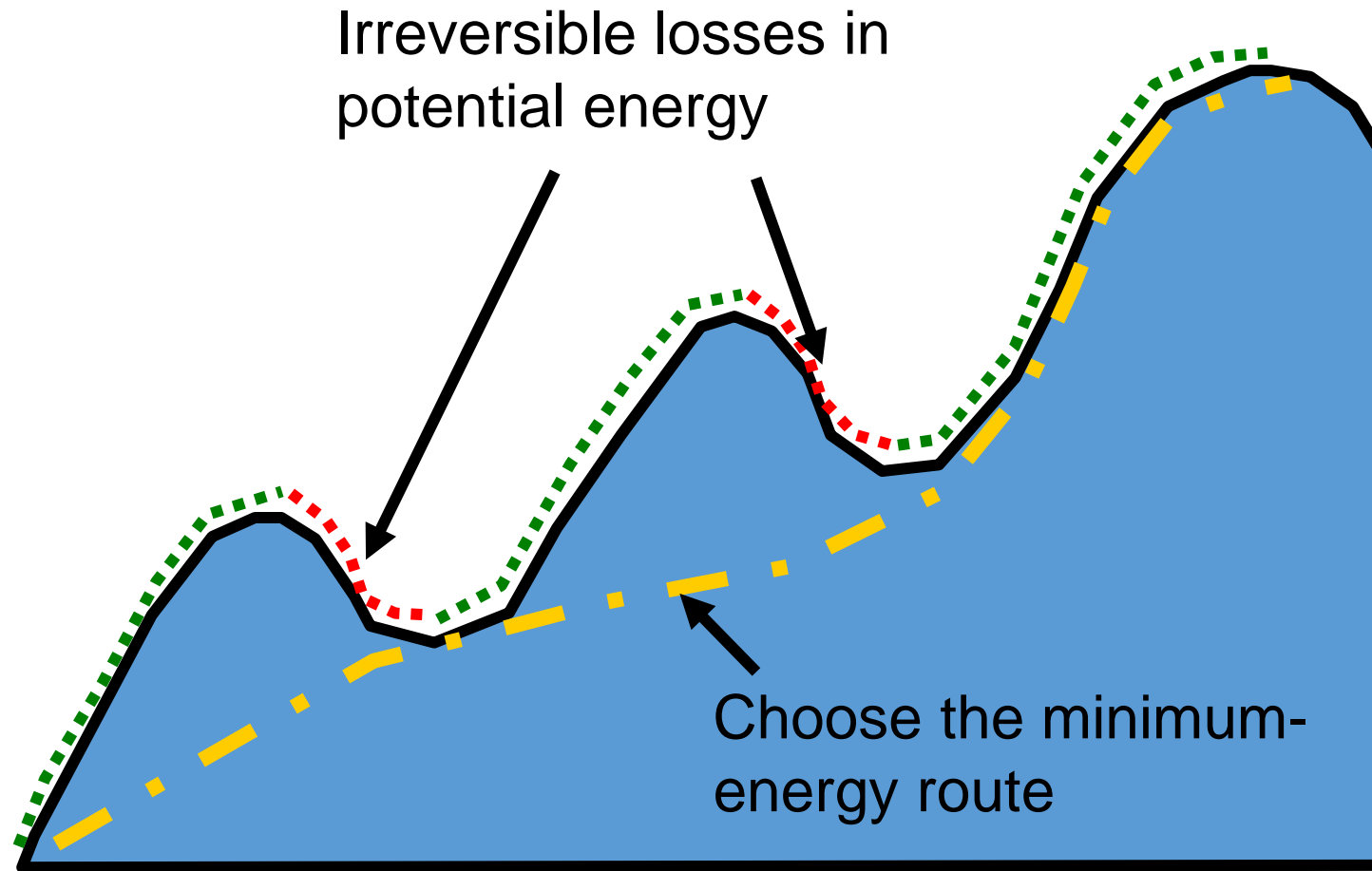


# Increasing purity require energy- Mixing gives irreversible loss

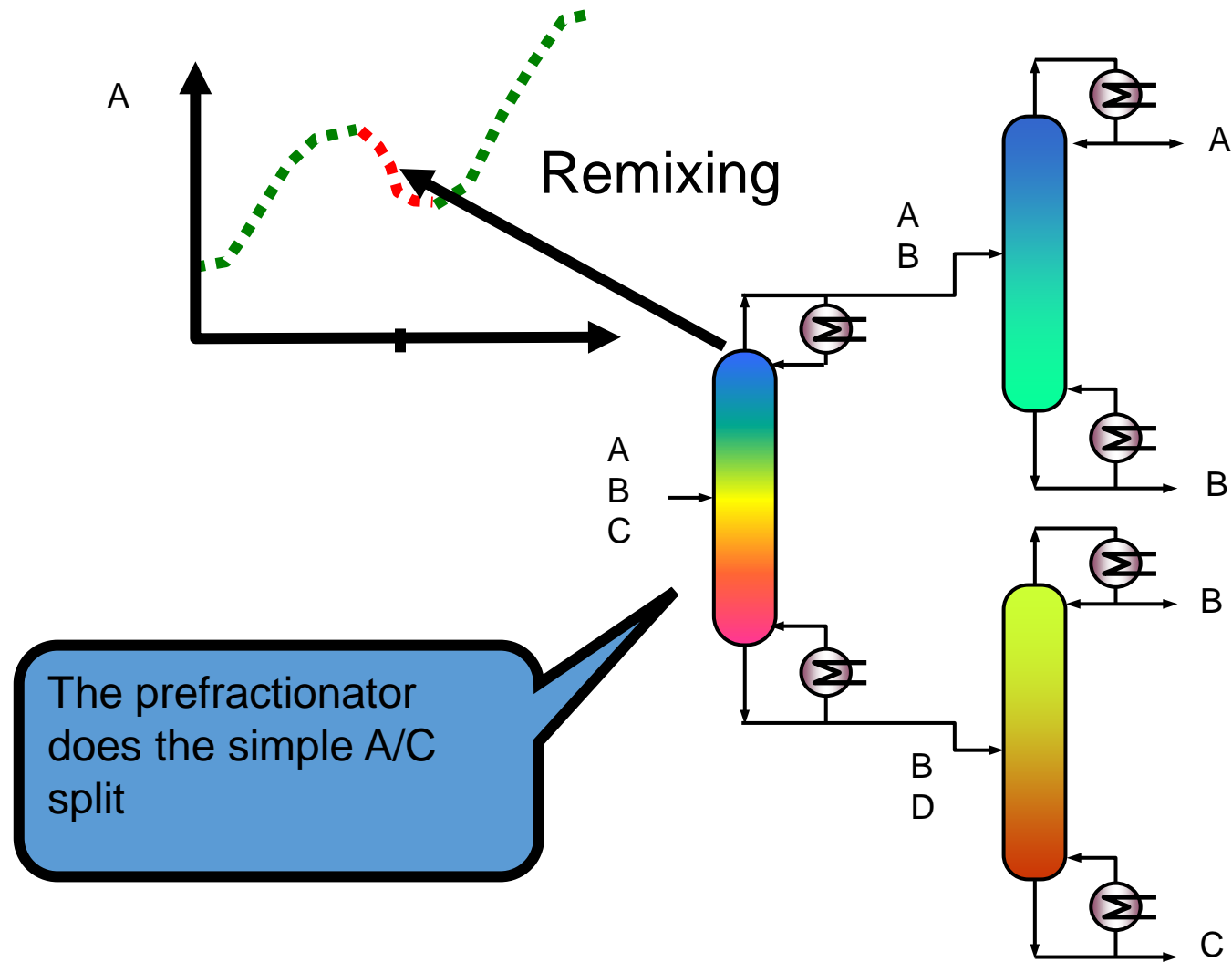




# Minimum energy path to the mountain top

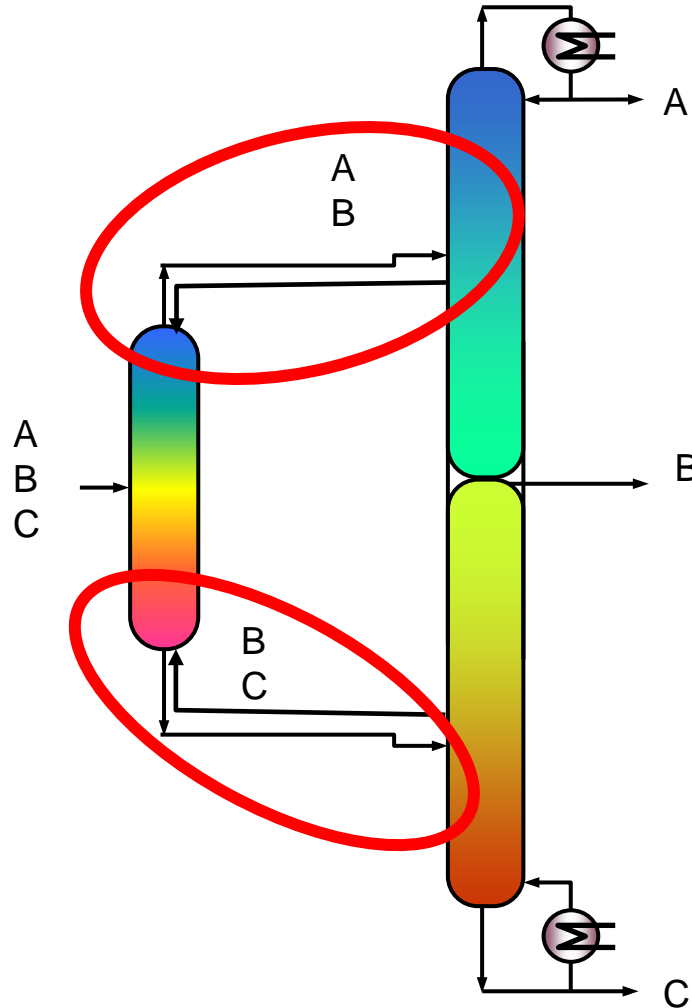
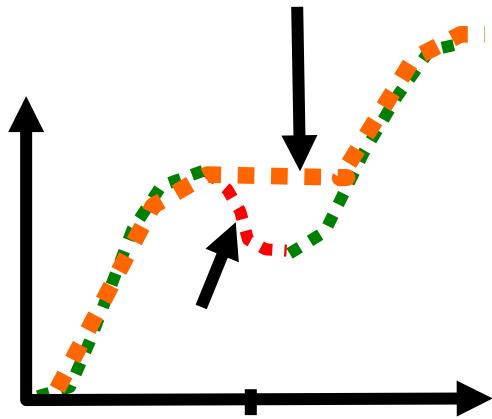


# Prefractionator arrangement



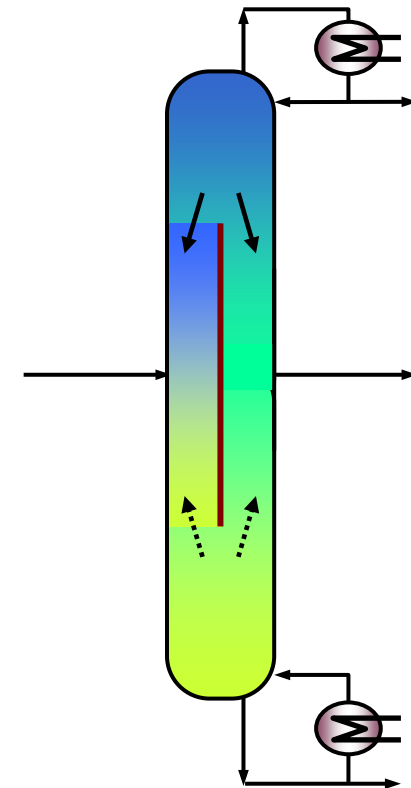
# Apply full thermal coupling

The Petlyuk column eliminates mixing loss at the interconnections.

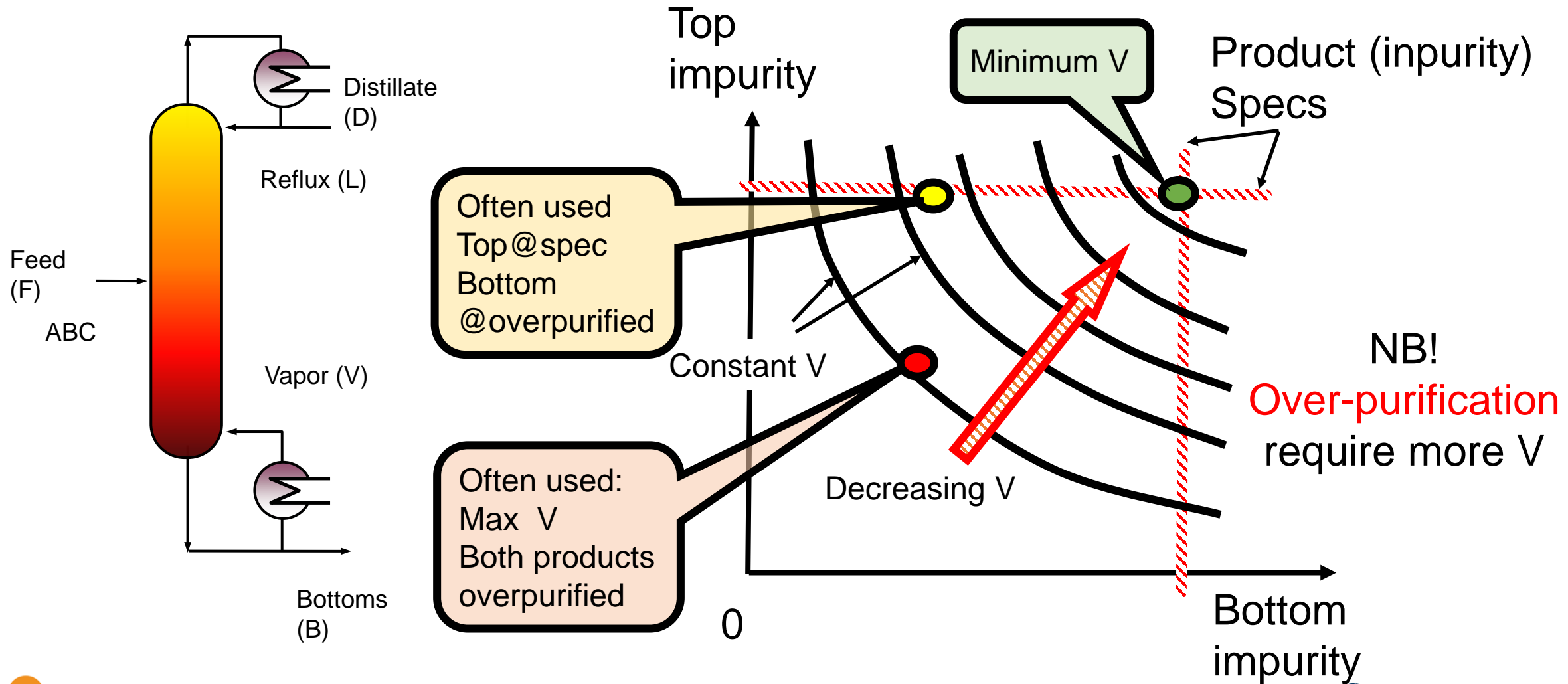


Implementation: DWC

The Dividing wall column

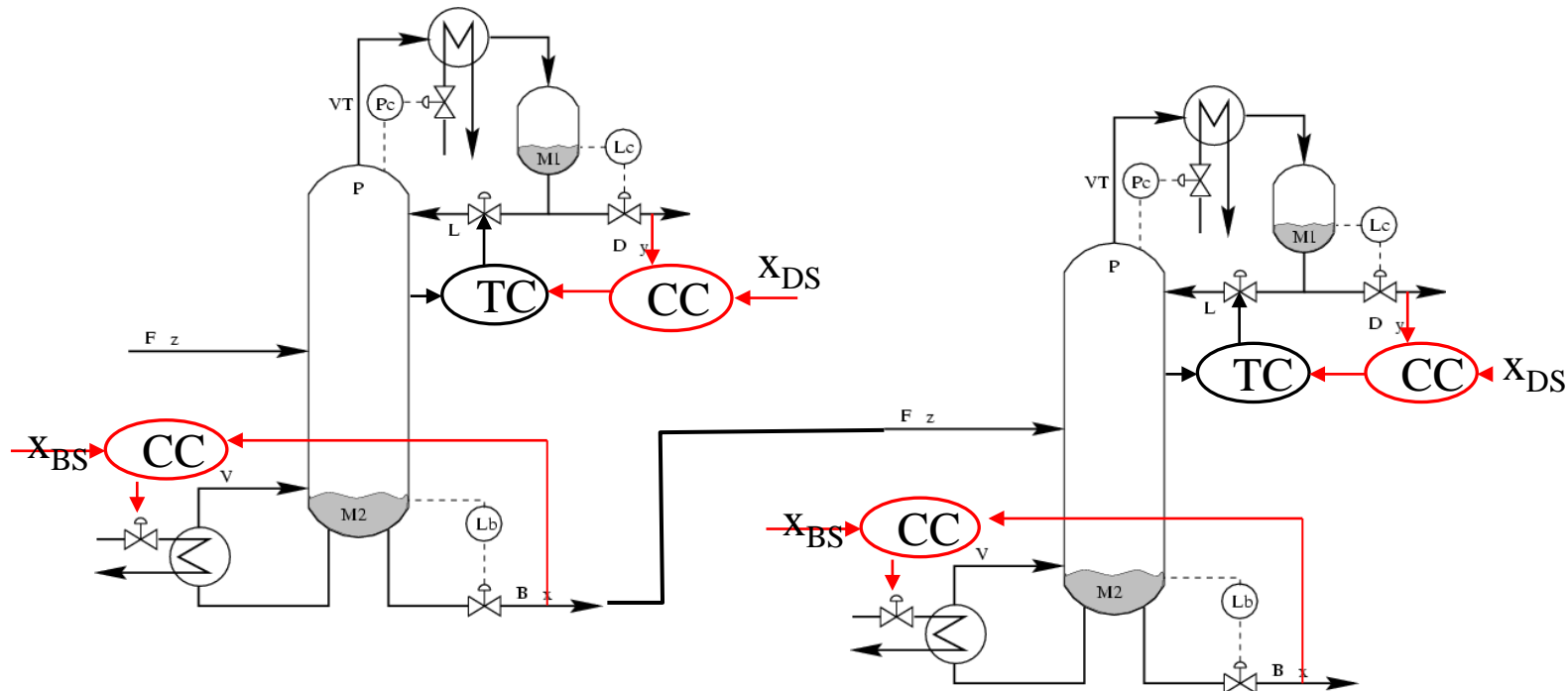


# Trivial mimimum energy for binary column



# Minimising energy in conventional binary sequence:

- Two-point composition control for each column => Minimum energy!



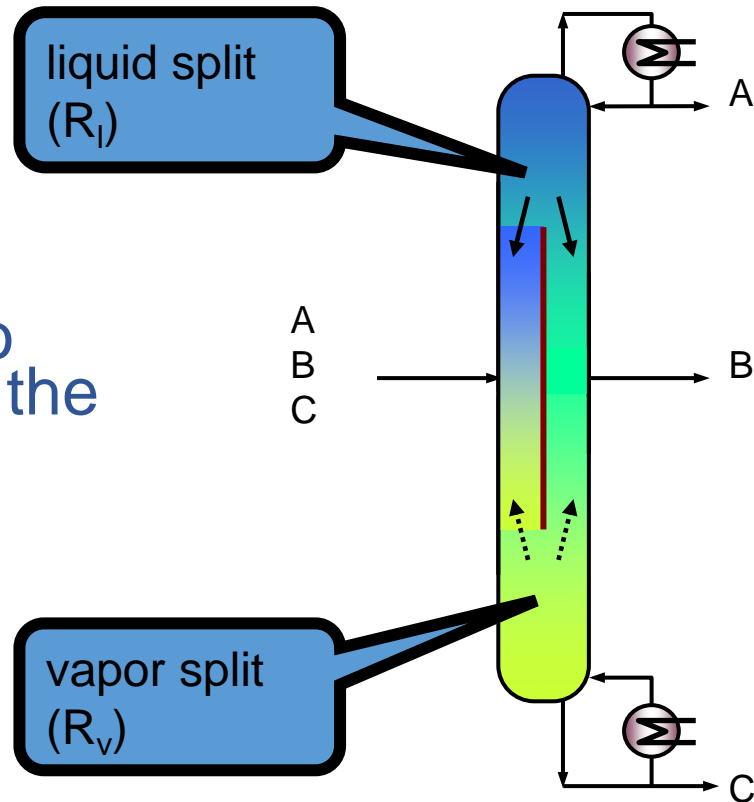
- No need for RTO (Real Time Optimisation)



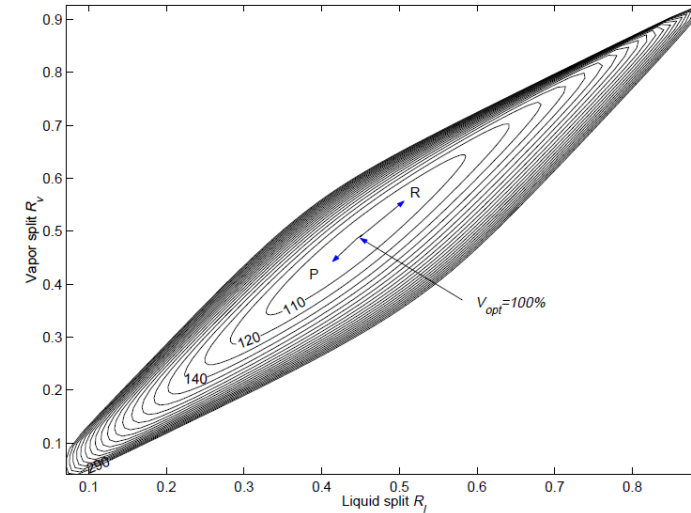
# Why is it not sufficient just to control products to spec in a DWC?

Reboiler vapor requirement depends strongly on the flow splits!

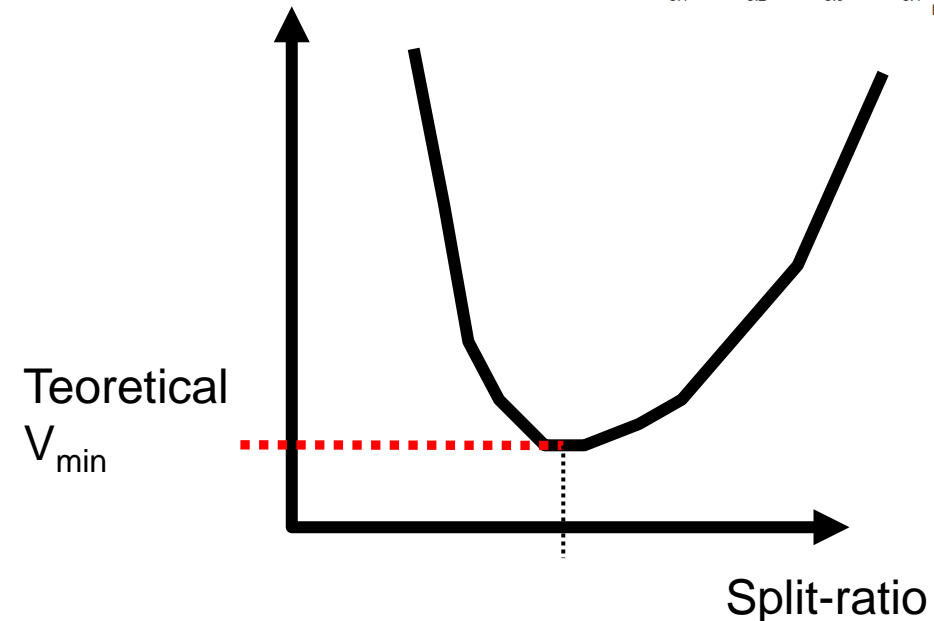
Need a strategy to set/adjust the splits!



Energy,  $V=f(\text{splits})$



Energy,  $V=f(\text{splits})$



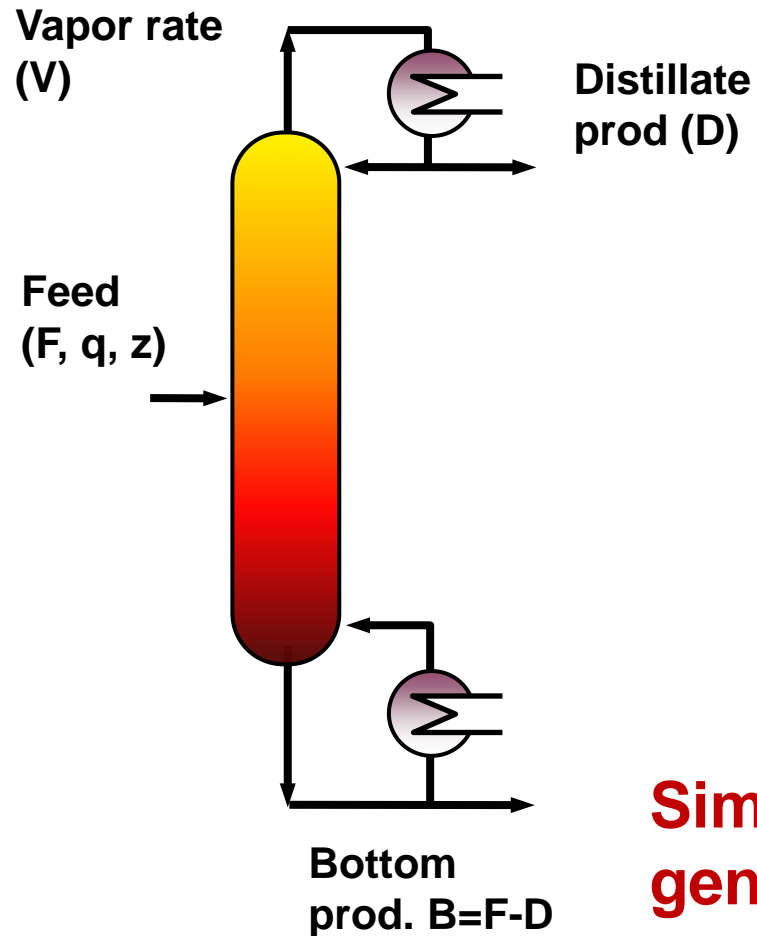
● ● ● — Key: Focus on prefractionator operation

# Tool for assessing Multicomponent separation – The $V_{min}$ diagram

- Start with assessment for a single binary column
- Extend to 3 products
- Extend to 4 products



# How will all components become distributed to products in a single binary column?



**Problem:**

**How to set boilup (V) and product flow (D) to obtain wanted recovery?**

**What is  $V_{min}$ ?**

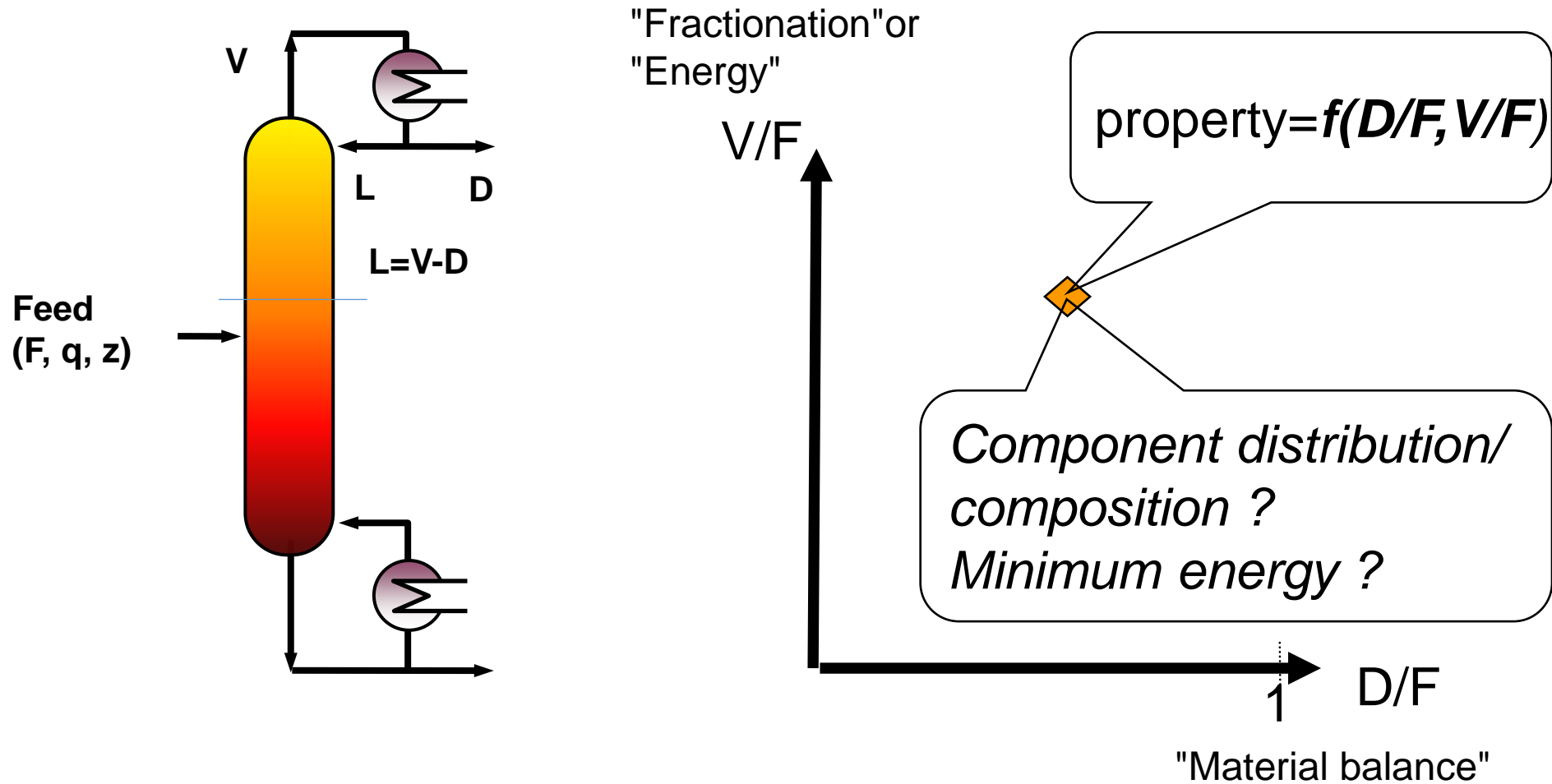
**Simple for binary feed, but what about general multicomponent feed?**



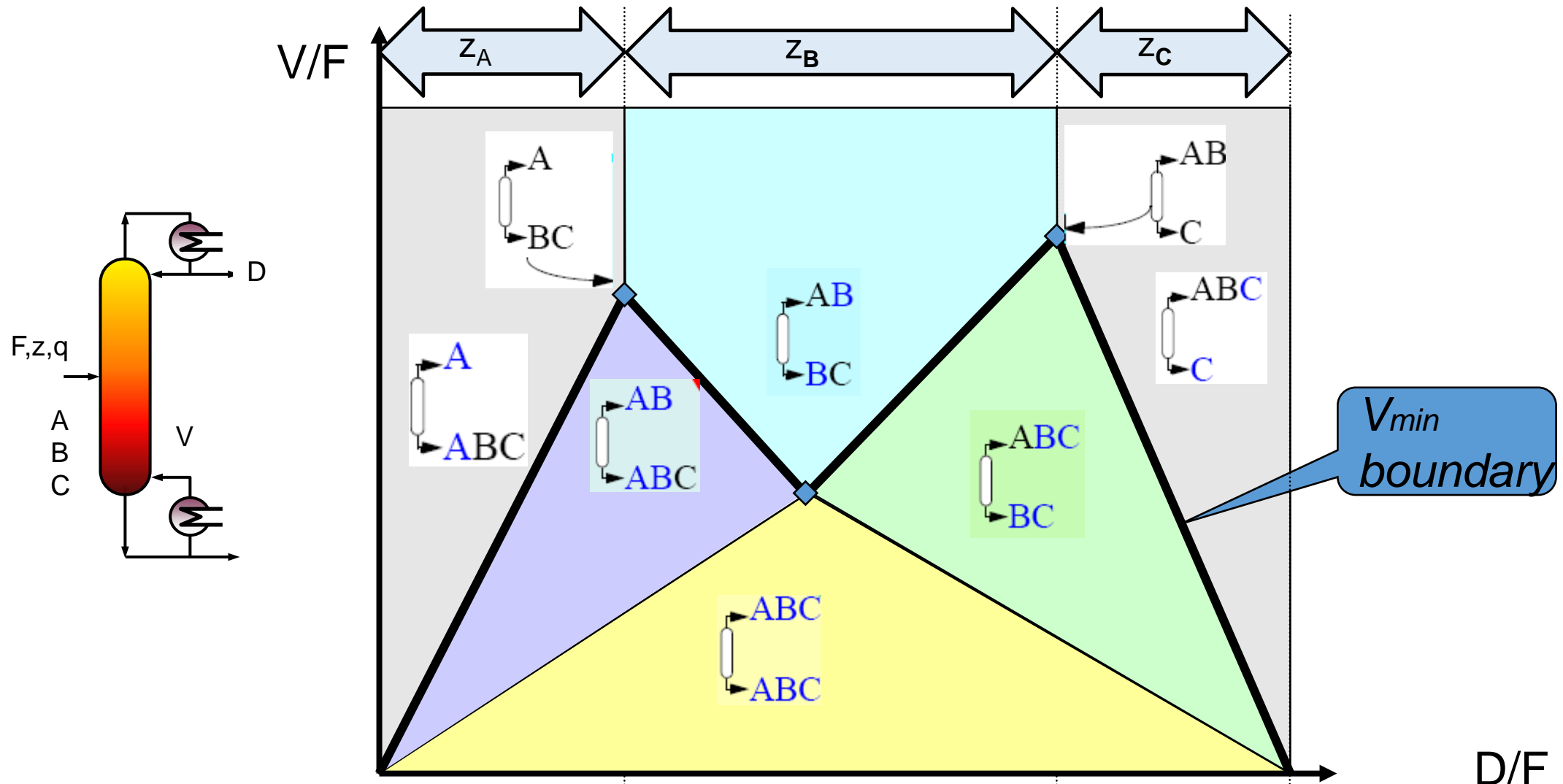


# The $V_{min}$ -diagram

Two degrees of freedom only.  
Here, choose:  $D/F, V/F$

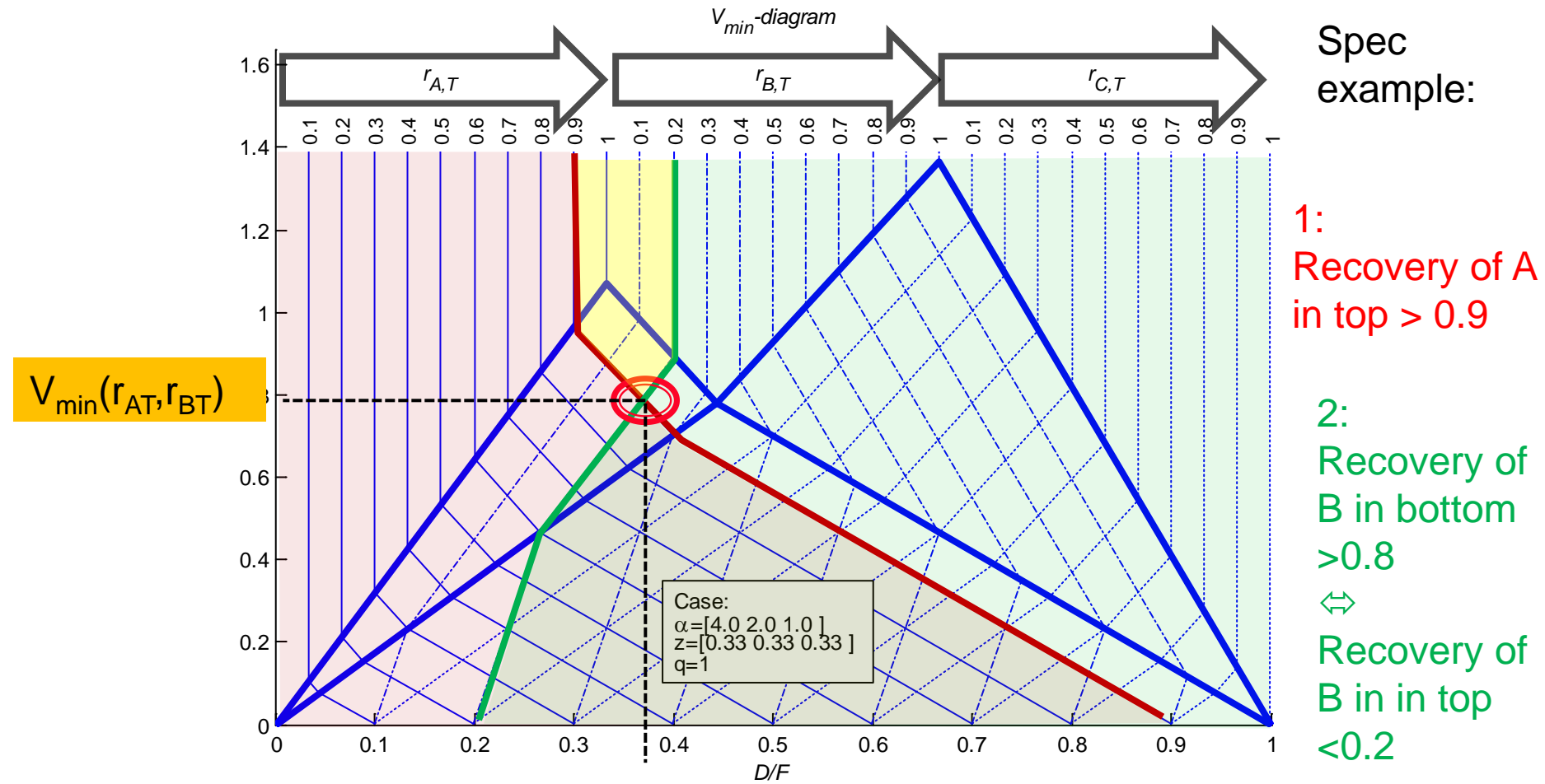


# The $V_{min}$ -diagram – 3 component example

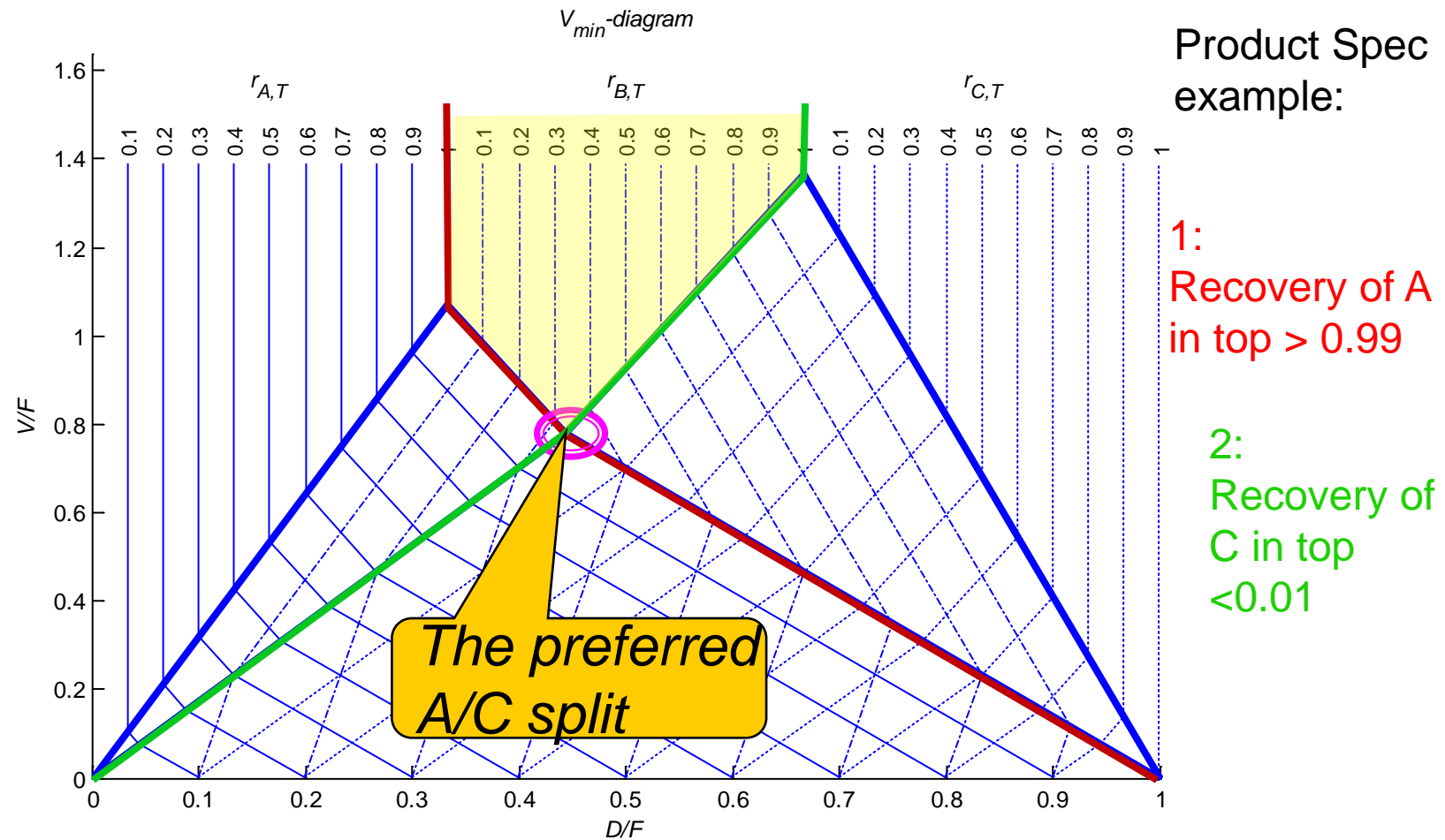


D/F

# The $V_{min}$ -diagram – split specification



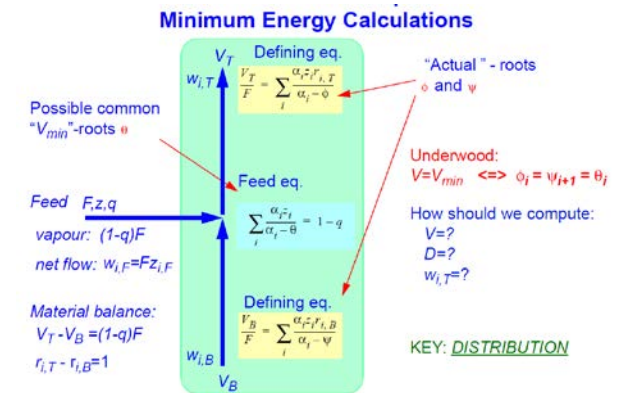
# The $V_{min}$ -diagram – The preferred A/C split



# How to obtain the Vmin-diagram

## A: Ideal assumptions:

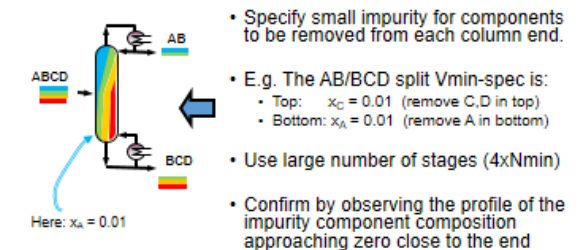
- Use analytic functions based on Underwood equations (See Halvorsen and Skogestad 2003) (Solved in milliseconds)
- Based on the following feed data only:
  - Molar fractions
  - Relative volatility (or K-values),
  - liquid fraction



## B: Real mixtures:

- Do one simulation for each point (A/BC, AB/C, AB/BC)
- Or – setup a simple sequence with special heat connection (will show later)
- Use  $N \sim 4N_{min}$  (Asses each section individually)
- Use sensible impurity specifications to define distribution boundaries. (Same spec. as used for calculating  $N_{min}$ )

How to find  $V_{min}$ -diagram by simulations on a conventional 2-product simulation

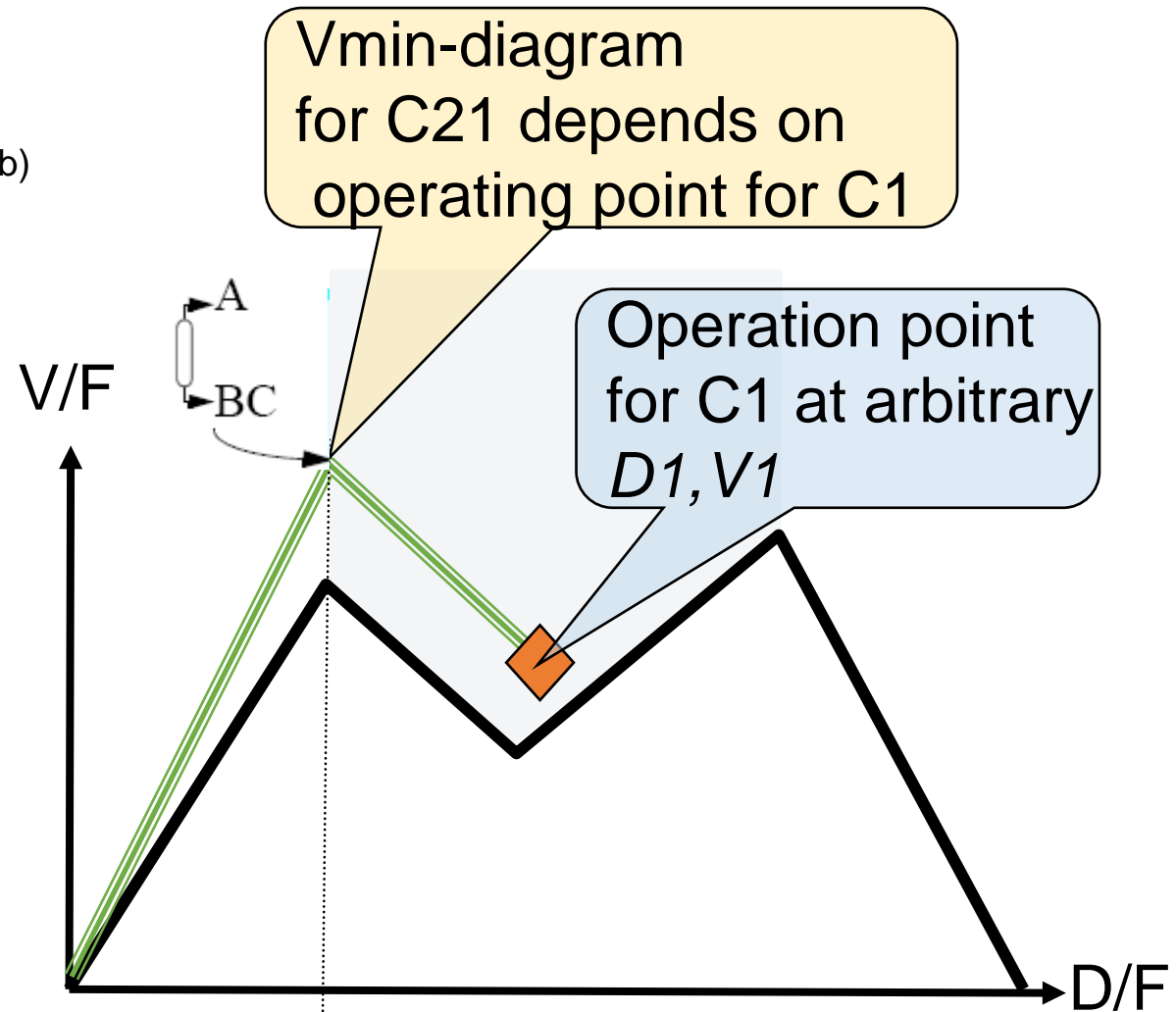
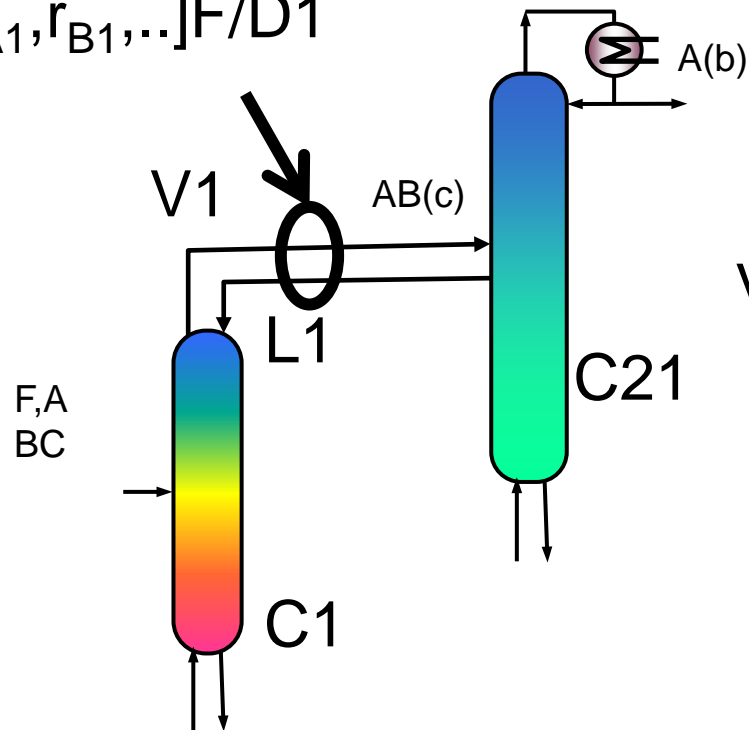


# The $V_{min}$ -diagram – for thermally coupled columns

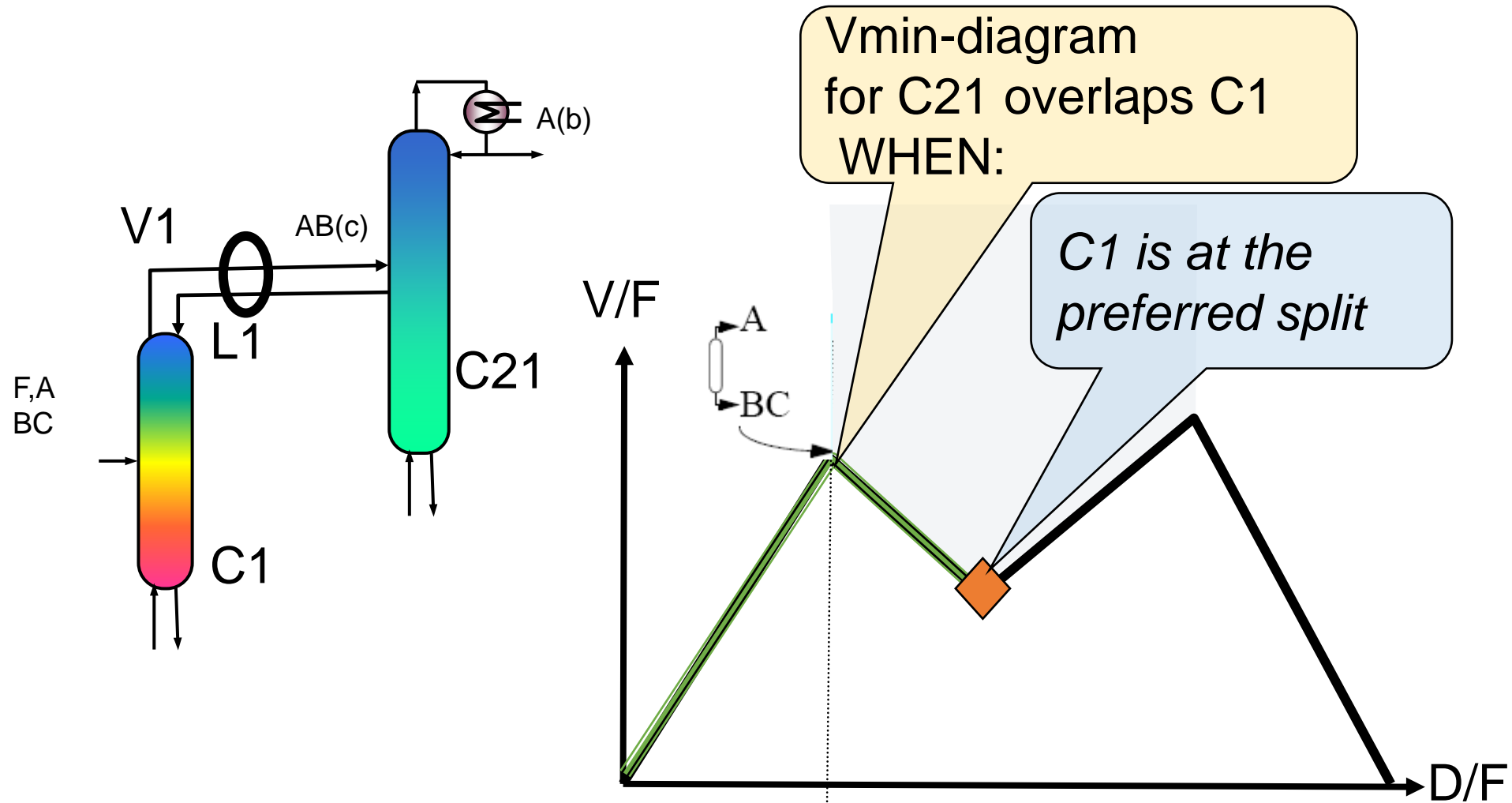
$$F_{21} = D_1 = V_1 - L_1$$

$$q_{21} = -L_1 / D_1$$

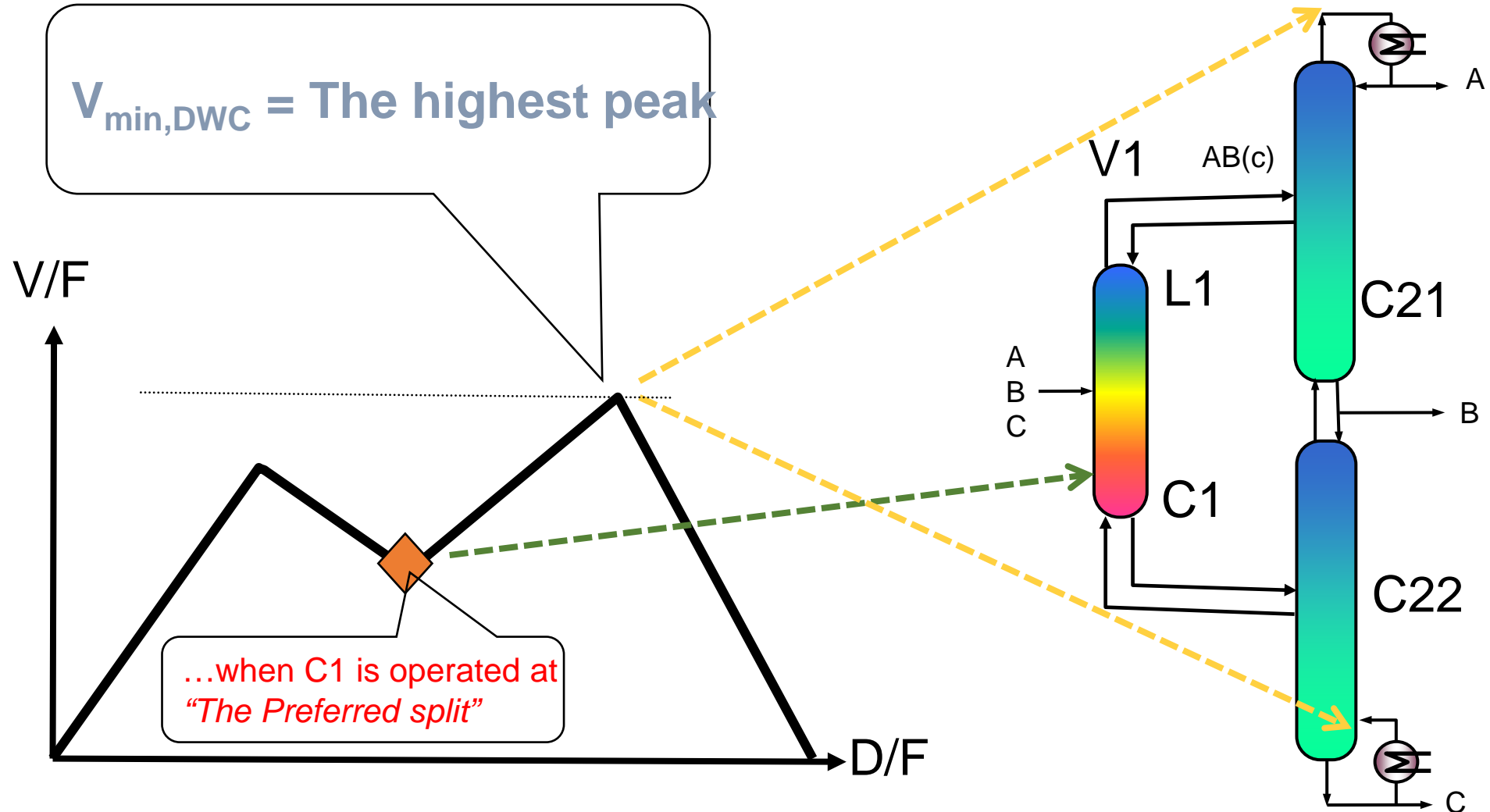
$$z_{21} = [r_{A1}, r_{B1}, \dots] F / D_1$$



# The $V_{min}$ -diagram – for thermally coupled columns

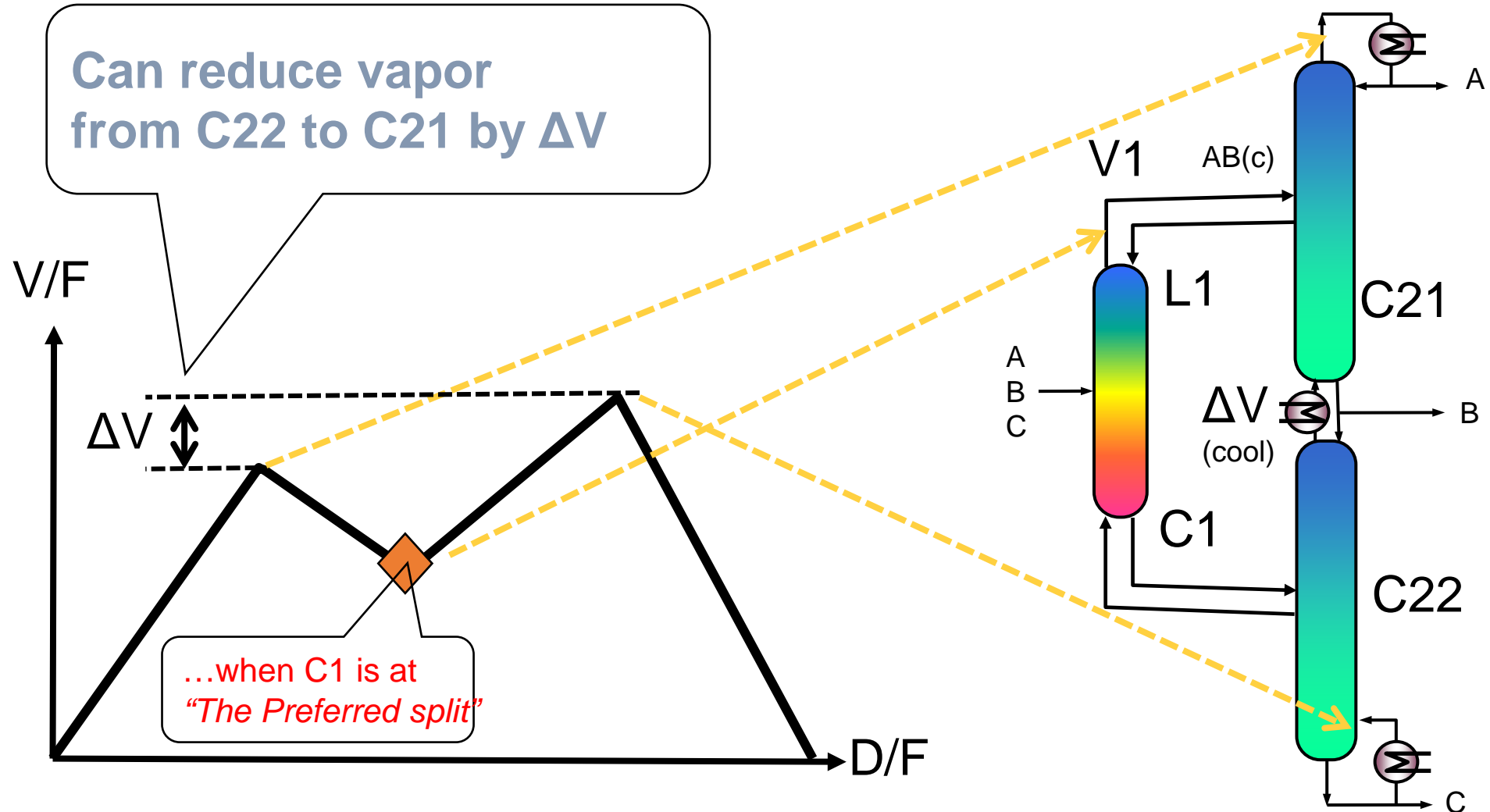


# The $V_{min}$ -diagram contains – optimal DWC flow rates



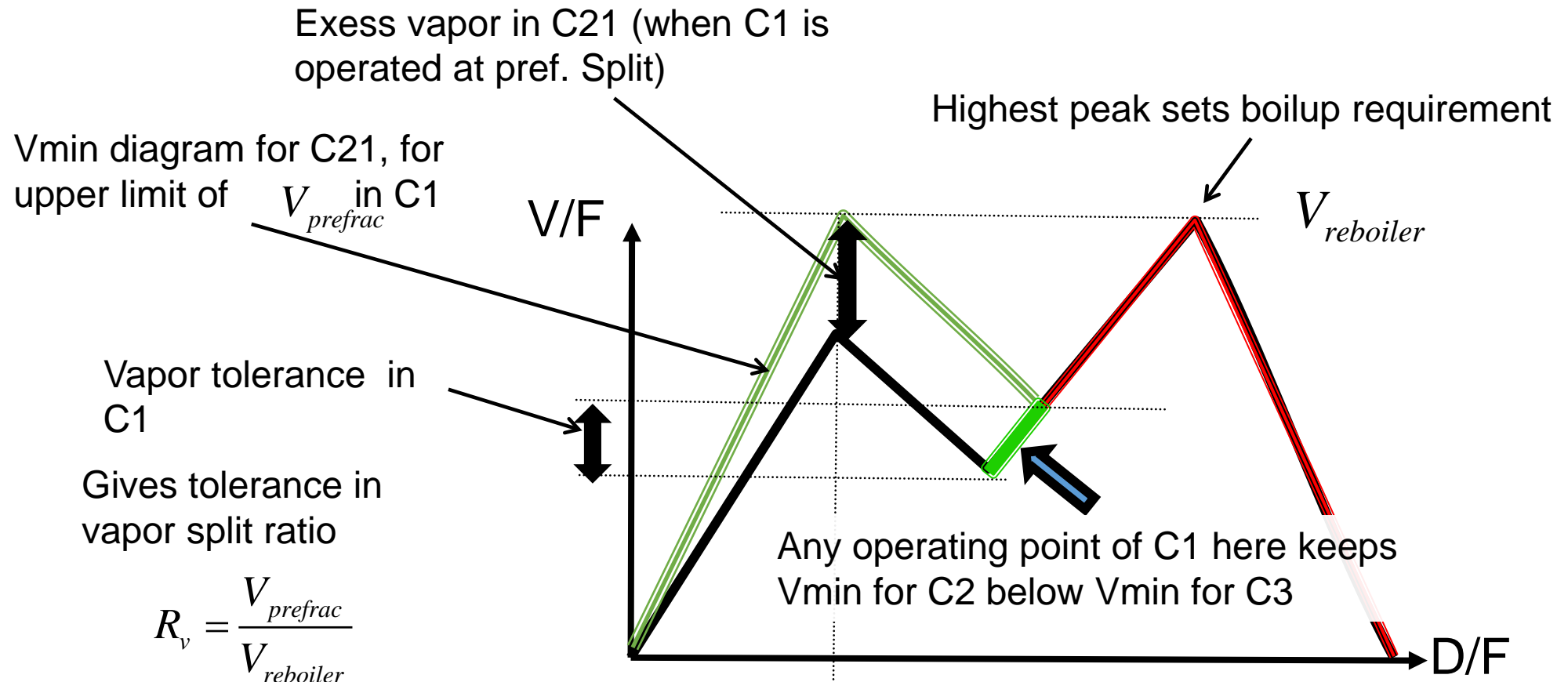


# The $V_{min}$ -diagram – Heatex at Sidestream location



# The $V_{min}$ -diagram – shows clearly DWC flexibility

**Key: Different height of the peaks gives tolerances in operation and design**



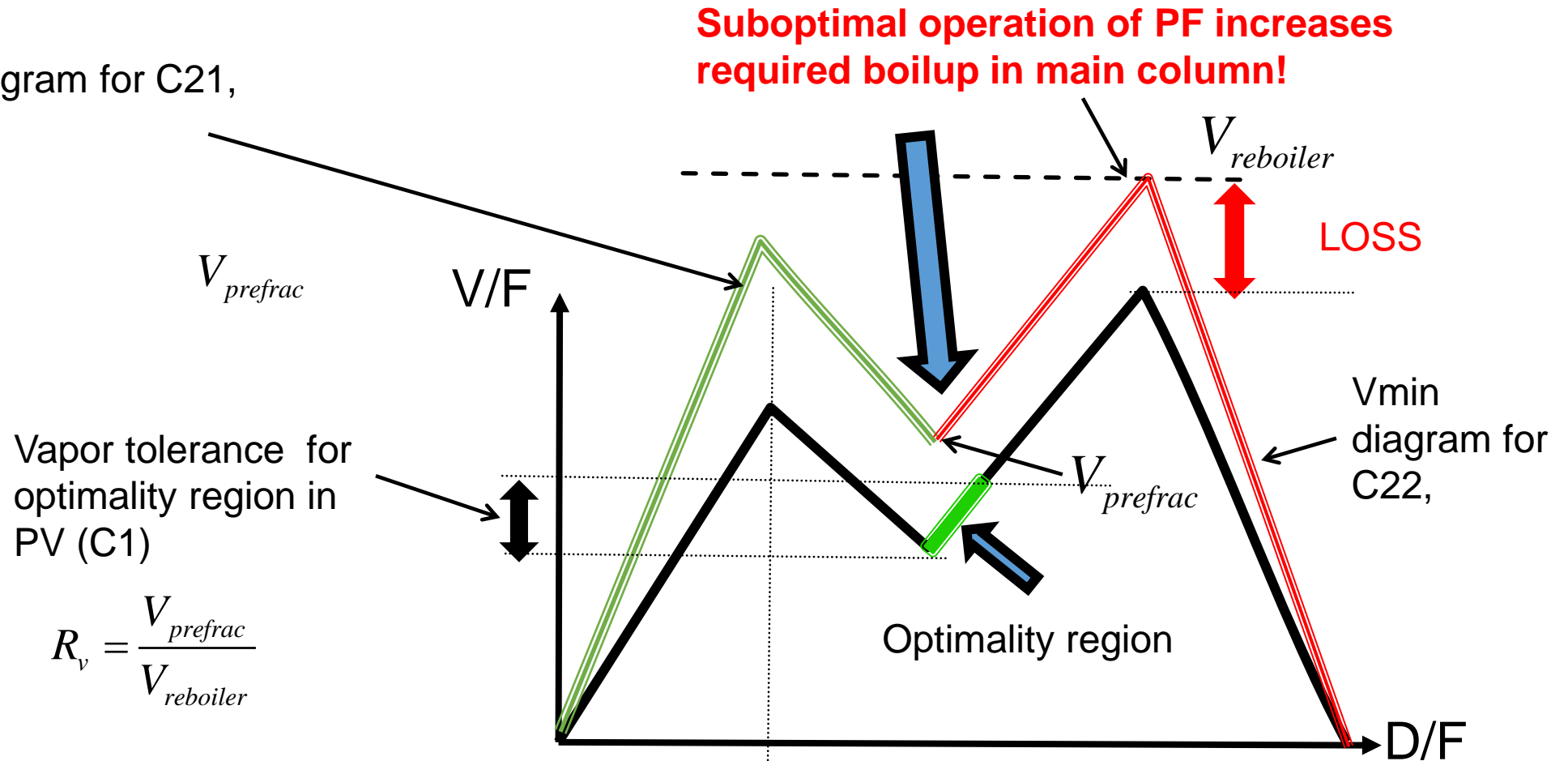
$$R_v = \frac{V_{prefrac}}{V_{reboiler}}$$



# The $V_{min}$ -diagram – How to operate prefractionator

**Key: Very important to operate prefractionator in optimality region**

Vmin diagram for C21,



Vapor tolerance for optimality region in PV (C1)

$$R_v = \frac{V_{prefrac}}{V_{reboiler}}$$



# The $V_{min}$ -diagram – How do the splits move the operating point in the prefractionator

Liquid split  $R_L = \frac{L_{prefrac}}{L_{condenser}}$

Vapor split  $R_v = \frac{V_{prefrac}}{V_{reboiler}}$

Prefractionator flowrates

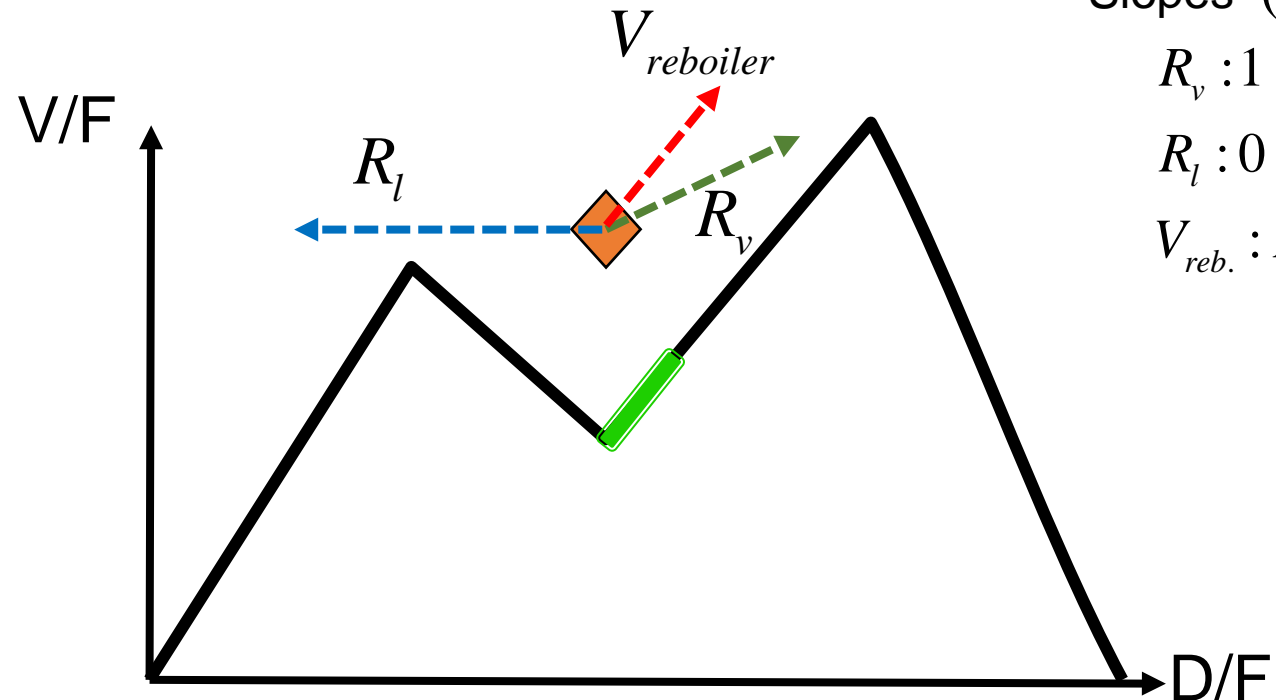
$$D_{prefrac} = R_v V_{reboiler} - R_l L_{condenser}$$

$$V_{prefrac} = R_v V_{reboiler}$$

$$L_{condenser} \approx V_{reboiler} - D_{condenser}$$

$$D_{prefrac} = V_{prefrac} - L_{prefrac}$$

How operating point is moved by increase in  $R_v, R_l, V_{reboiler}$



Slopes ( $\Delta V / \Delta D$ )

$$R_v : 1$$

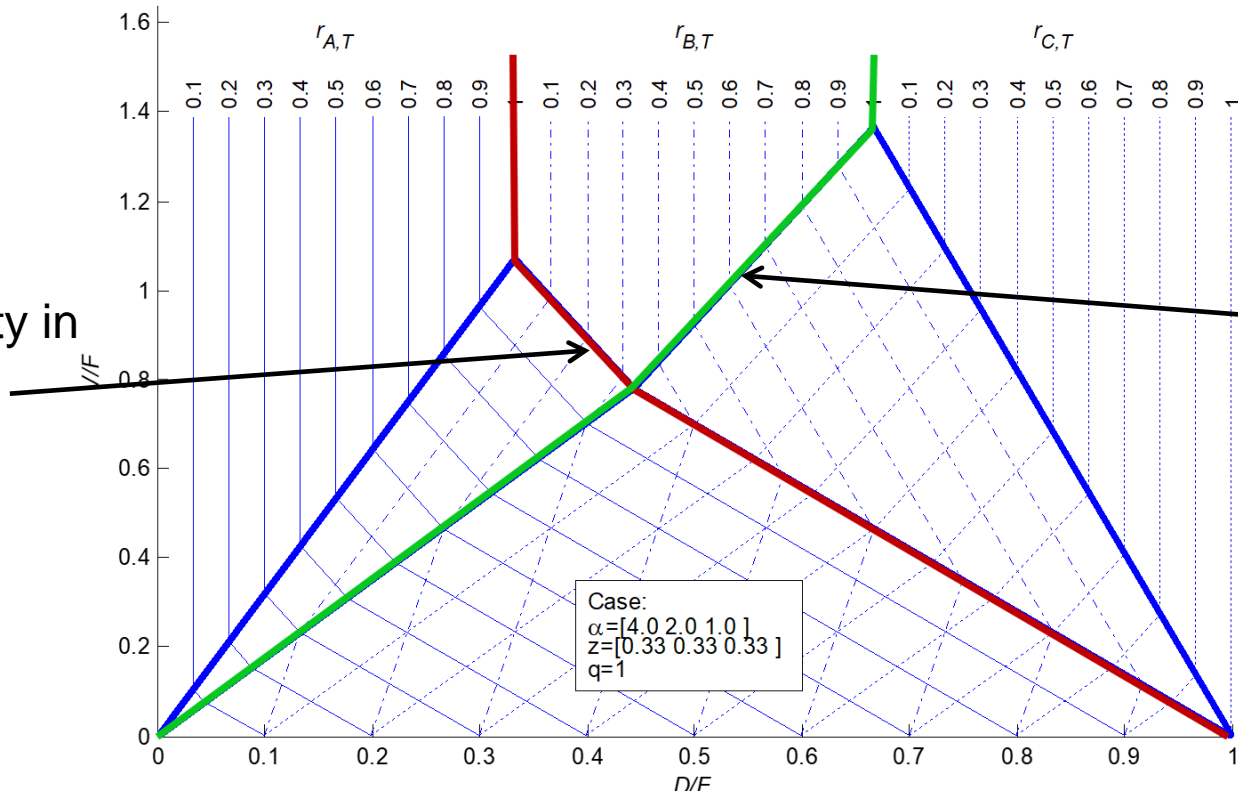
$$R_l : 0$$

$$V_{reb.} : R_v / (R_v - R_l)$$



# How to recognize that operation is close to a distribution boundary

Line where A-impurity in bottom is small (e.g. about 0.1%)



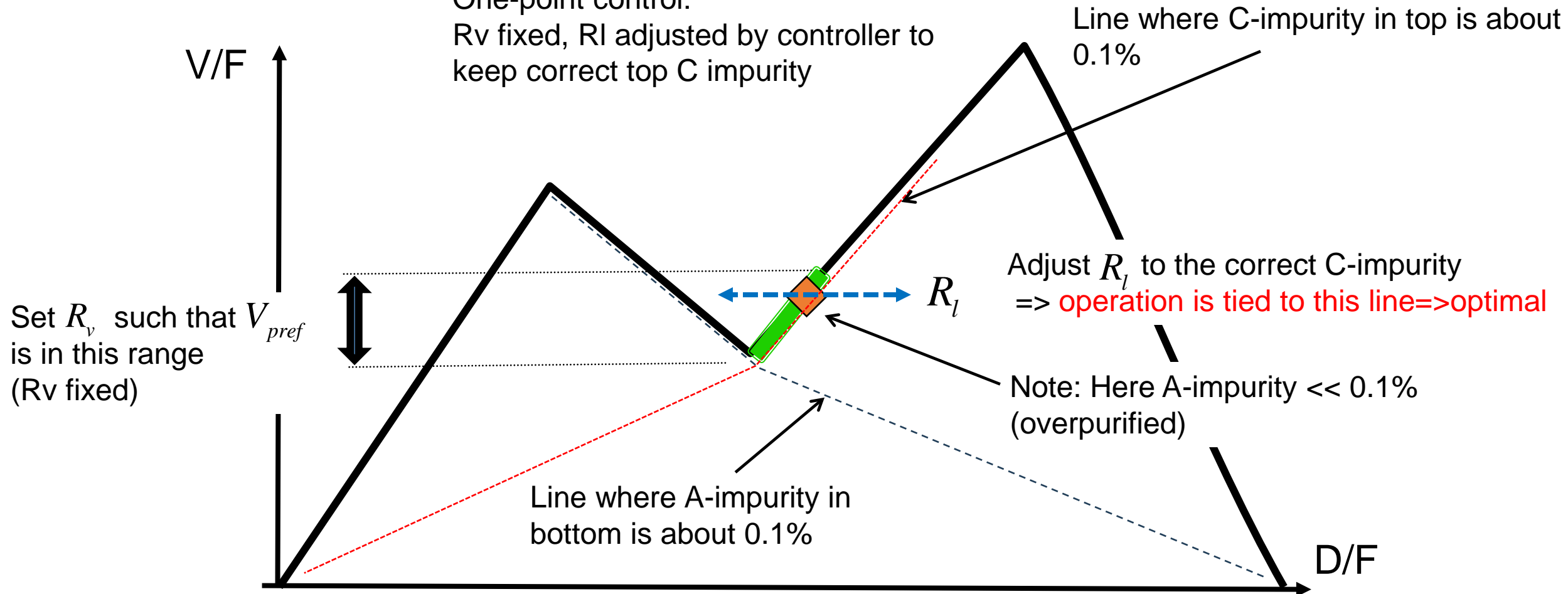
Line where C-impurity in top is small (e.g. about 0.1%)

Distribution boundary: A component is at the limit of disappearing in one end – this is characterised by a small impurity – but not overpurification!



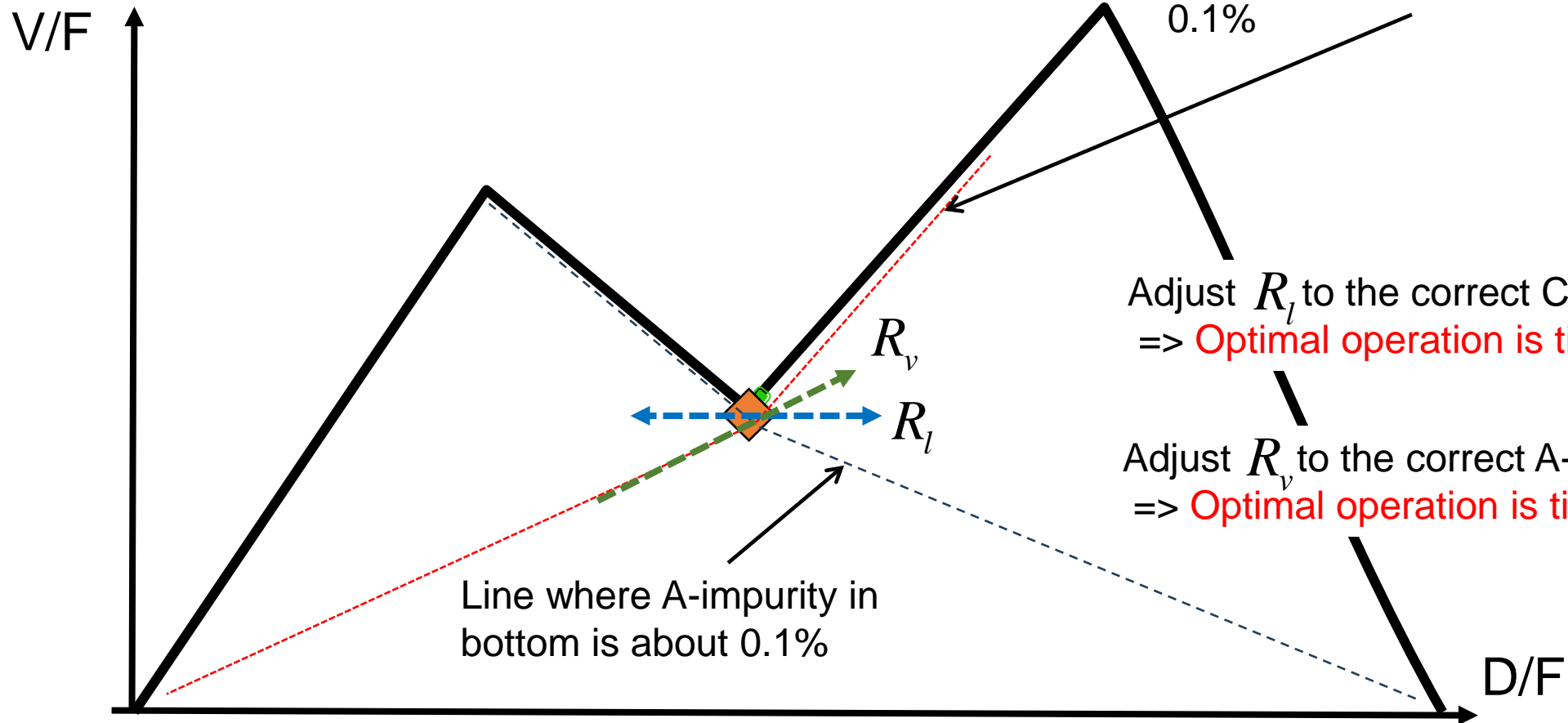
# How to select controlled variables in prefrac.

Typical:  
One-point control:  
 $R_v$  fixed,  $R_l$  adjusted by controller to keep correct top C impurity



# How to select controlled variables in prefrac.

Want preferred split => Require Two-point control:  
R<sub>l</sub> adjusted by controller to keep correct top C  
R<sub>v</sub> adjusted by controller to keep correct bottom A



Adjust  $R_l$  to the correct C-impurity  
=> Optimal operation is tied to the line

Adjust  $R_v$  to the correct A-impurity  
=> Optimal operation is tied to the line



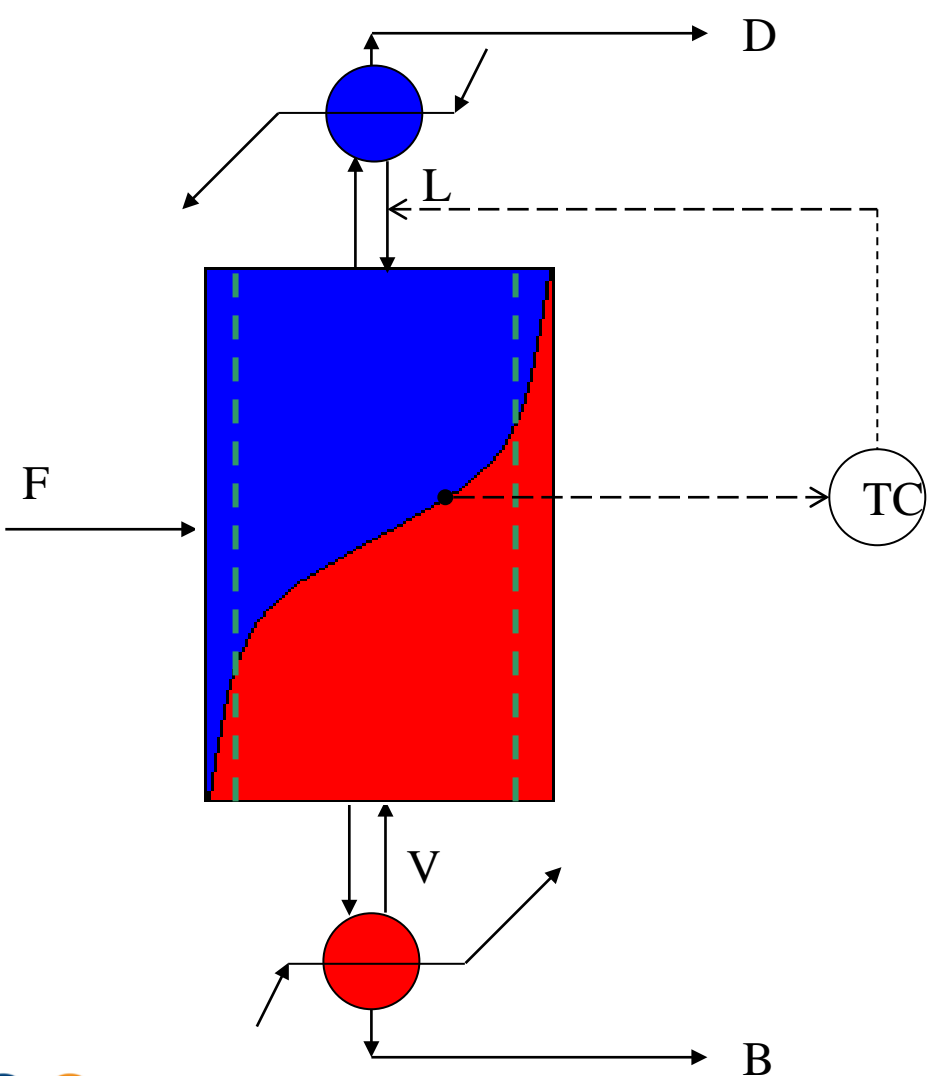
# Practical control: Use temperatures

- Direct composition control is not common
- Use temperature profile to infer composition estimate
- May also use combination of temperature points

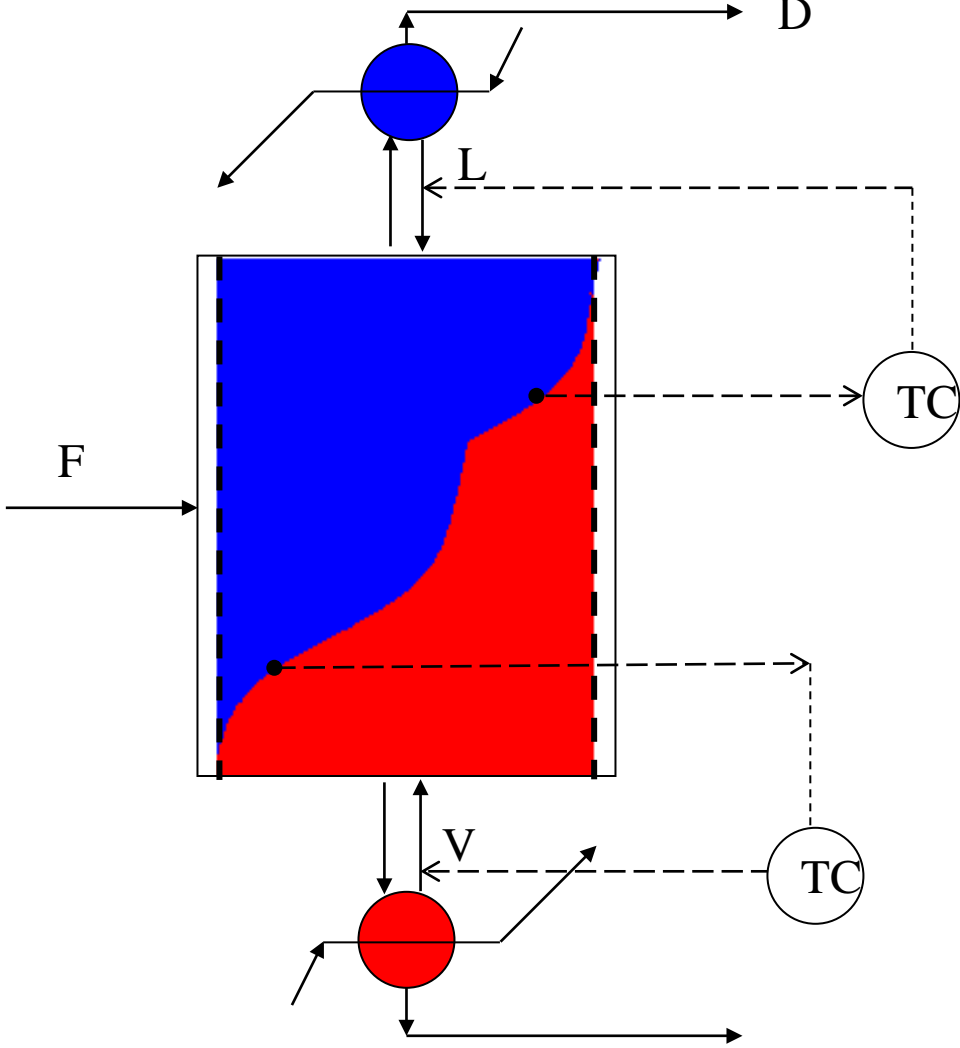




# One-point control



# Two-point control



# When is active vapor split beneficial ?

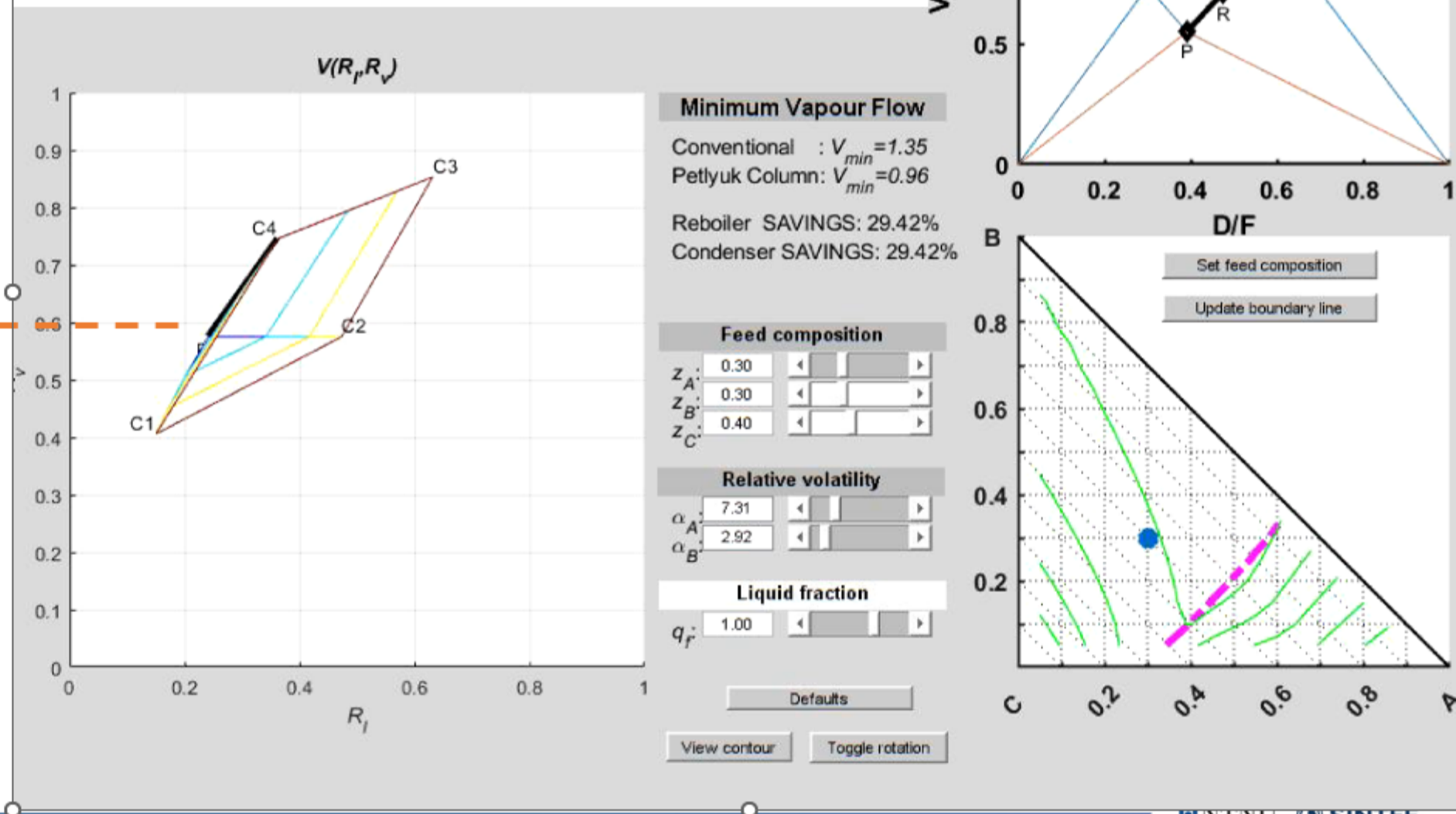


# Optimality is obtained only in a narrow region for the flow splits

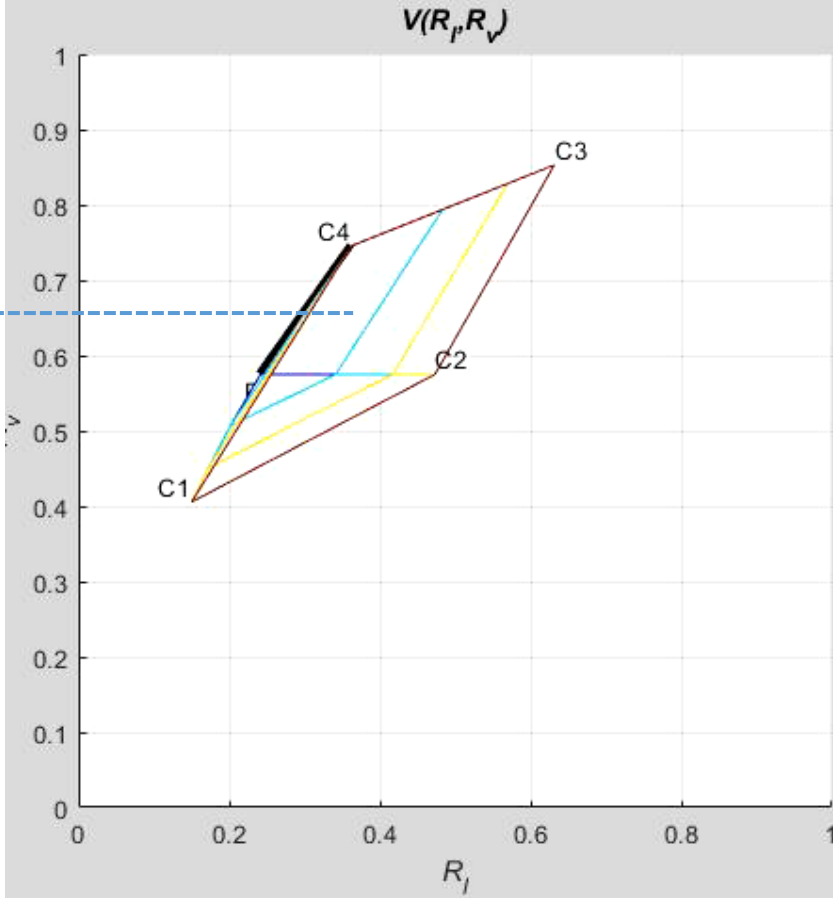
How manipulation of feed liquid fraction can move the optimal vapor- and liquid-splits

Ex: Fix  $R_v=0.6$

Avoid uncontrolled variations in feed liquid fraction



# Petlyuk column boilup (V) as function of split ratios



## Minimum Vapour Flow

Conventional :  $V_{min} = 1.35$   
 Petlyuk Column:  $V_{min} = 0.96$

Reboiler SAVINGS: 29.42%  
 Condenser SAVINGS: 29.42%

## Feed composition

$z_A$ : 0.30  
 $z_B$ : 0.30  
 $z_C$ : 0.40

## Relative volatility

$\alpha_A$ : 7.31  
 $\alpha_B$ : 2.92

## Liquid fraction

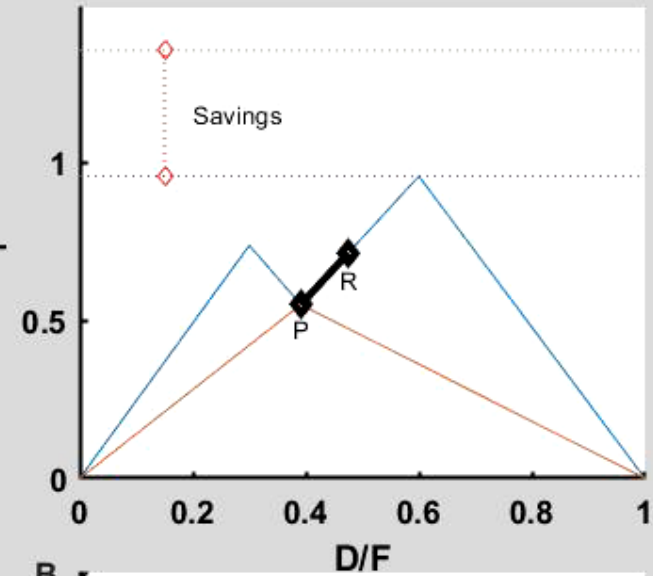
$q_f$ : 1.00

Defaults

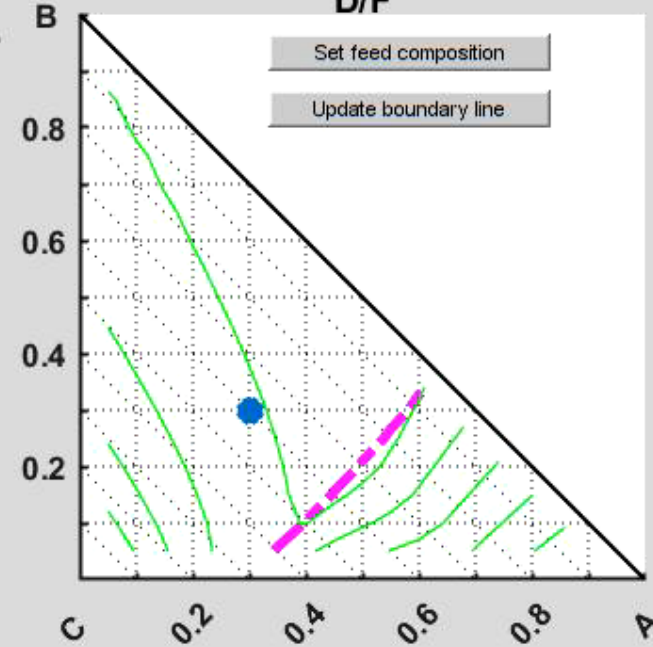
View contour

Toggle rotation

$V_{T,i}$



B



May fix Rv

Adjust RI from 0.25-0.38 to track optimum



# About the need for on-line adjustment of Vapor split

- Most (all) industrial 3-product DWCs in the world use fixed  $R_v$
- This is OK for the majority of cases.
- E.g.:  $V_{min}$ -diagram peaks are of different height.
- And when changes in feed properties (composition and liquid fraction) are limited
  
- And, if some reduced energy saving is accepted
- Or if the some sidestream impurity is accepted



# Use active vapor split when:

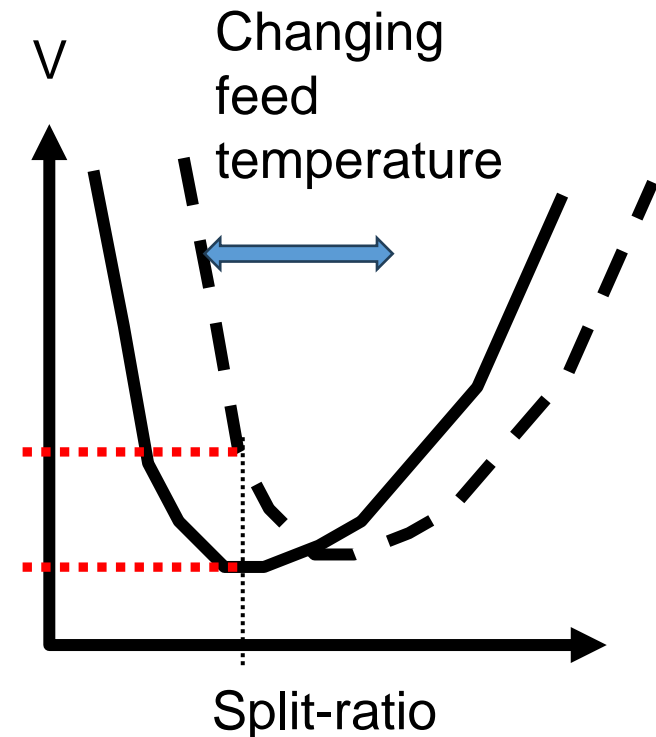
- The peaks in the  $V_{\min}$  diagram are of similar height, and/or:
  - When significant changes in feed composition is expected
  - When full energy saving is required
  - When sidestream impurity is undesirable

(Assume that number of stages is selected to enable the desired purity. )

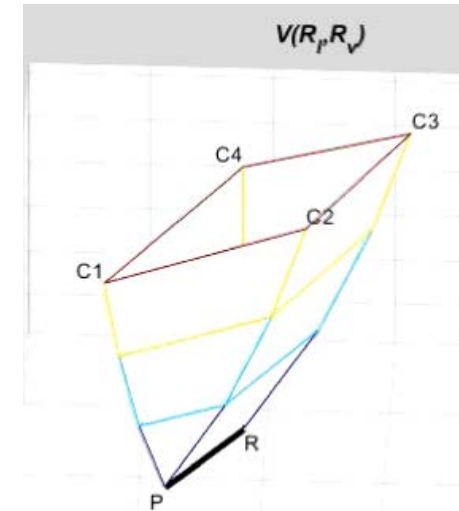
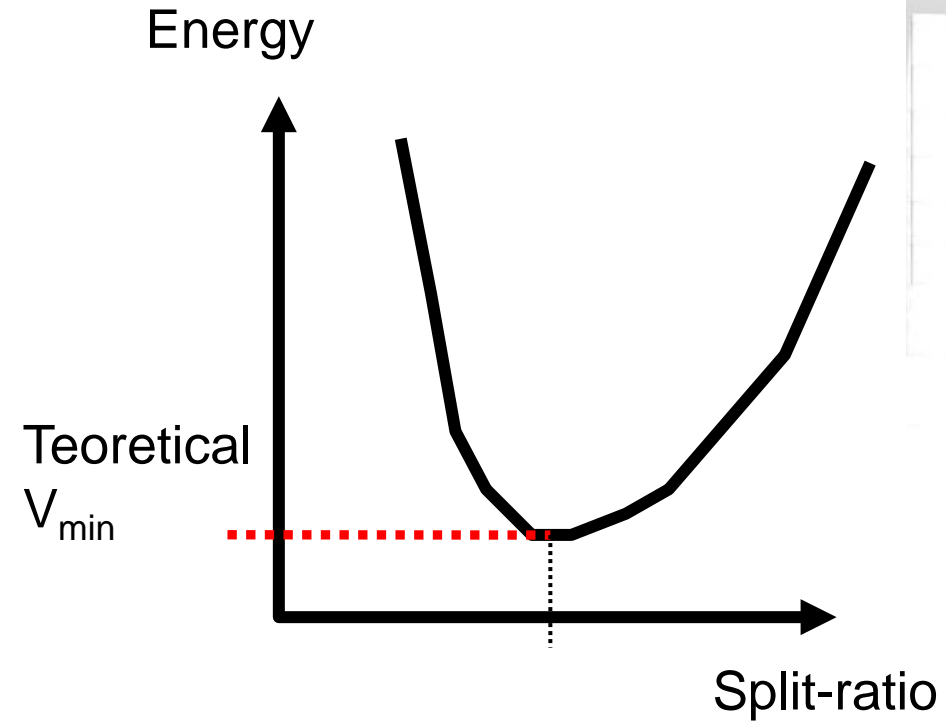
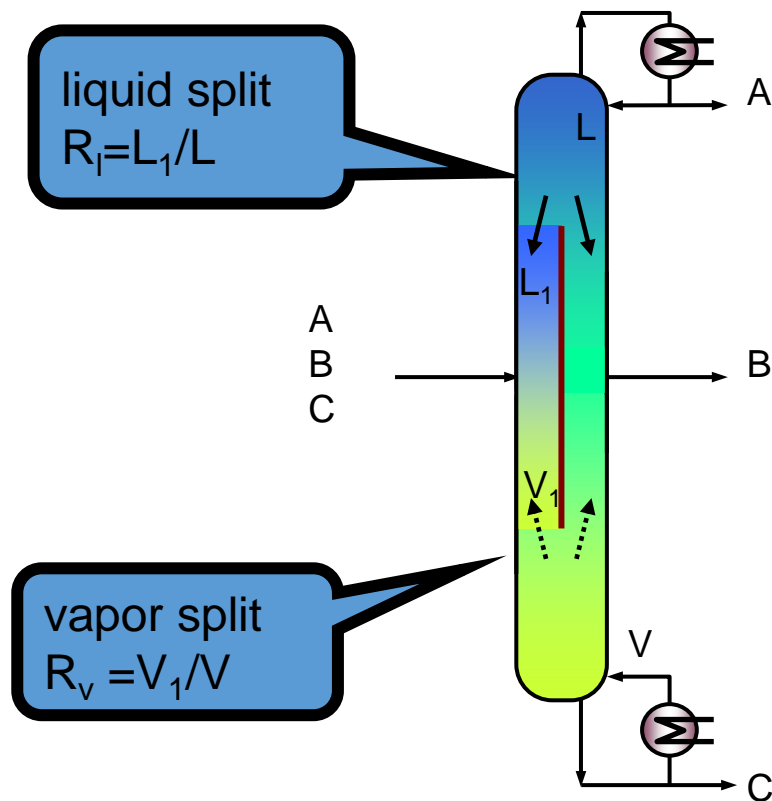


# Adjust the feed temperature: The hidden "vapor split adjustment"

- The optimality region is strongly affected by Feed liquid fraction
- **Uncontrolled Feed temperature variations are severe disturbances**
- Thus: It is strongly recommended to control feed temperature to a setpoint
- The feed temperature controller setpoint becomes an additional degree of freedom!
- The impact is not by affecting the internal split, but to **MOVE** the whole **OPTIMALITY** region such that the actual column split becomes **INSIDE** the optimality region!

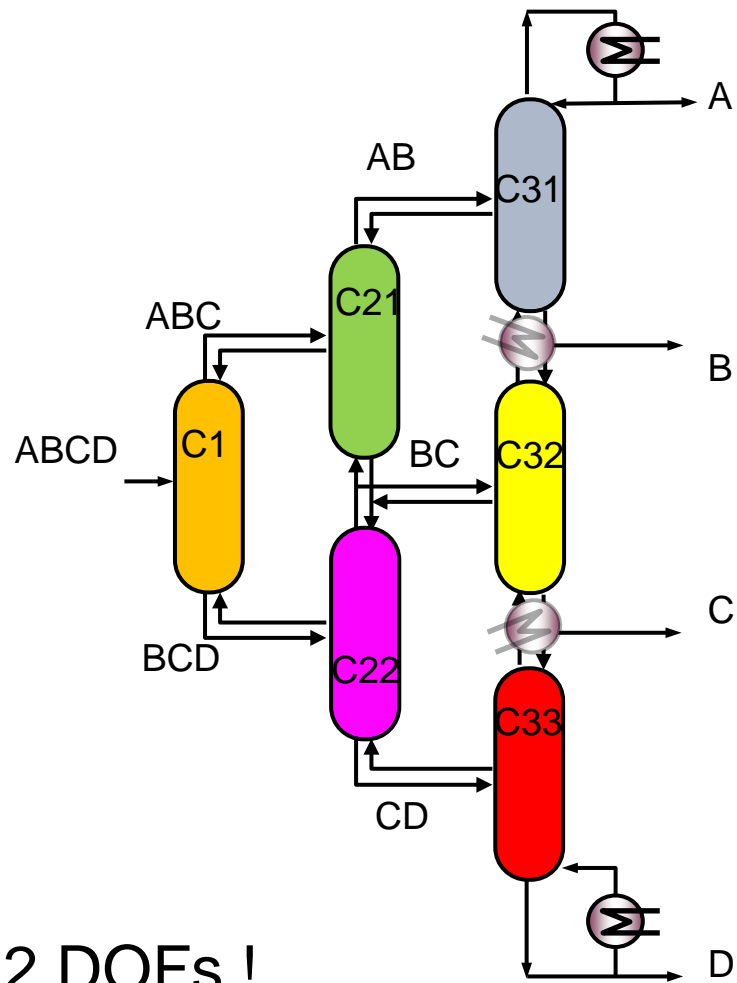


Important for obtaining savings in practice:  
**Adjust/Control the splits. At least one!**



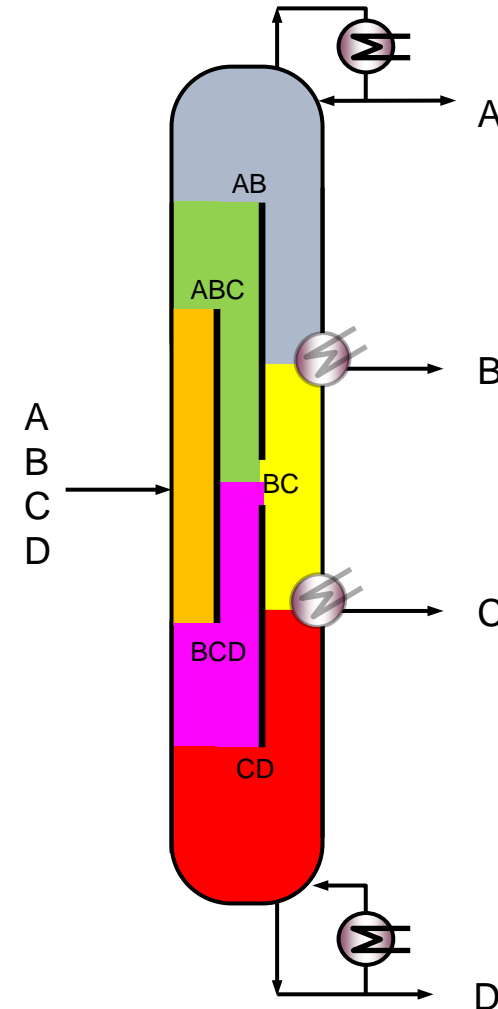


# Generalized 4-product DWC

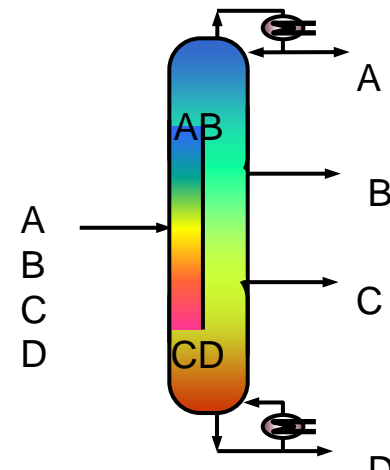
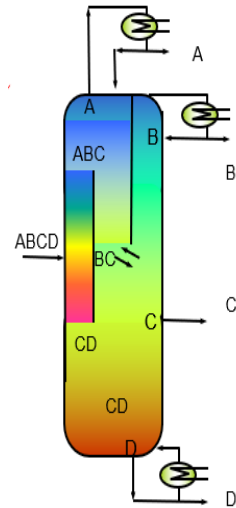
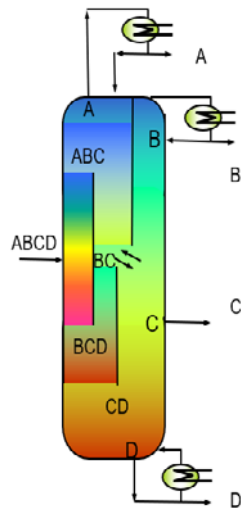
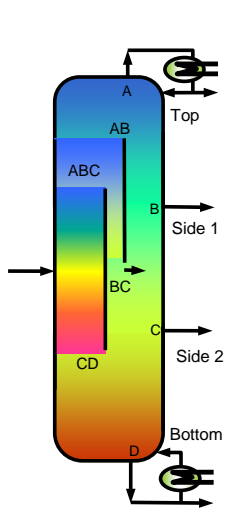
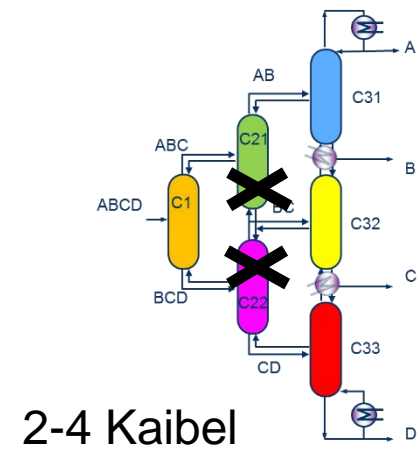
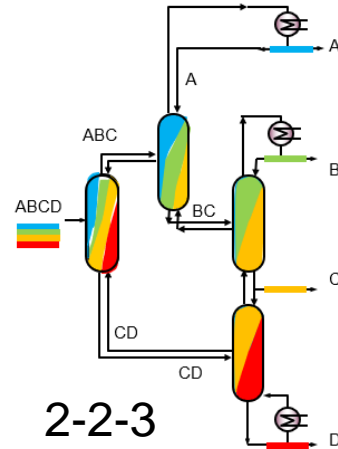
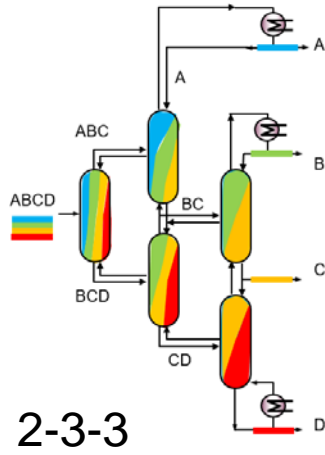
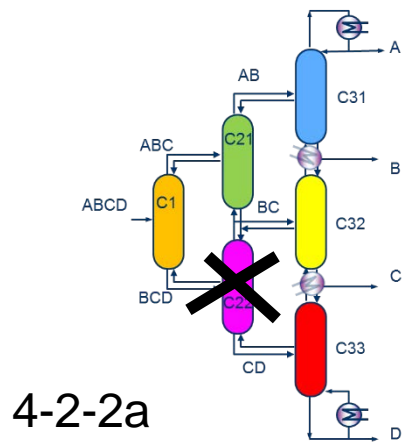


12 DOFs !

The Vmin-diagram can be used to identify possible simplifications for specific classes of feeds



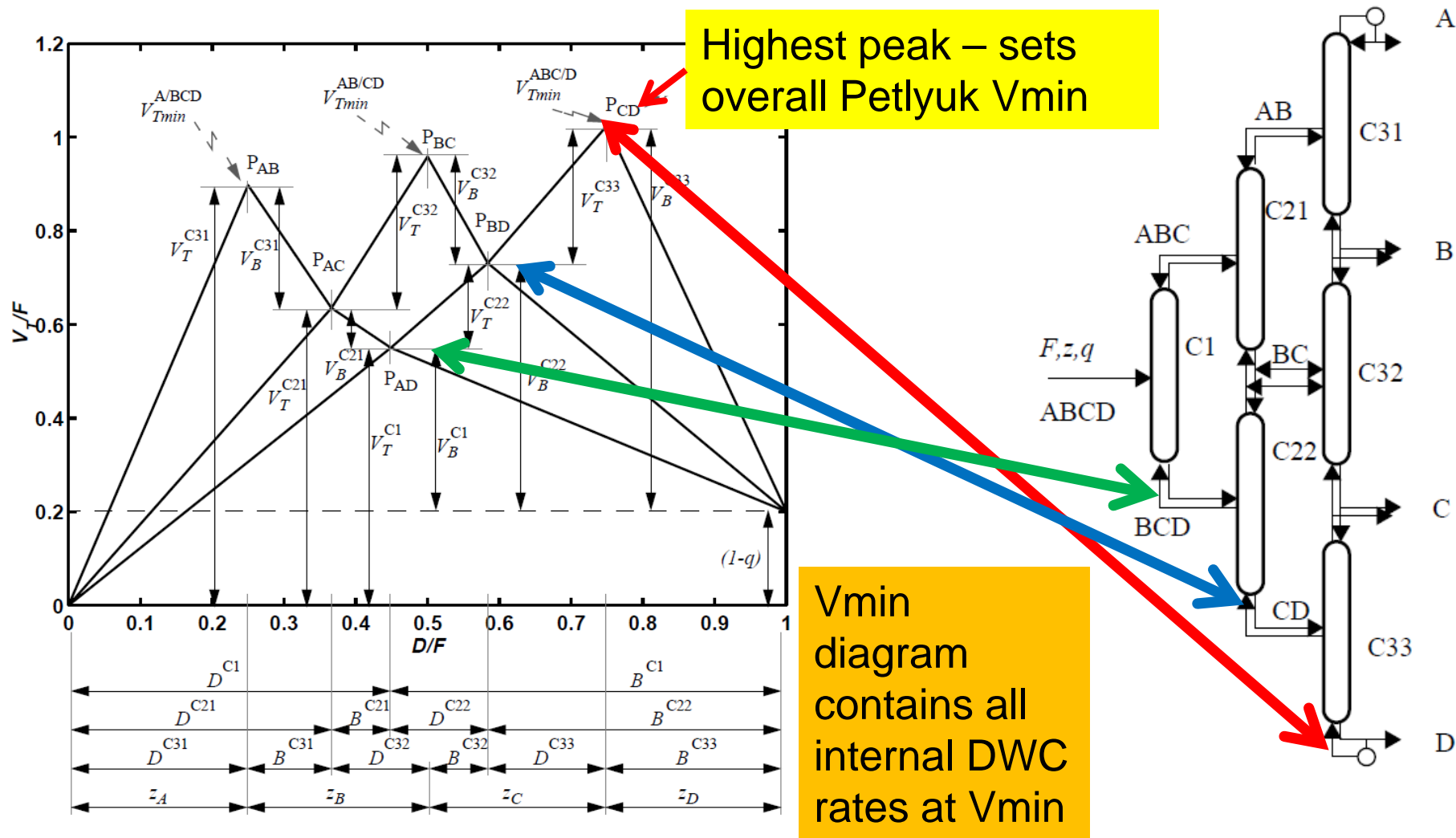
# Several different 4-component arrangements can be obtained by simplifying the general arr.



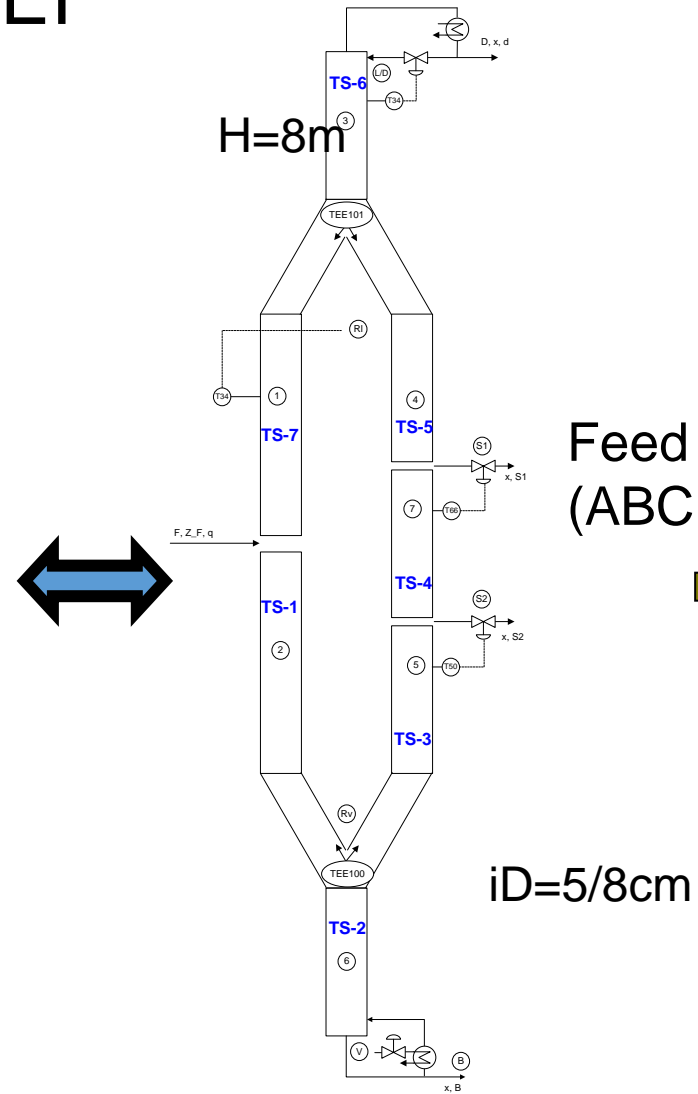
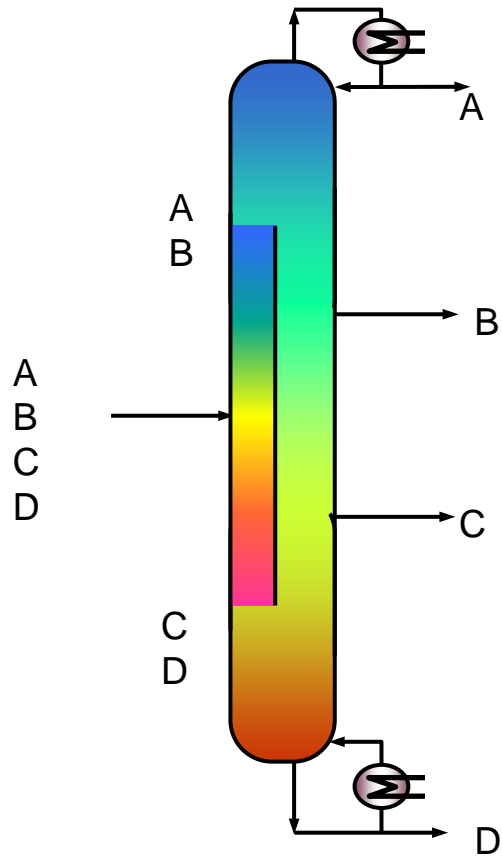
Can reach same savings as full 4p structure (for some feeds)

Less savings

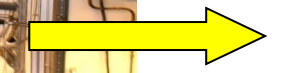
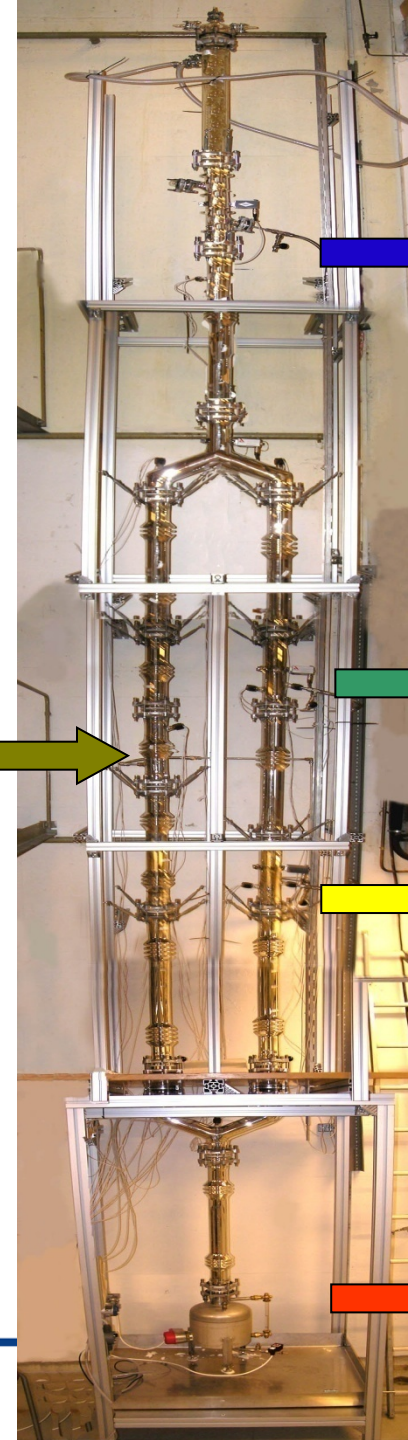
# Vmin diagram for 4-product DWC/Petlyuk



# The Kaibel column at NTNU/SINTEF



Feed (ABCD)



A

B

C

D



# Vmin diagram – Kaibel column

**Kaibel Column:**

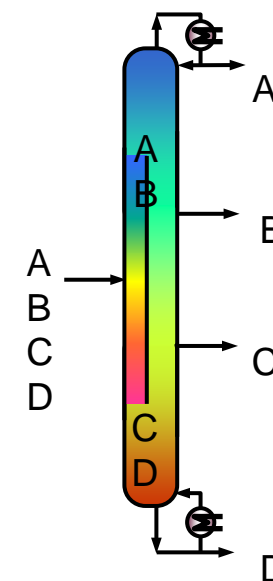
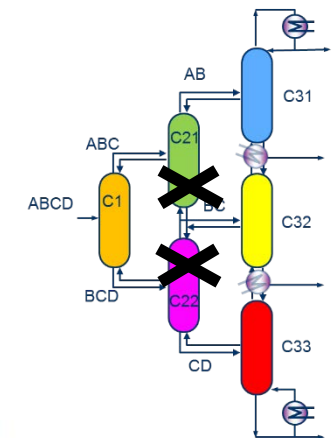
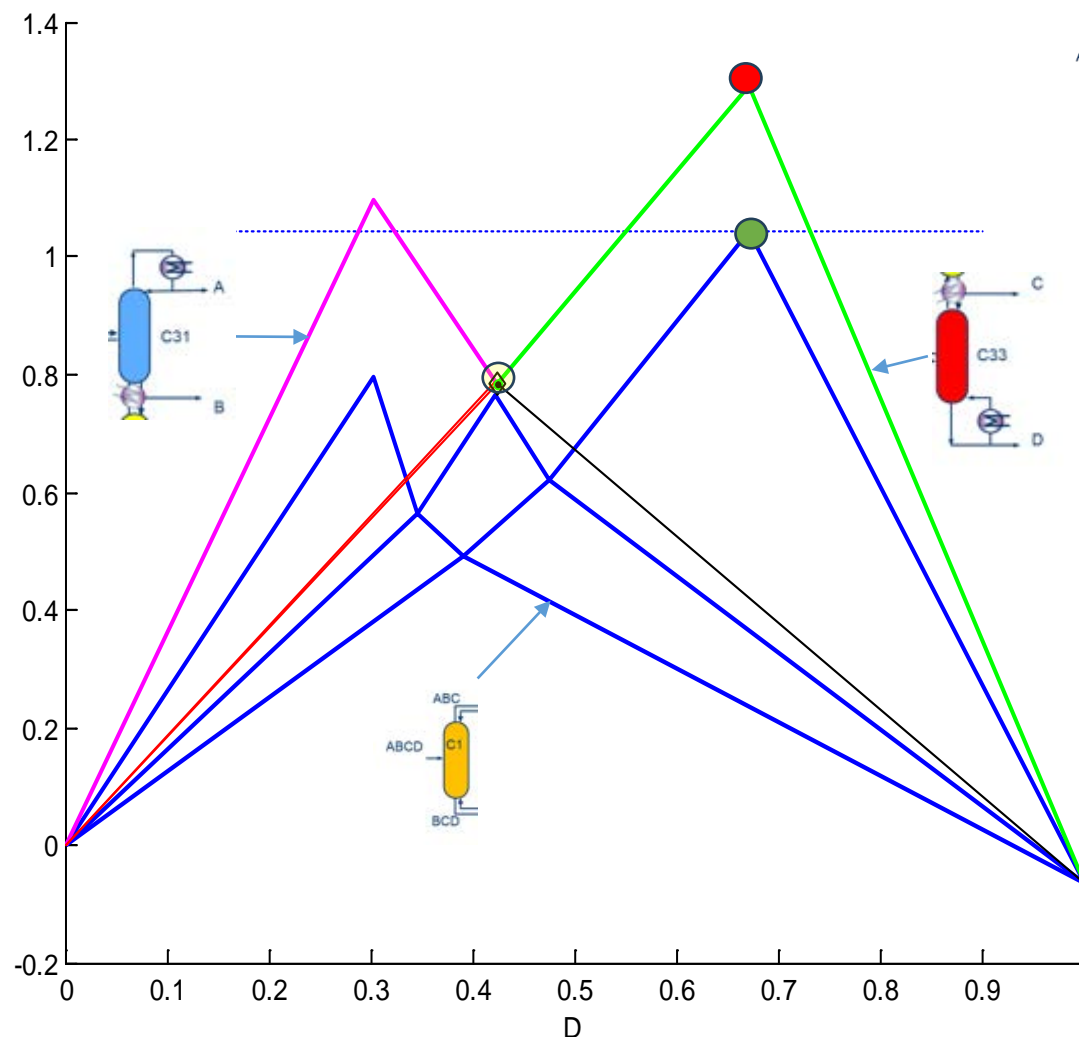
Do sharp AB/BC split in C1

⇒

Lifted peaks and minimum boilup

⇒

But can remove a partition wall!  
(C21+ C22)



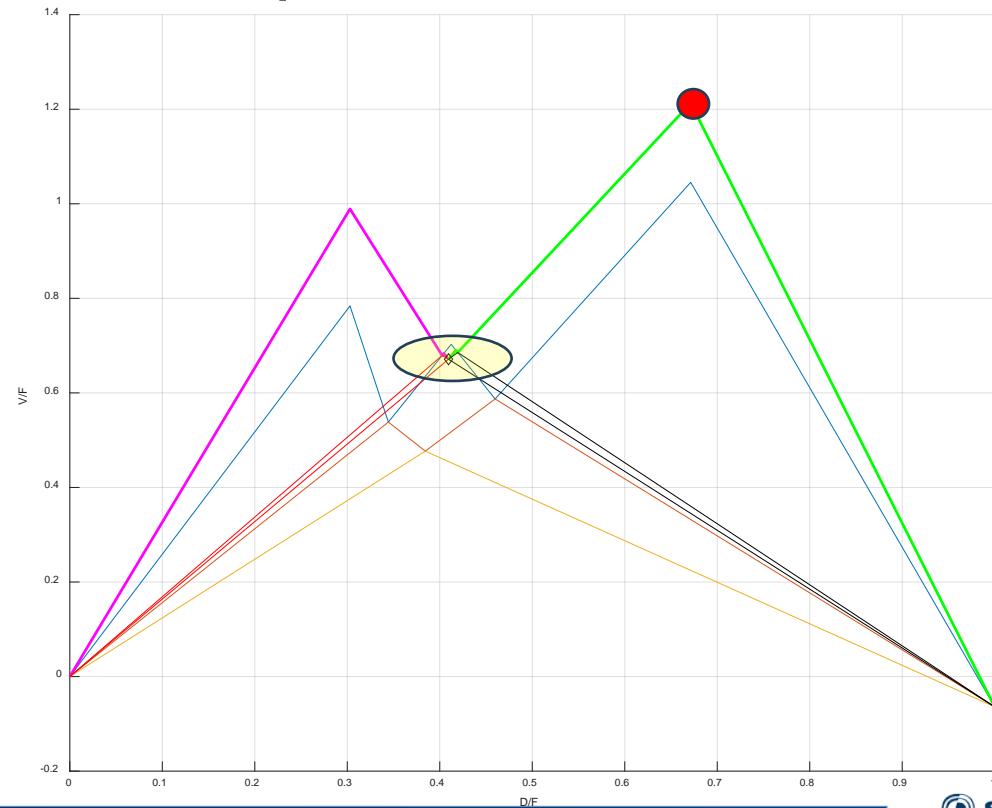
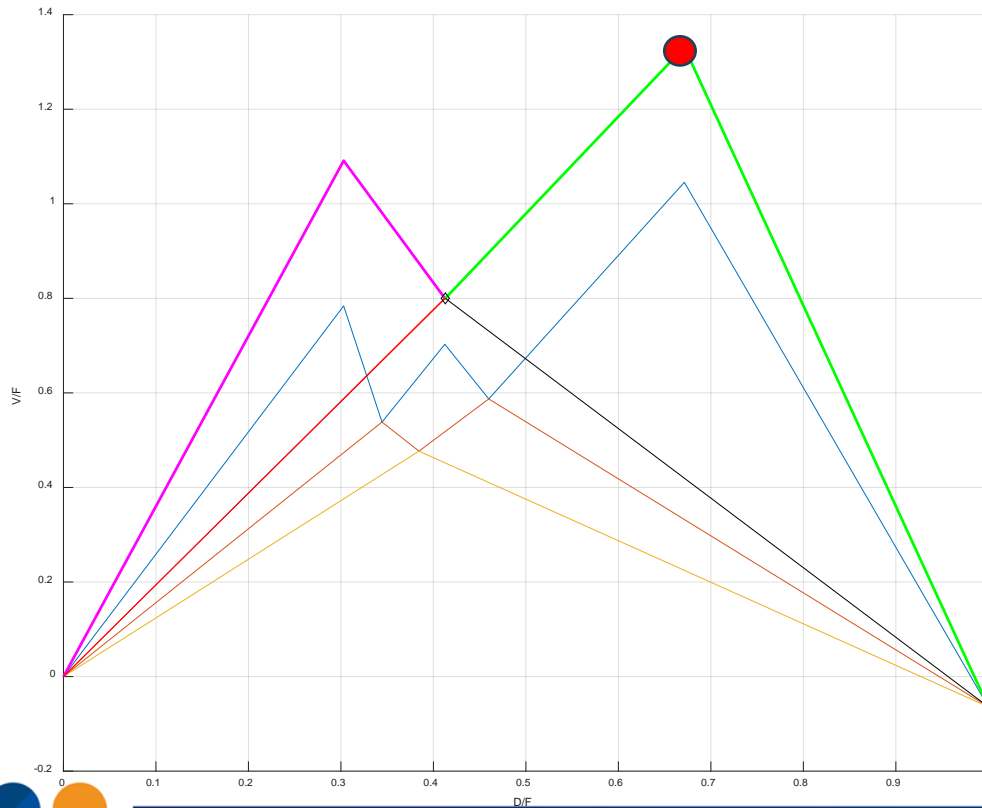
Kaibel  
2-4



# Options with one-point control

- Higher energy in prefrac=> Higher reboiler duty

- Impure AB/CD split =>
- Lower reboiler duty, but impure side streams



# Kaibel column needs active use of both splits to achieve potential energy savings

- There is not a "wide optimality region" for the Kaibel-column
- Optimal operation of the pefractionator is exactly at the B/C split.
- Require two-point control for achievement of full savings
- One-point control can be used if increase in total reboiler duty can be accepted. (Reduced effective savings)
- Or, if significant impurities can be accepted in the side-streams



# Conclusion

- DWC columns are attractive for savings in both energy & capital
- Some separations are particularly well suited and easy to control
- Some separations require more precise control of the prefractionator, including on-line adjustment of vapor split
- As we will show in the following: Feedback control by manipulating vapor split is very important



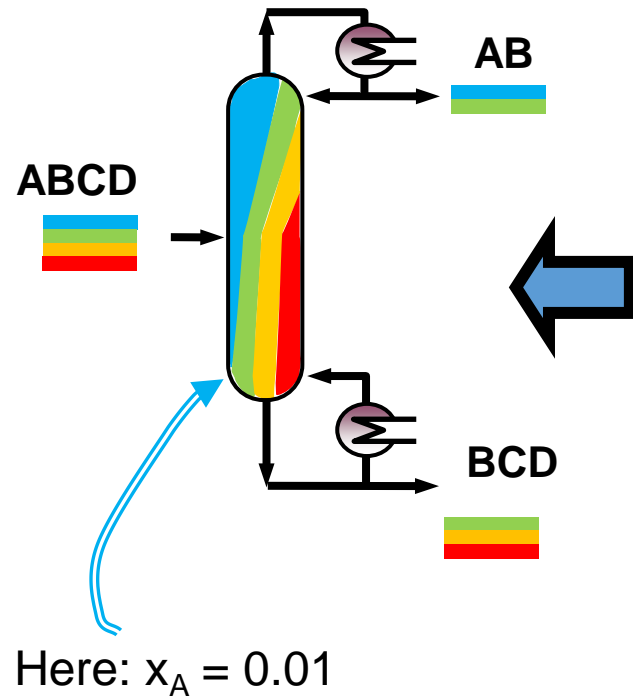


# Extras



# How to find $V_{\min}$ -diagram by simulations on a conventional 2-product simulation

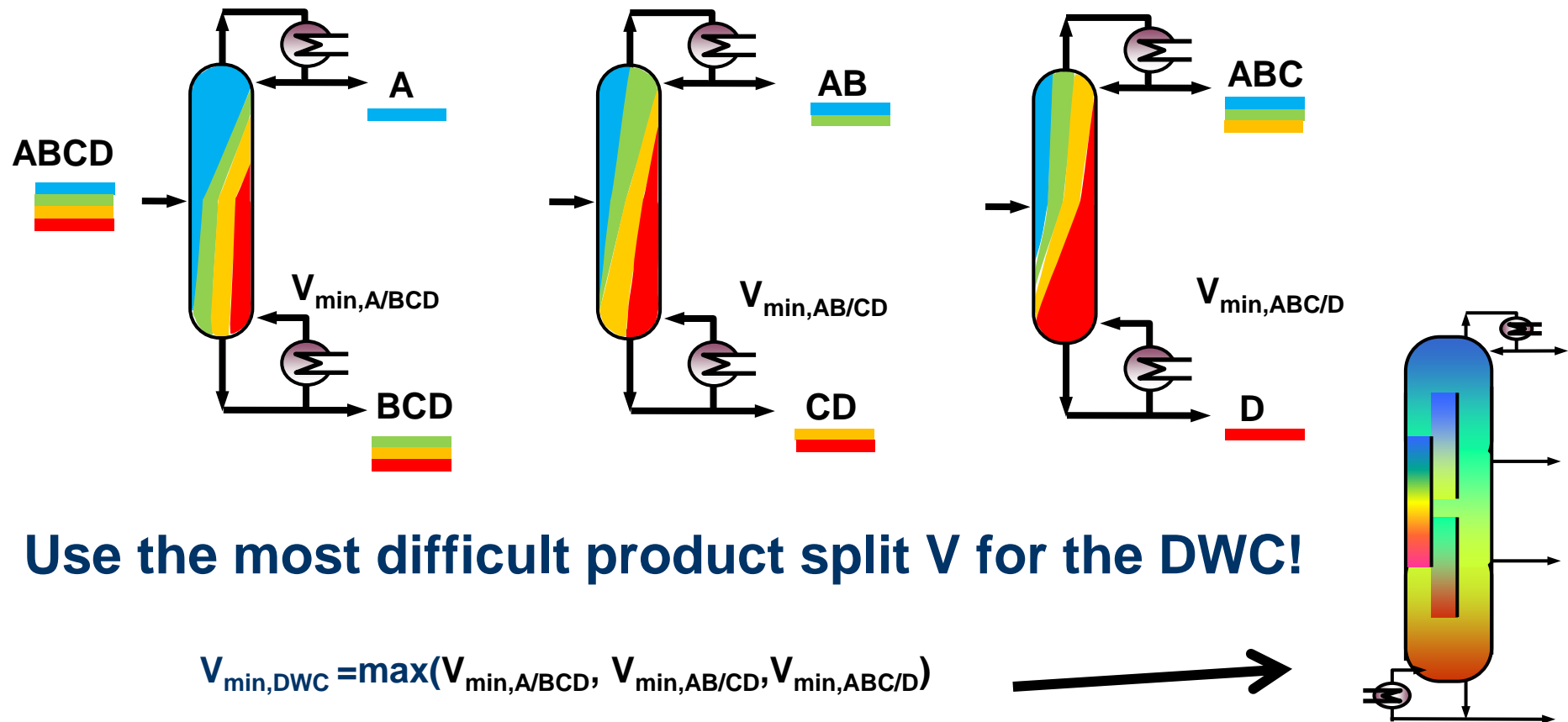
## Method no 1



- Specify small impurity for components to be removed from each column end.
- E.g. The AB/BCD split  $V_{\min}$ -spec is:
  - Top:  $x_C = 0.01$  (remove C,D in top)
  - Bottom:  $x_A = 0.01$  (remove A in bottom)
- Use large number of stages ( $4 \times N_{\min}$ )
- Confirm by observing the profile of the impurity component composition approaching zero close to the end

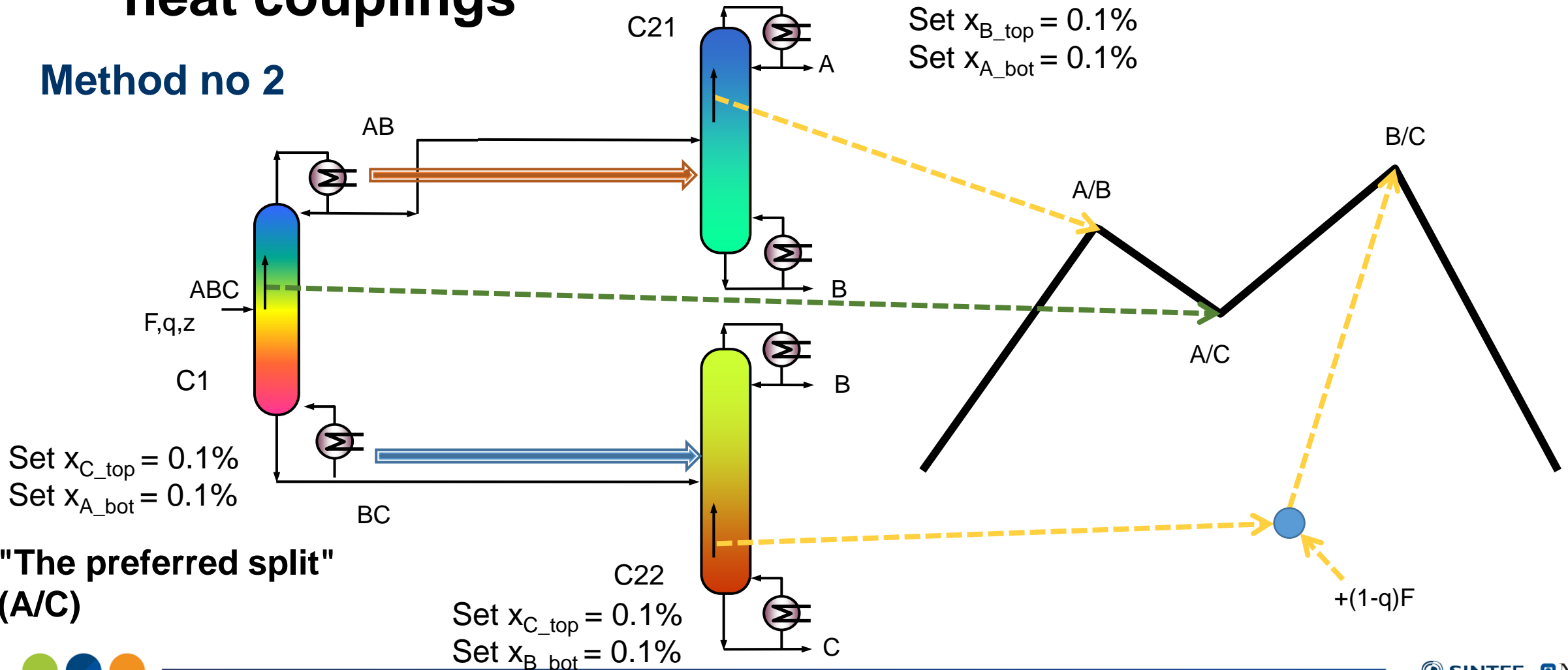
# Amazingly simple to find $V_{\min}$ for DWC

4-product example, just consider 3 separate sharp split cases:



# The Vmin-diagram can be found directly from internal flows of the "equivalent conventional columns with heat couplings"

## Method no 2



"The preferred split" (A/C)



# How to get around complex simulation initialisation and simulator recycle blocks

- Simulate for the Vmin-diagram with real mixtures by using equivalent sequences of heat integrated conventional columns
- Initial specifications: Every column should run at its "local" preferred spec.
- This will reveal which internal separation that is most demanding
- Operation of the other columns in the arrangement can then be altered until their operation "moves" and increases the most demanding
- Main advantages
  - Simple one-pass conventional column simulations without need for "simulation recycle blocks"
  - Obtain flow rates for direct initialisation of thermally coupled sections (use two model twins, one with conventional equivalents and one with the physical correct setup).



# Based on proposal from Halvorsen (2001):

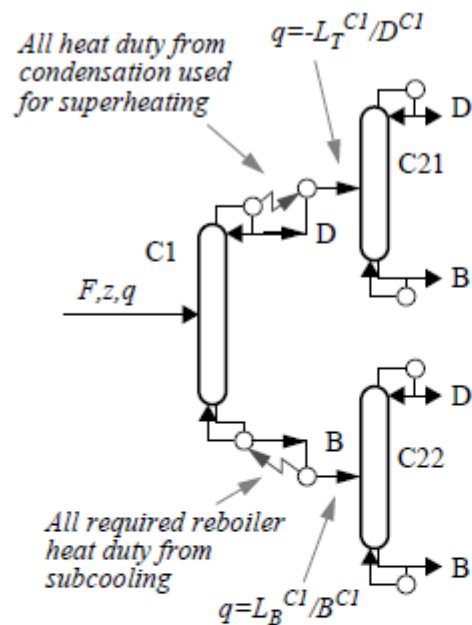


Figure D.1:  
Computational equivalent to  
the Petlyuk arrangement

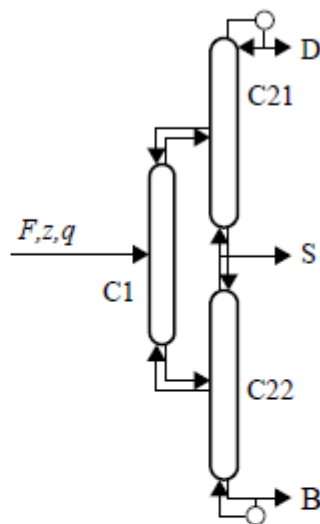


Figure D.2:  
Petlyuk arrangement

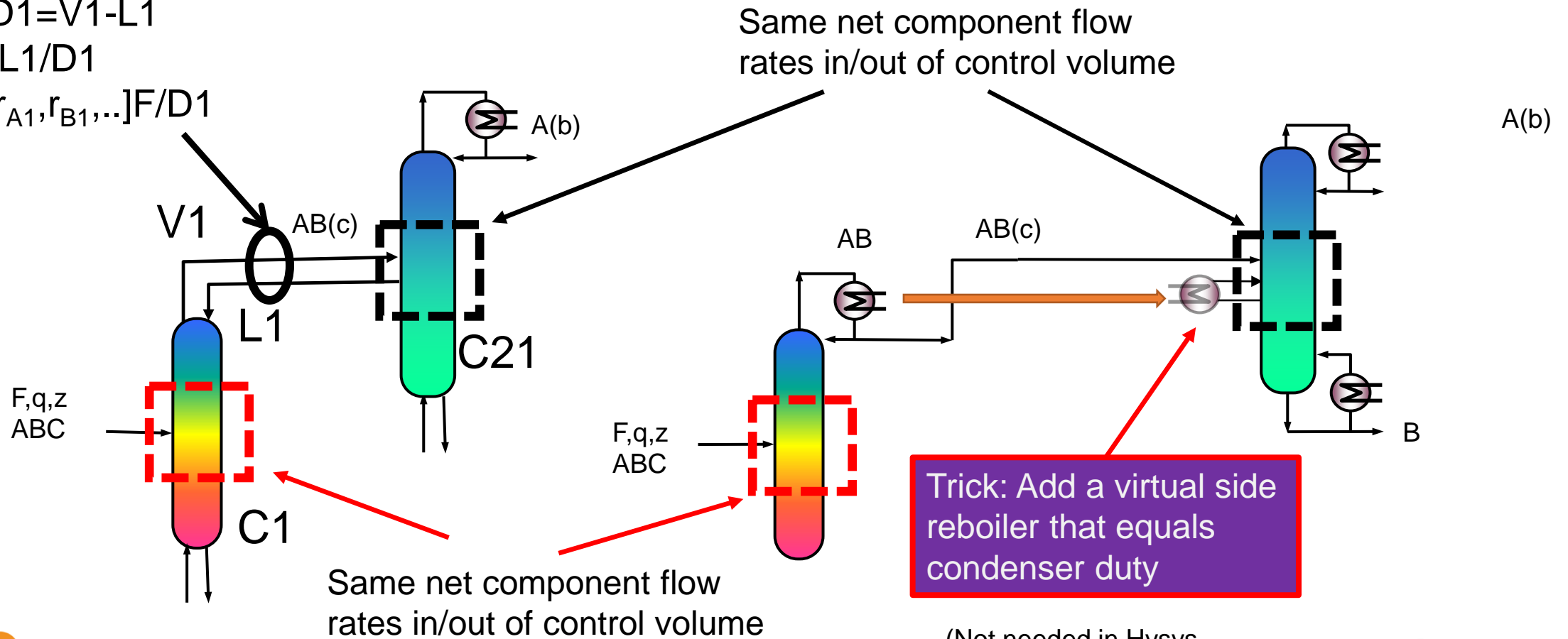
- Use the same internal flow rates in both configurations
- The two-way full thermal coupling is equivalent to direct coupling + virtual heat coupling (some restrictions apply)
- E.g.: Hysys allows direct heat coupling (no need for extra side condenser/reboiler devices)

# The thermal coupling can be "replaced" with a "virtual" direct heat coupling

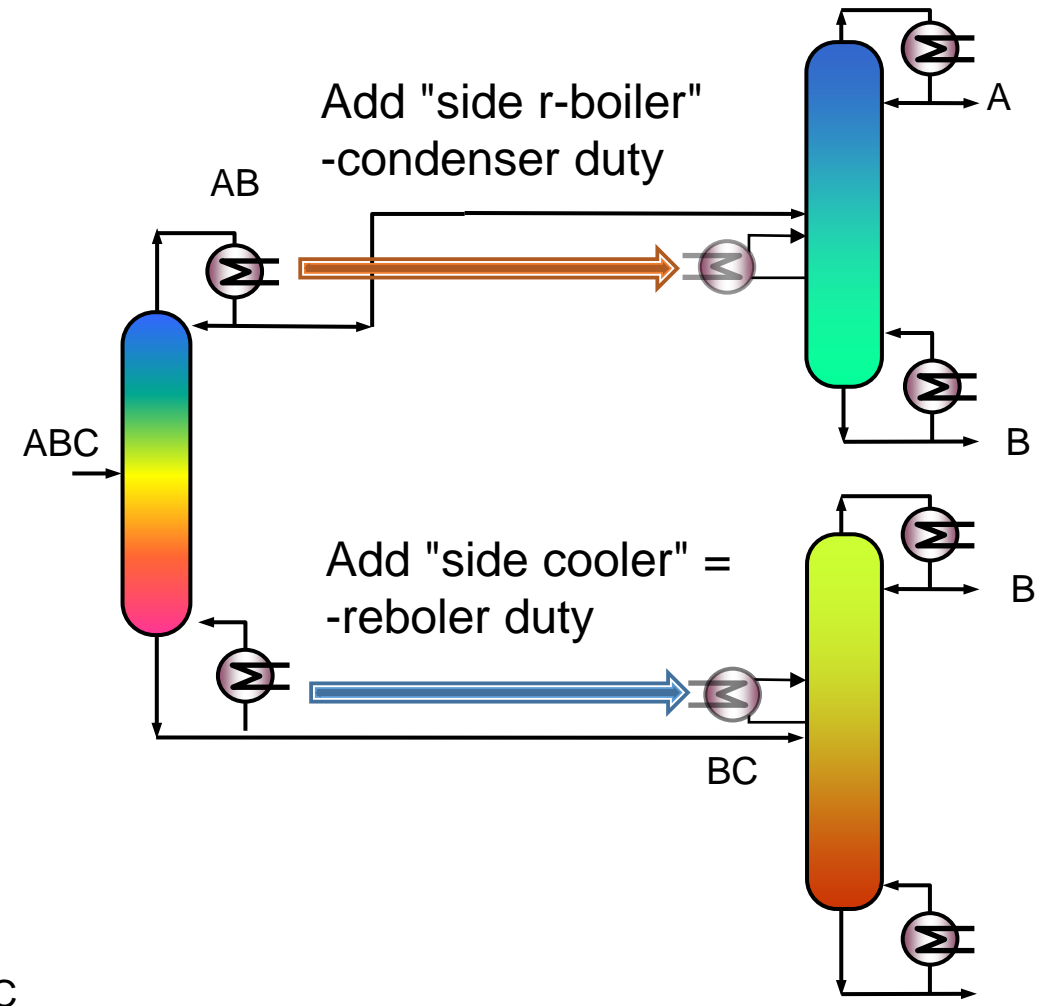
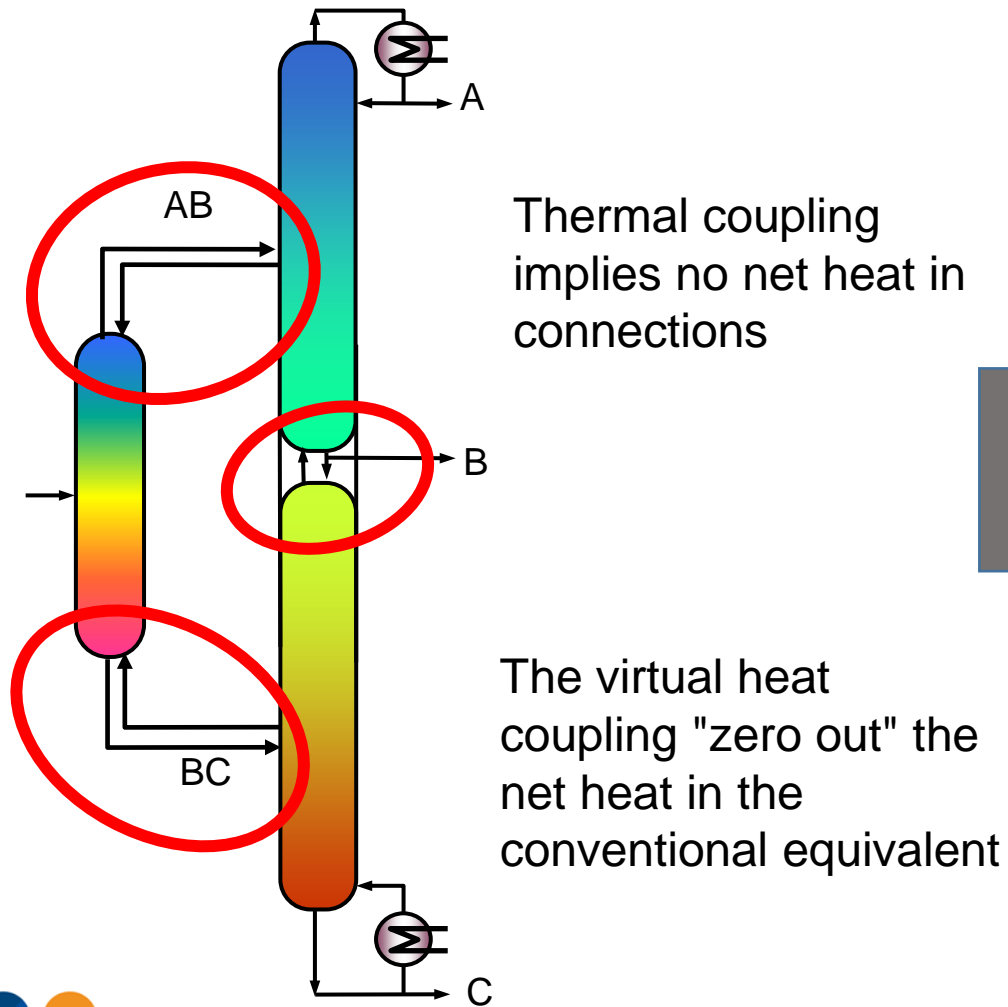
$$F_{21} = D_1 = V_1 - L_1$$

$$q_{21} = -L_1 / D_1$$

$$z_{21} = [r_{A1}, r_{B1}, \dots] F / D_1$$

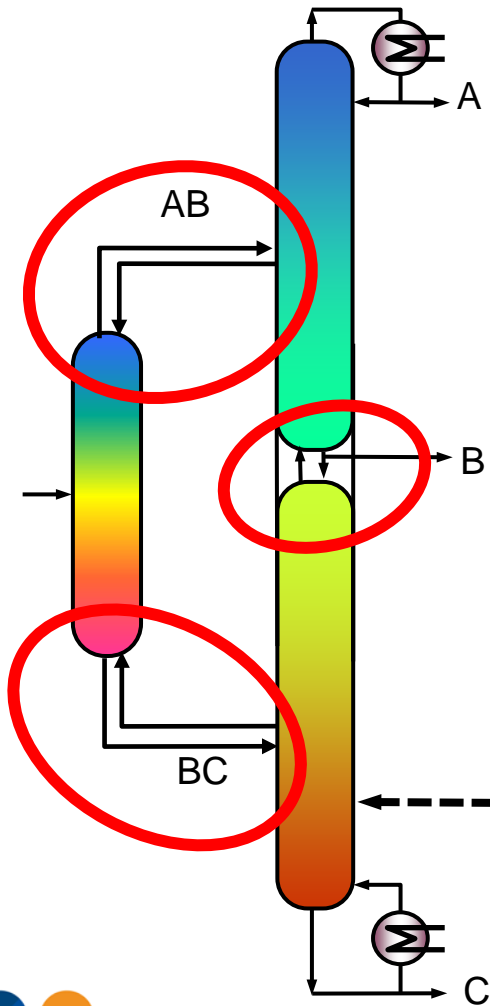


# A DWC can be simulated by a conventional sequence with virtual heat connections





# What will be different?



1) Remixing zones in top/bottom

(may require some extra stages in conventional equivalent)

3) Cannot handle additional feeds into succeeding columns

Must handle 1) but 2&3 cause normally no problems

2) Only positive net component flow rates

