Minimum Energy Requirements in Complex Distillation Arrangements

A thesis submitted for the degree of dr. ing.

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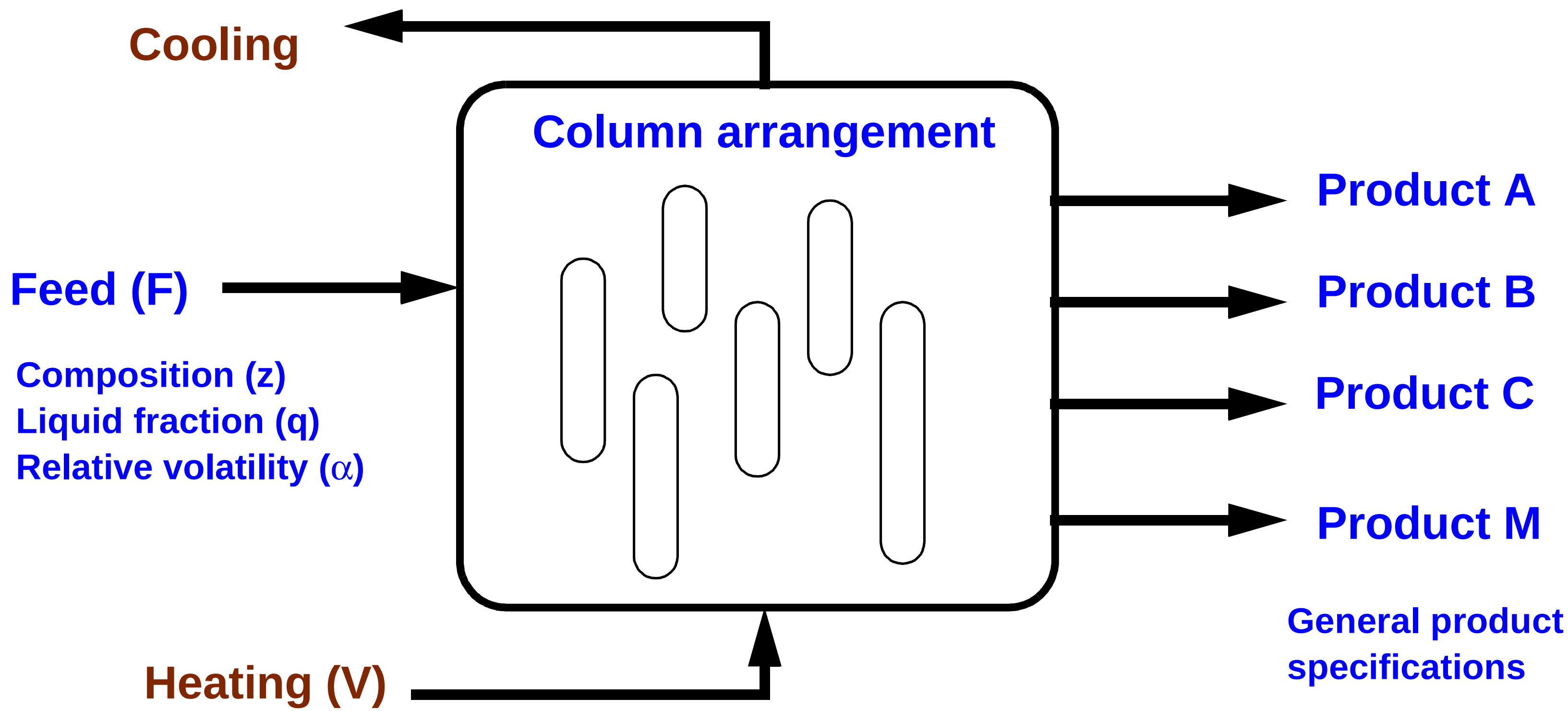
by

Ivar J. Halvorsen

Outline of talk:

1. Introduction and main contributions
2. Part I : Design (Chapters 2-6)
3. Part II: Operation (Chapters 7-11)
4. Demonstration
5. Summary

Introduction: The Distillation Design Problem



Minimum energy (V_{min}) ?

Internal flows ?

Intermediate recoveries ?

Control strategy?

Minimum Energy

Definition:

The minimum external heat supply required to achieve a given set of product specifications when we consider a column arrangement with infinite number of equilibrium stages in each section.

The total vapour flow (V) generated in reboilers is used as the energy measure.

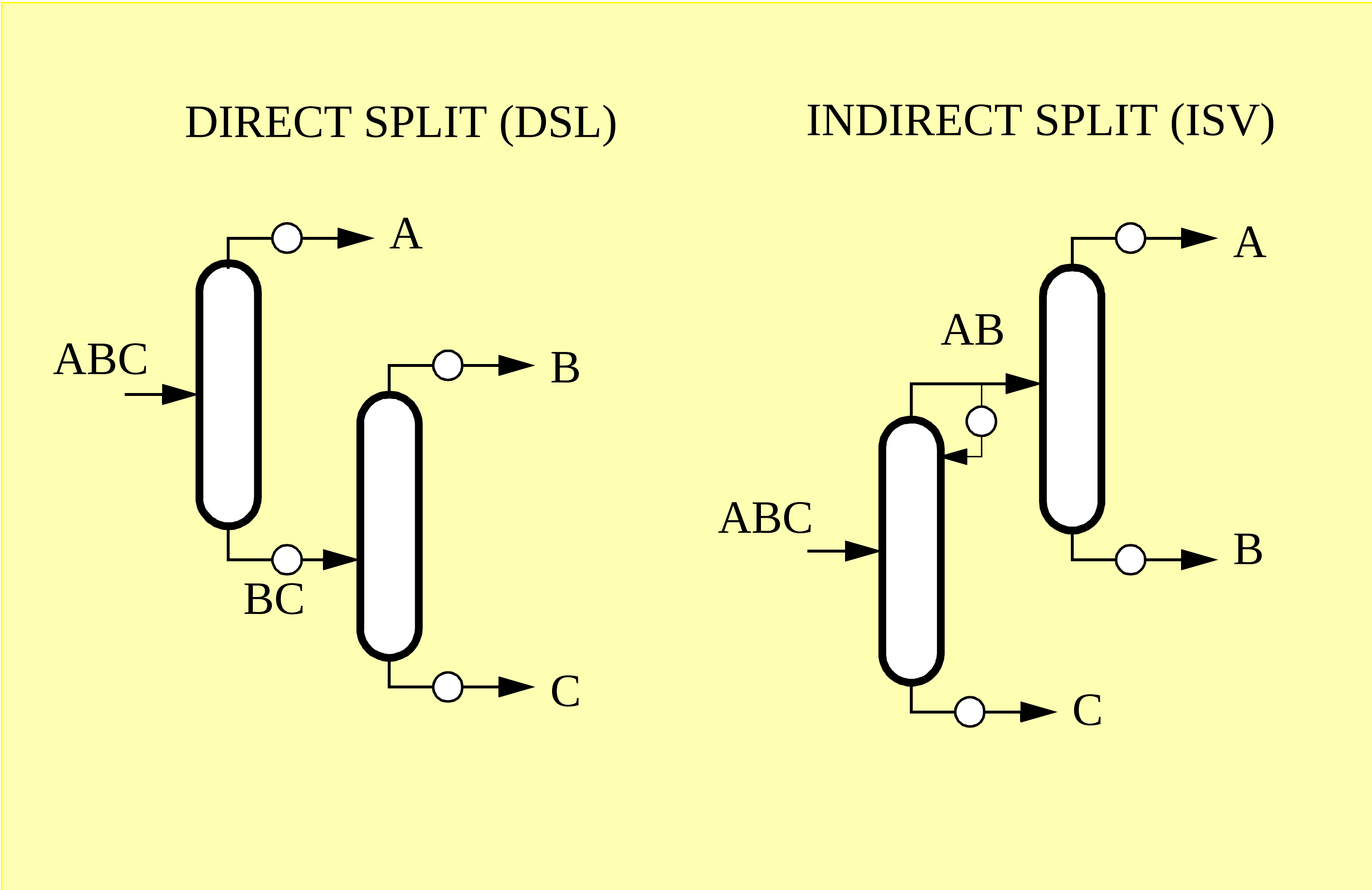
Simplifying assumptions:

- constant relative volatilities (α)
- constant molar flows
- constant pressure and zero pressure drop
- no internal heat exchange (relaxed in Chapter 6)
- zero loss in heat exchangers

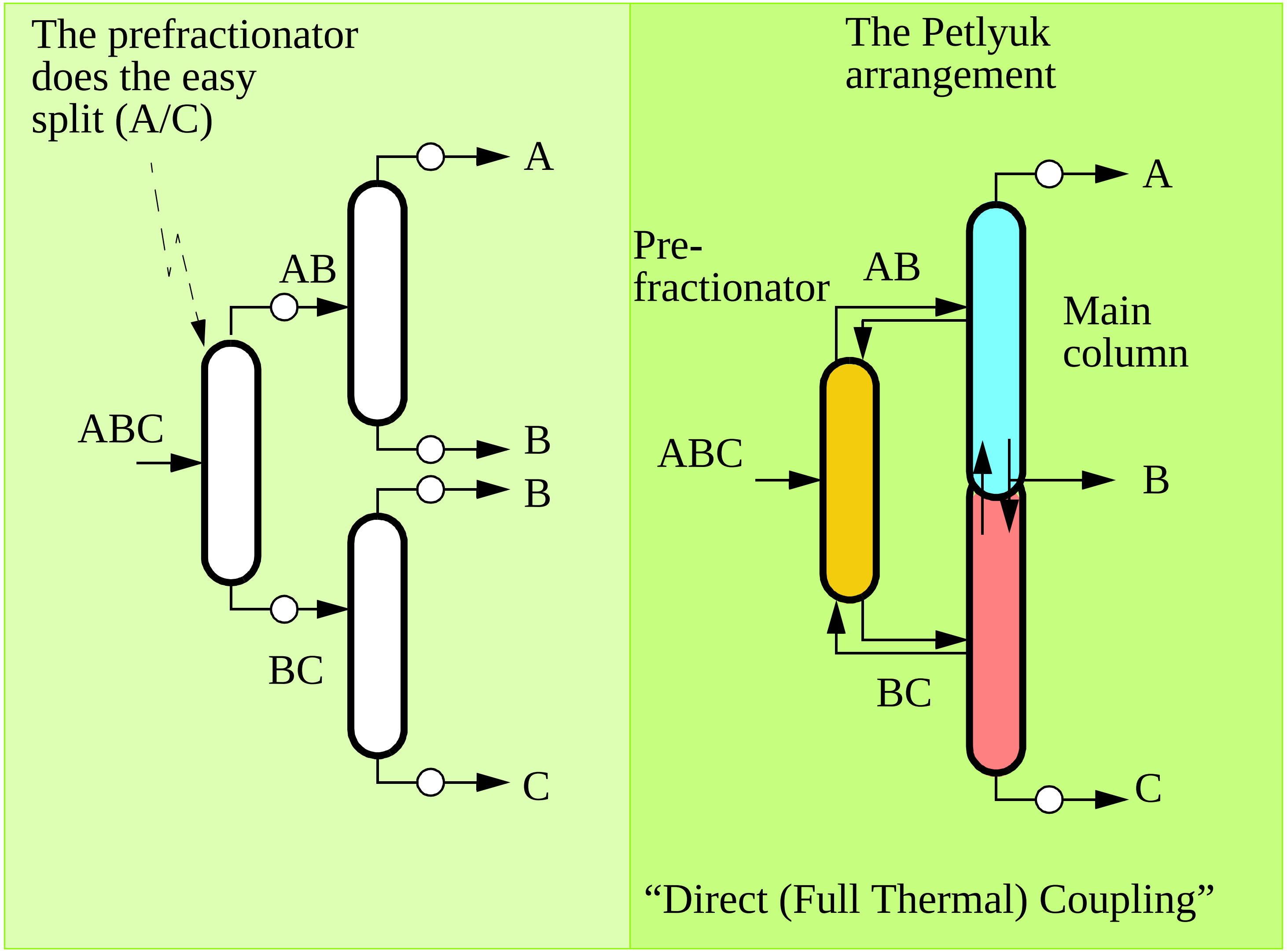
NOTE: The main properties of the results will also be valid for real mixtures

Alternatives for 3-component separation:

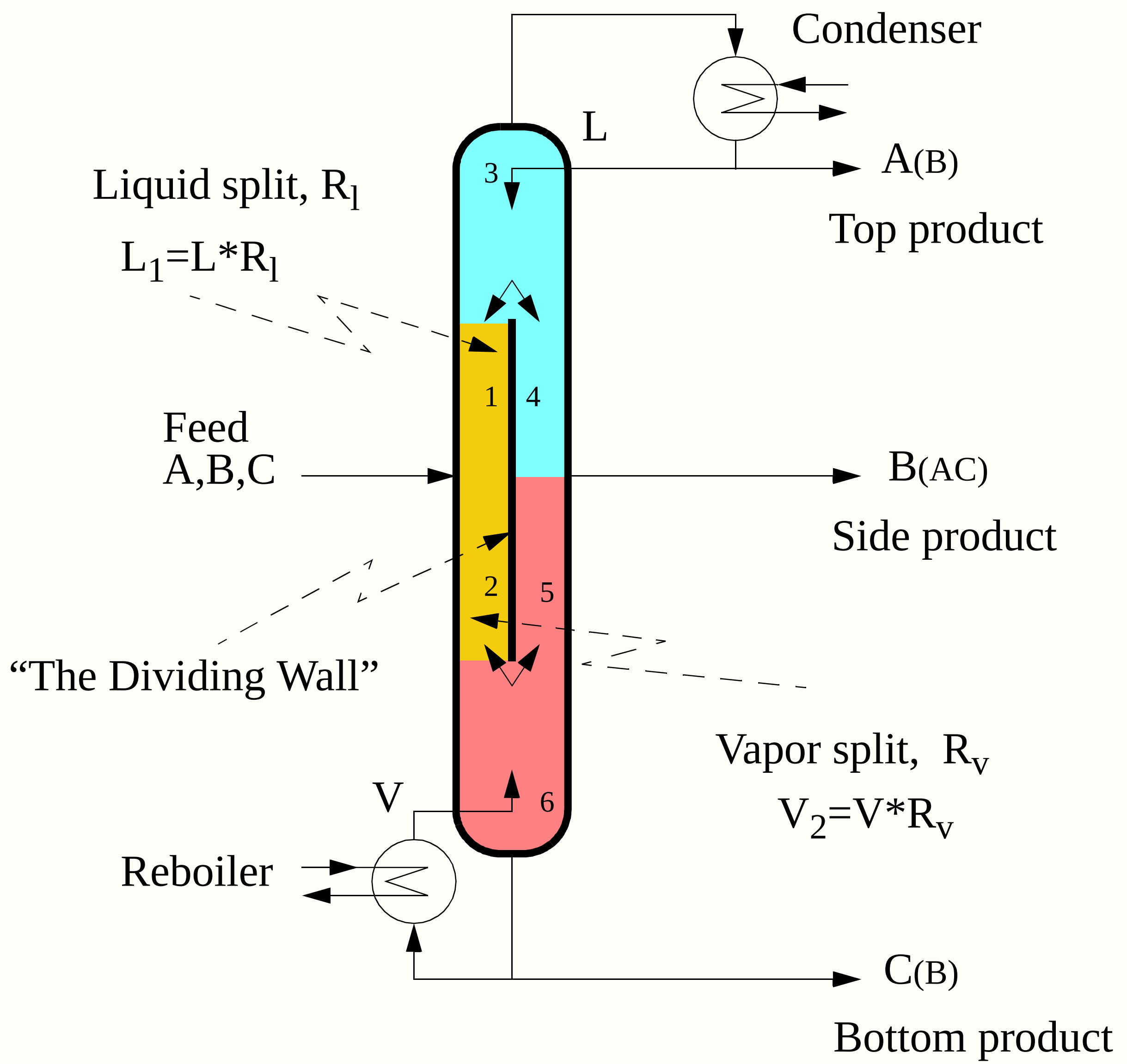
Conventional configurations:



Prefractionator Arrangements:



Petlyuk Column in a single shell: The Dividing Wall Column:



Motivation

Why consider directly integrated columns:

1. Large potential for reduced energy consumption.
   Savings of 20-40% reboiler duty can be achieved for 3-product Petlyuk columns compared to conventional column sequences.
2. The Dividing Wall Column (DWC) has also a potential for reduced capital costs.
3. Growing industrial interest, by German companies in particular.

Obstacles:

1. Industrial reluctance due to reported difficulties in control and lacking design procedures.
2. No analytical results have been available for more than ternary mixtures

Conclusion: Better Understanding is Required

Main contributions:

Part I, Design:

- Exact analytical solution for minimum energy in directly coupled distillation arrangements (Petlyuk columns, fully thermally coupled columns)
  - Valid for N>3 components and M>3 products
  - Handles non-sharp product splits
- The V_{min}-diagram
  - Effective visualization tool
  - Simple assessment of multicomponent separation tasks

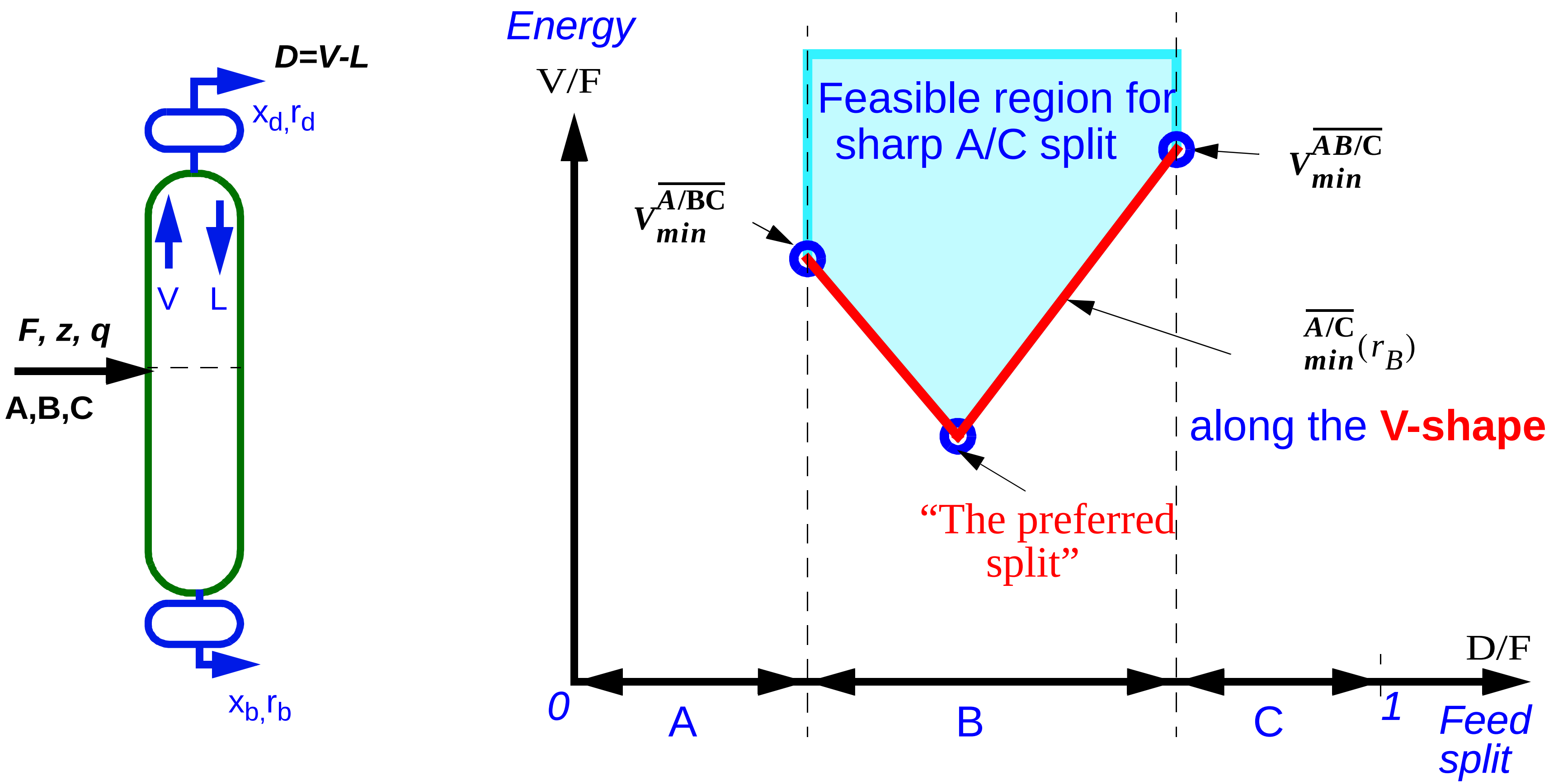
Part II, Operation:

- Analysis of Self-optimizing Control for control structure design
  - Applied to the Petlyuk column
- Improved understanding of control requirements for Petlyuk columns
- The reported industrial control problems for Petlyuk columns are probably due to bad control structures.

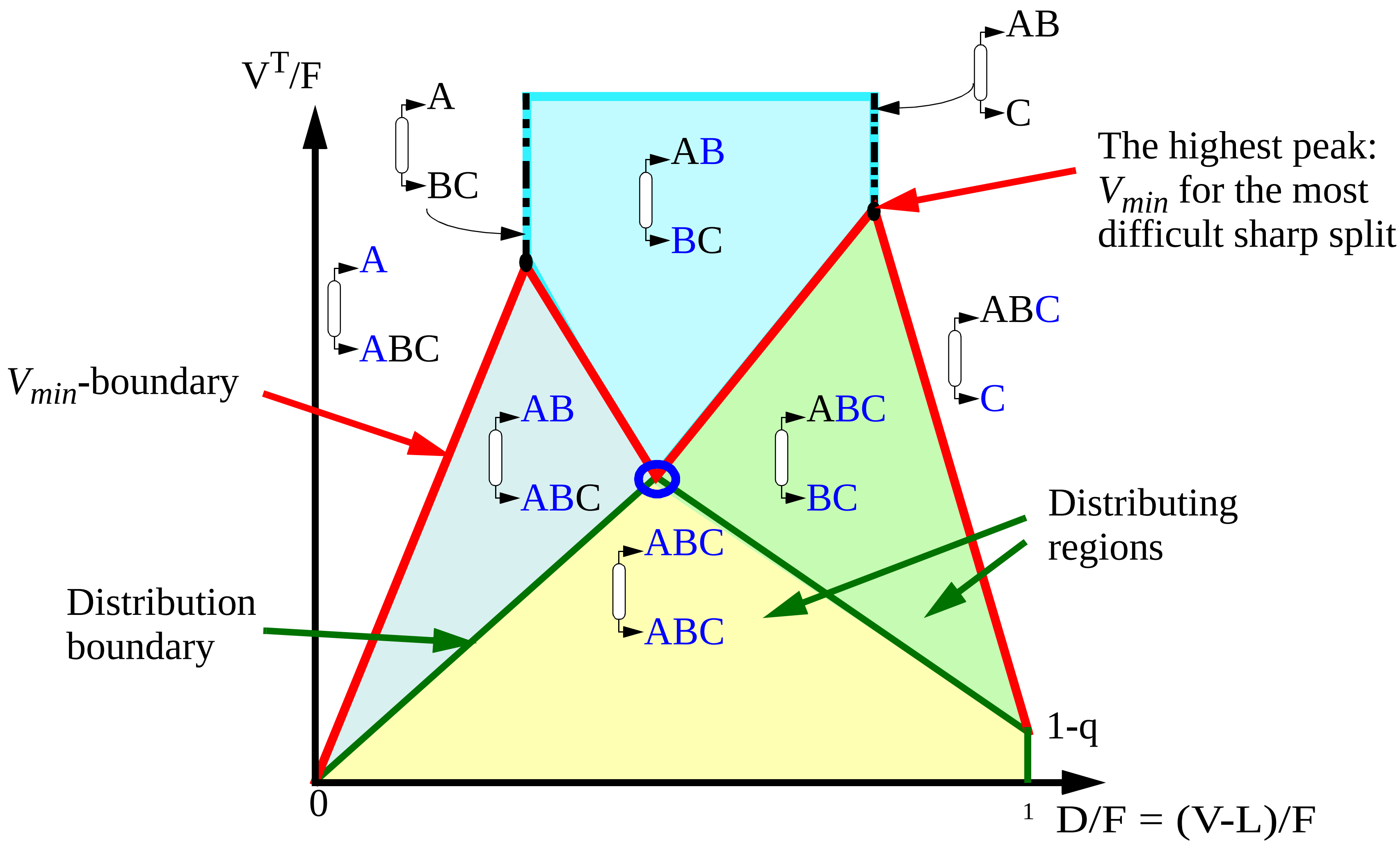
The understanding of directly integrated columns is improved

Chapter 3: The two-product column

has only two degrees of freedom in operation ==> We can visualize all possible operating points in the D-V plane:



The V_{min}-diagram



Revisit of Underwood's Equations for Minimum Energy Calculations

Possible common "V_{min}"-roots θ

Feed F,z,q

vapour: (1-q)F

net flow: $w_{i,F}=Fz_{i,F}$

Material balance:

$V_T - V_B = (1-q)F$

$r_{i,T} - r_{i,B} = 1$

V_T

$w_{i,T}$

Defining eq.

$$\frac{V_T}{F} = \sum_i \frac{\alpha_i z_i r_{i,T}}{\alpha_i - \phi}$$

Feed eq.

$$\sum_i \frac{\alpha_i z_i}{\alpha_i - \theta} = 1 - q$$

Defining eq.

$$\frac{V_B}{F} = \sum_i \frac{\alpha_i z_i r_{i,B}}{\alpha_i - \psi}$$

$w_{i,B}$

V_B

"Actual " - roots ϕ and ψ

Underwood:

$V=V_{min}$ **<=>** $\phi_i = \psi_{i+1} = \theta_i$

How should we compute:

$V=?$

$D=?$

$w_{i,T}=?$

KEY: *DISTRIBUTION*

How to use Underwood's minimum energy results:

Problem: Given 2 specifications, find {$\boldsymbol{V, r_{1,D}, r_{2,D}, \ldots r_{N,D}}$ } (N-1 unknowns).

1. Compute all the *common root s (N-1)* from the feed equation (polynomial roots):

$$(1-q) = \sum_i \frac{\alpha_i z_i}{(\alpha_i - \theta)}$$

2. Determine the total set (N_D) of the *distributed components*

   There will be $N_A = N_D - 1$ active Underwood roots

3. Apply the set of definition equations (in the top or in the bottom) corresponding to each active root.

   This is N_A **linear** equations in N_A unknowns
   (The non-distributed components have recoveries of either 1 or 0)

$$V^T_{min} = \sum_{i=1}^{N_c} \frac{\alpha_i r_{i,D} z_i}{(\alpha_i - \theta_{a1})}$$

$$\bullet$$

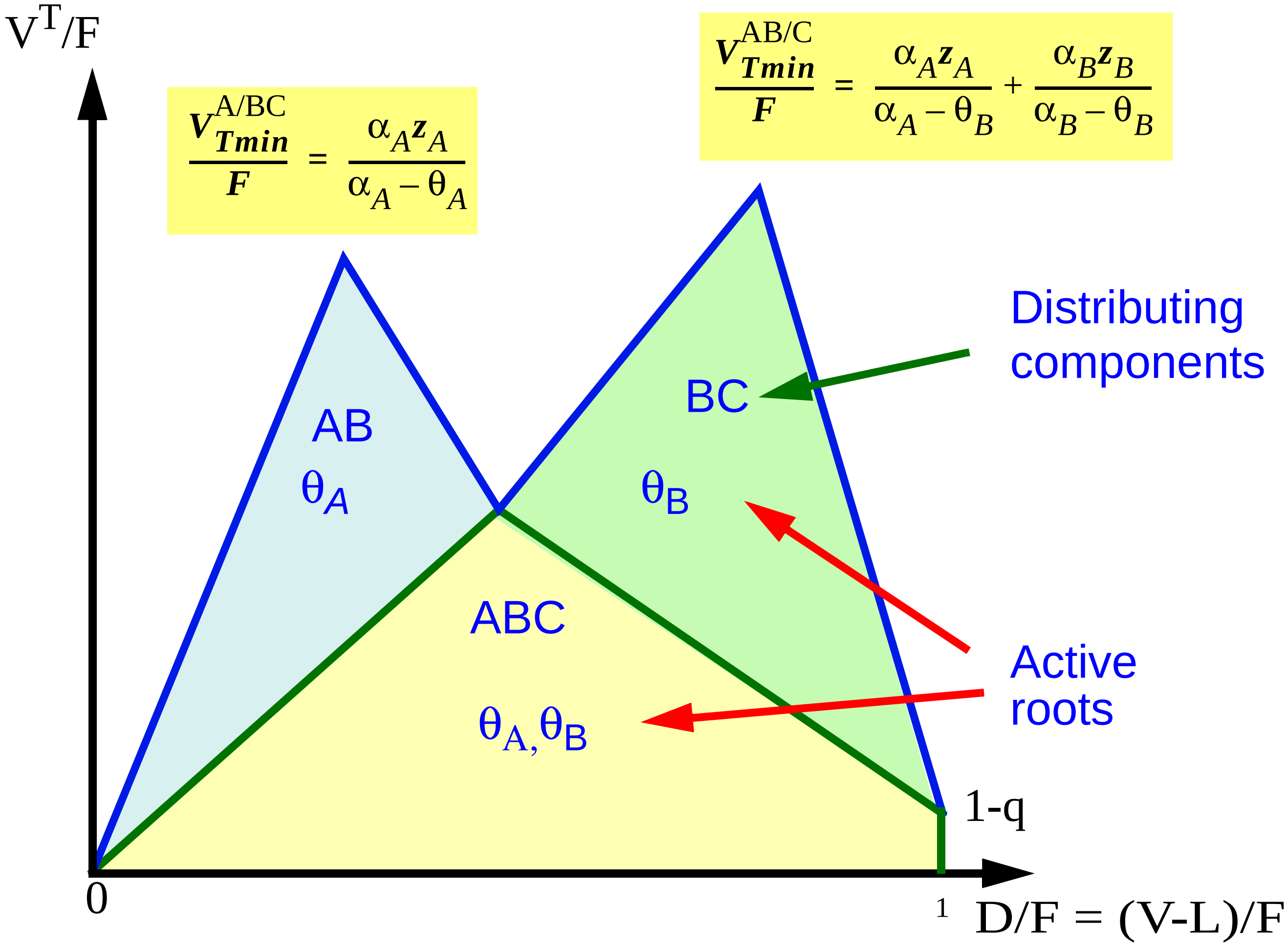
$$\bullet$$

$$V^T_{min} = \sum_{i=1}^{N_c} \frac{\alpha_i r_{i,D} z_i}{(\alpha_i - \theta_{aN_a})}$$

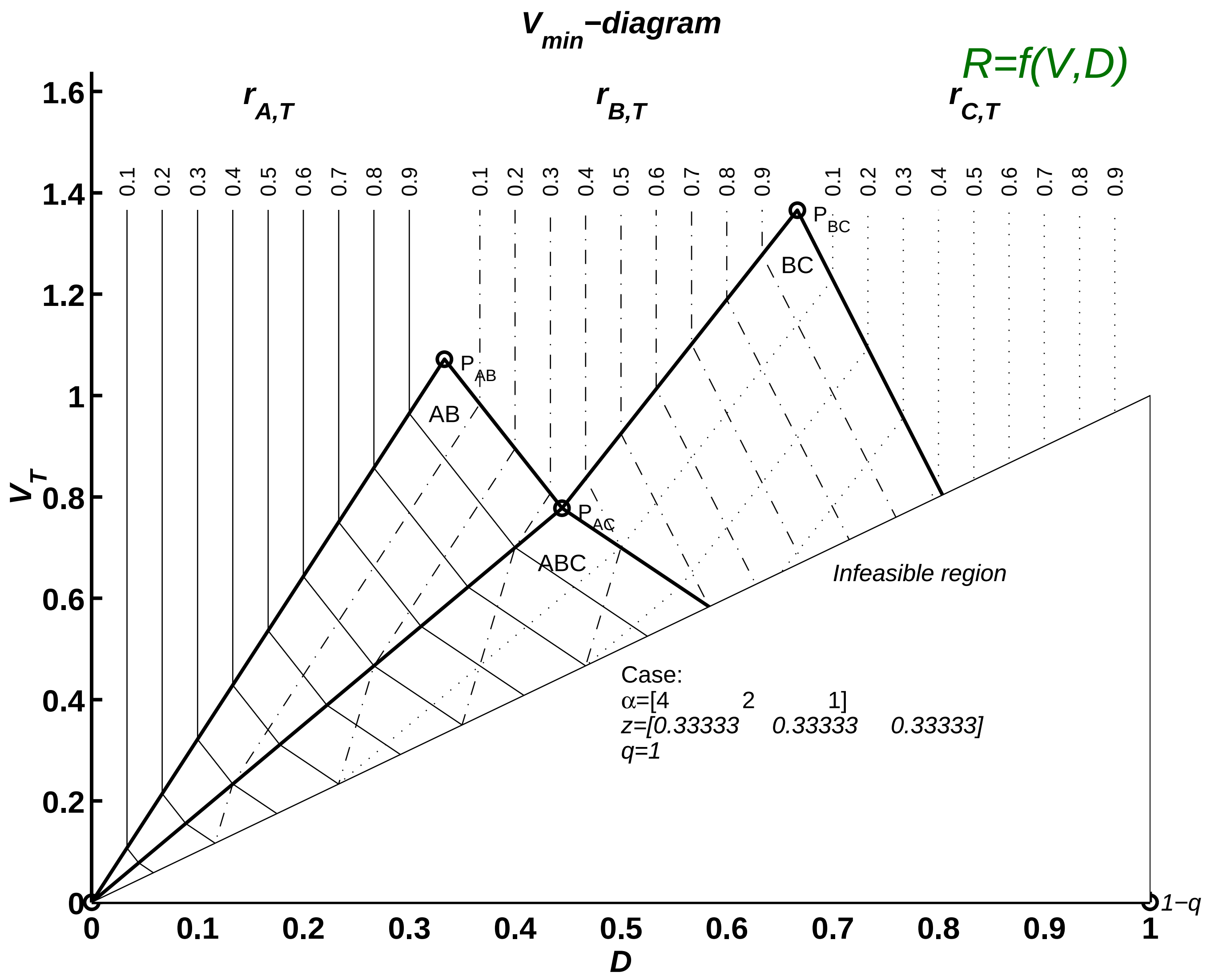
This procedure particularly simple for sharp component splits (r_i=1 and r_j=0)

Analytic Results with the Underwood equations

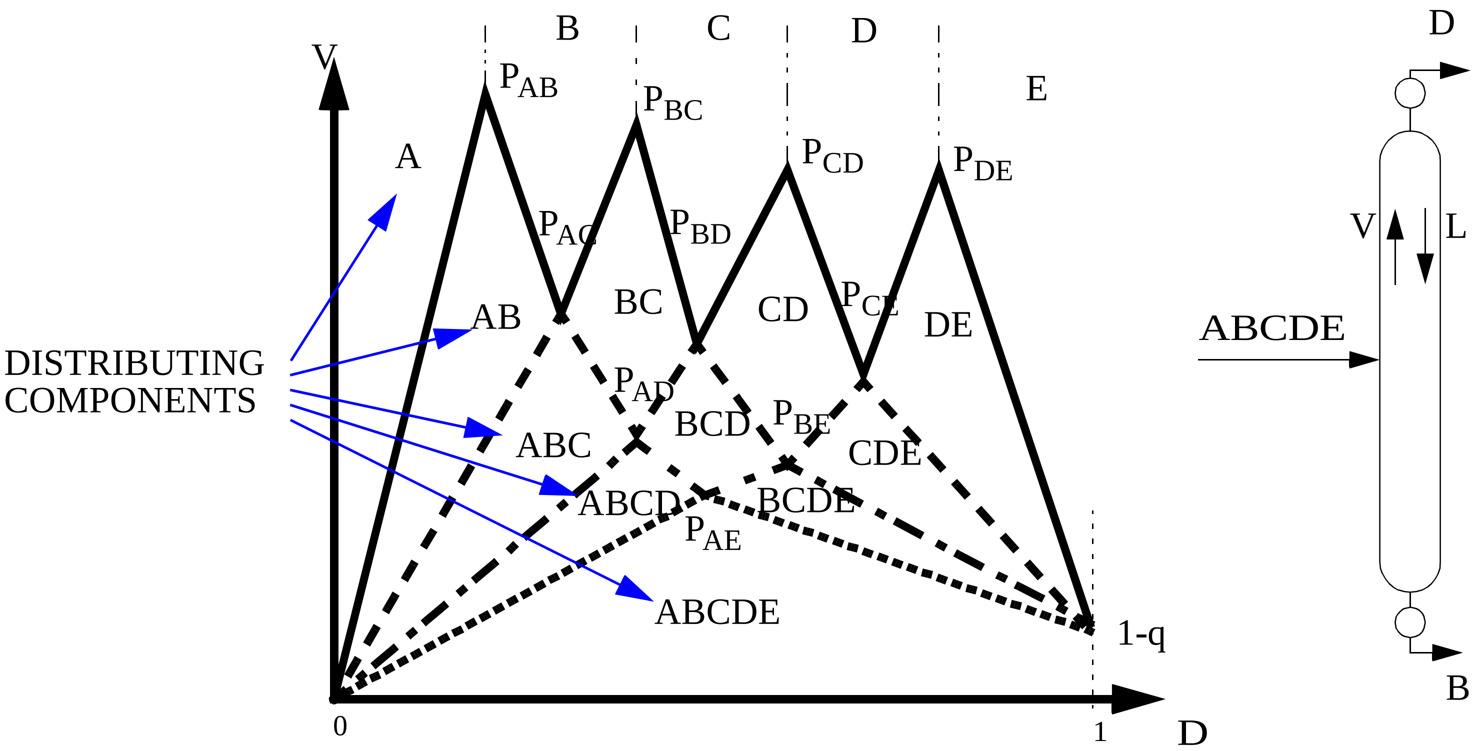
The peaks:



Example: Possible recoveries in the top product



5-Component example:

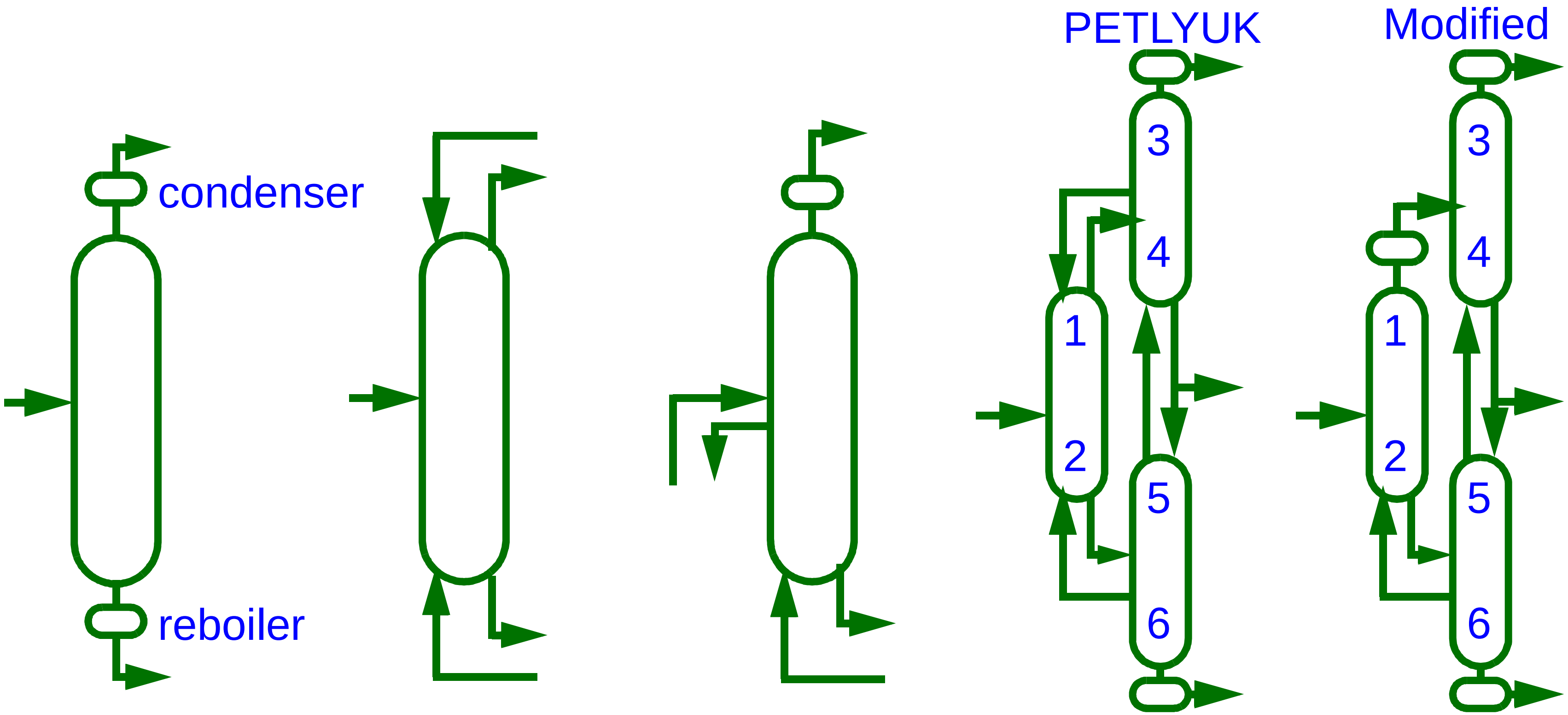


P_{ij} marks V_{min} for sharp split of keys i, j.
$V > V_{min}$ all above the "mountains"

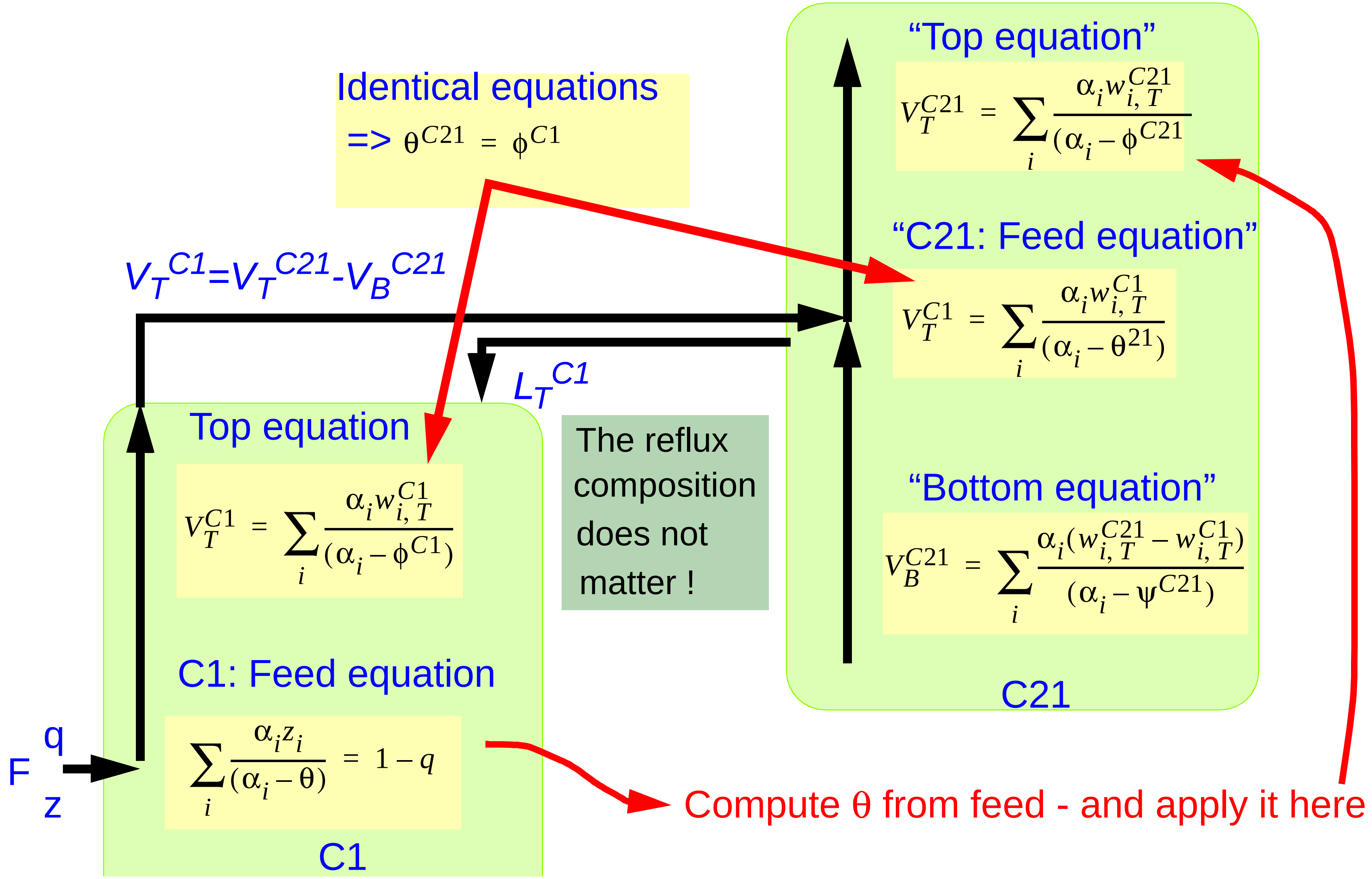
All computations are simple and the solution is exact (infinite number of stages).

Chapter 4:
Application to directly (fully thermally) coupled columns:

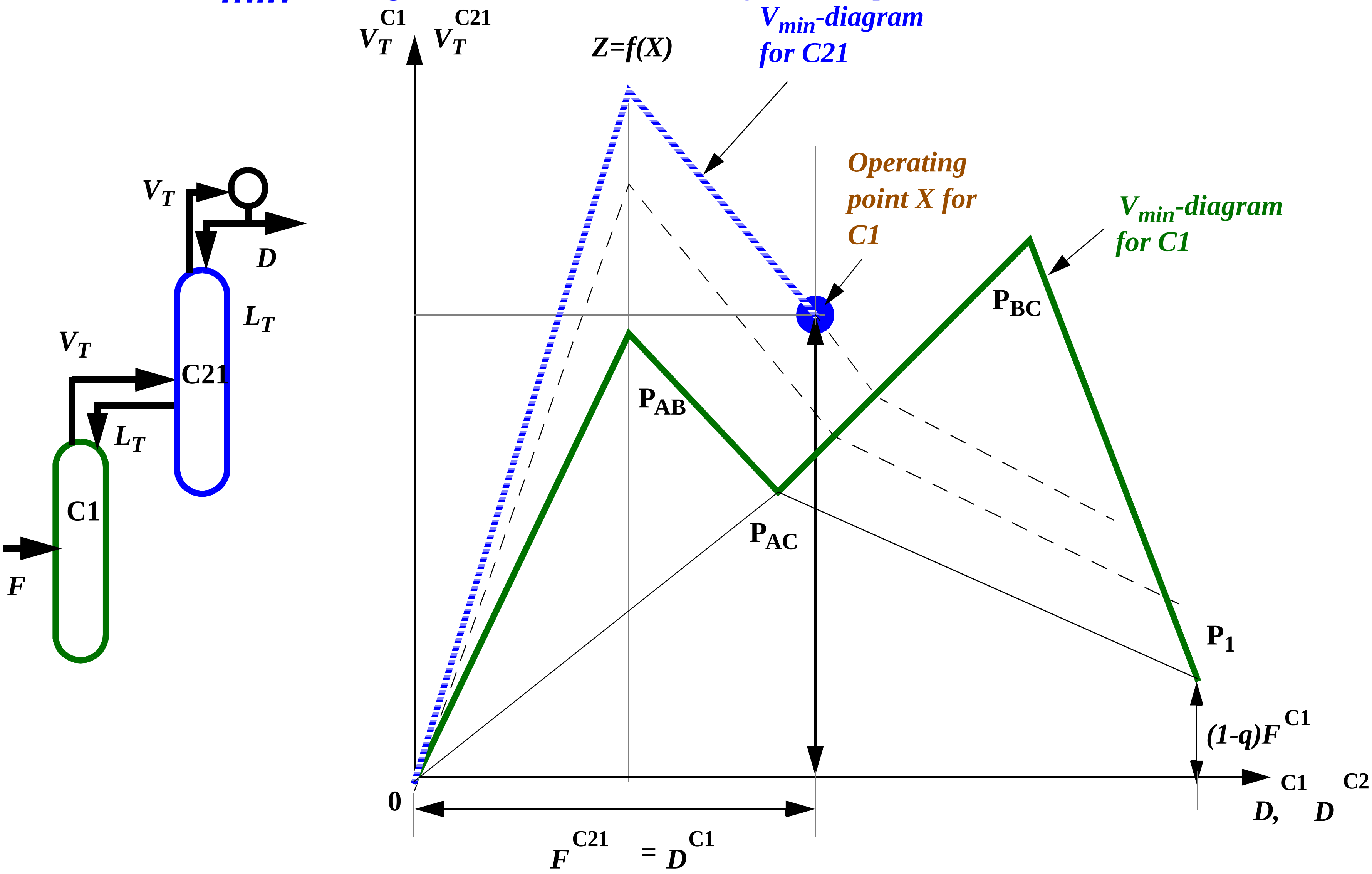
:



Underwood roots "carry over" to the next column through the direct (full thermal) coupling

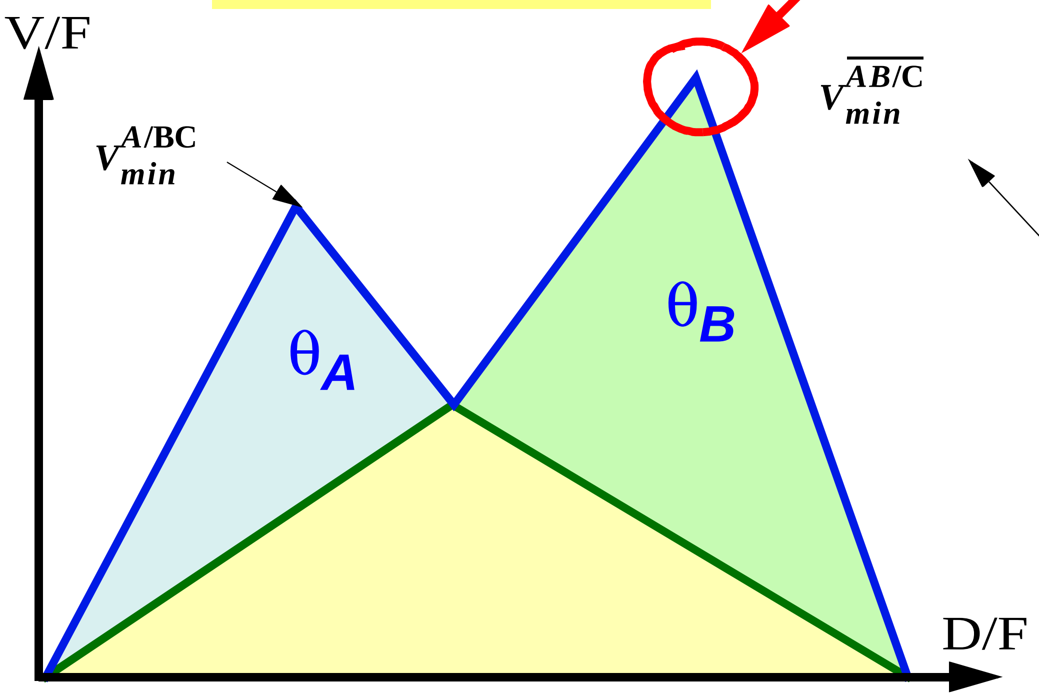


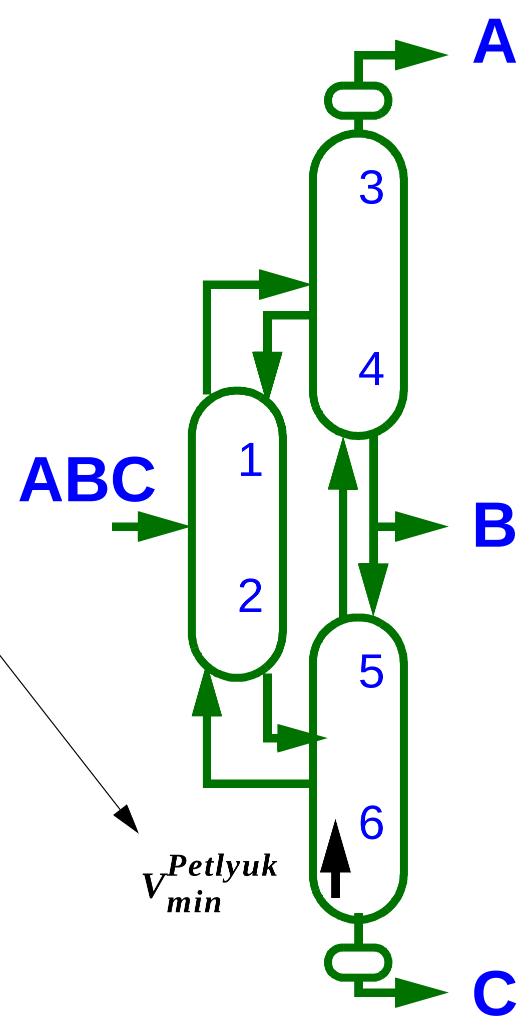
V_{min}-diagram for directly coupled columns



V_{min} for the Petlyuk column: The highest peak:

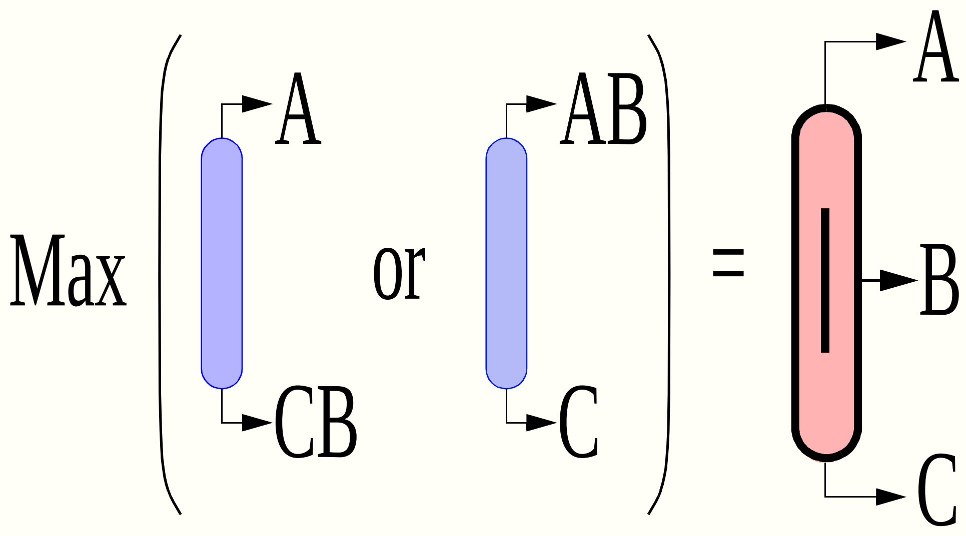
$$\frac{V_{Tmin}}{F} = \max_j \left(\sum_{i=1}^{j} \frac{\alpha_i z_i}{\alpha_i - \theta_j} \right)$$





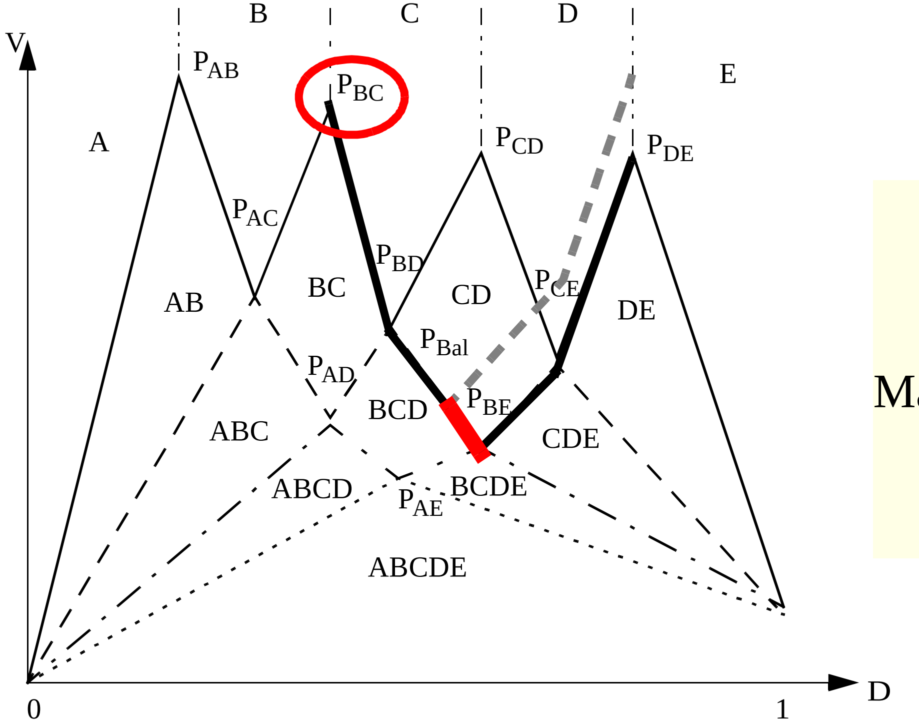
V_{min}-diagram

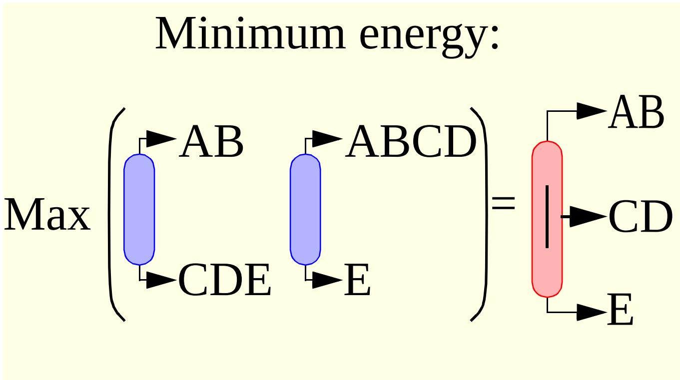
Petlyuk column: V_{min} = the most difficult binary split



Example: 5-component feed

We want pure A+B in the top, and pure C+D in the side and pure E in the bottom

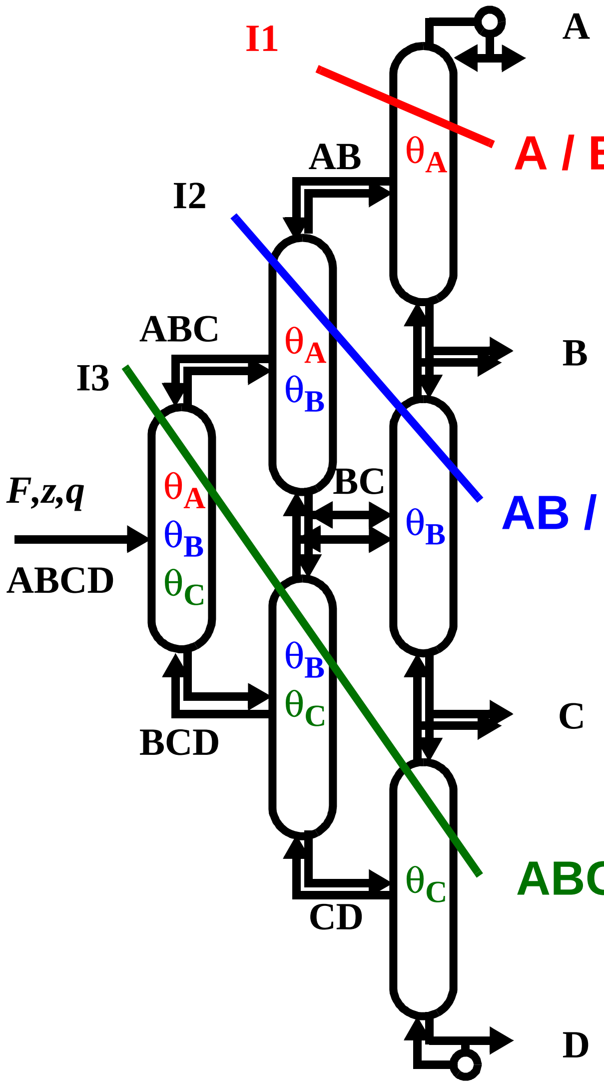




Solution: Operate the prefractionator between P_{Bal} and P_{BE}

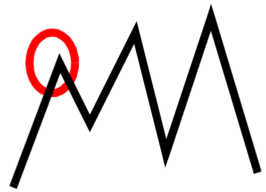
The energy requirement to the Petlyuk column is found as $\max(P_{BC}, P_{DE}) = P_{BC}$

Chapter 5: Proof for the general N-component case



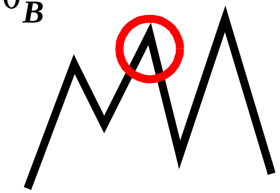
A / BCD - split

$$V_{min} = \frac{\alpha_A z_A}{\alpha_A - \theta_A} = \sum_{i=A}^{A} \frac{\alpha_i z_i}{\alpha_i - \theta_A}$$



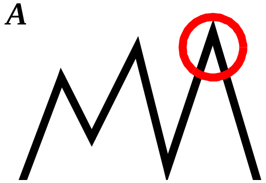
AB / CD - split

$$V_{min} = \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B}{\alpha_B - \theta_B} = \sum_{i=A}^{B} \frac{\alpha_i z_i}{\alpha_i - \theta_B}$$



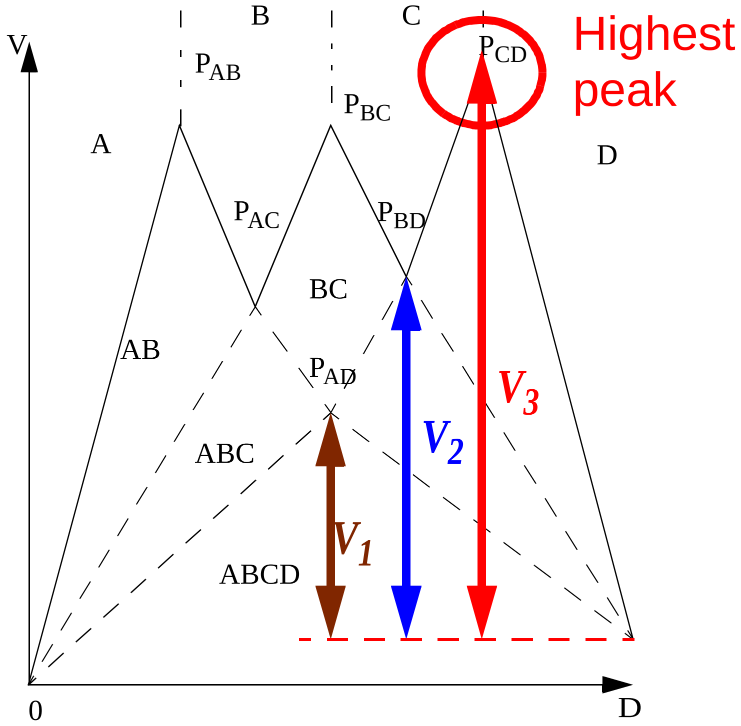
ABC / D - split

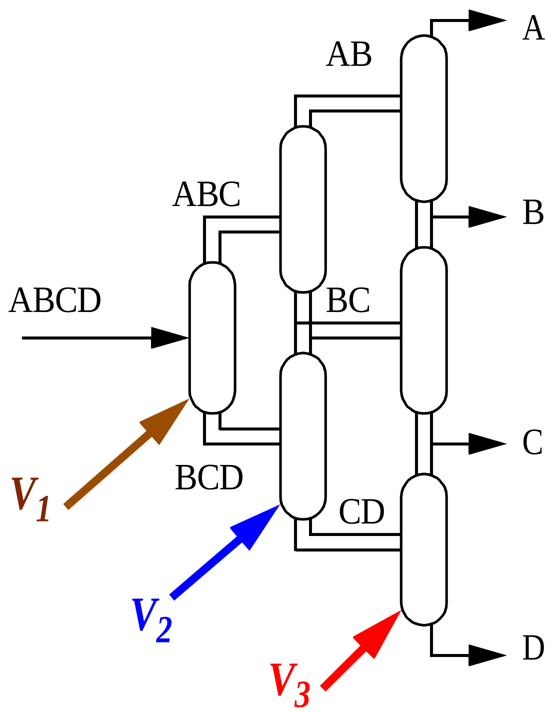
$$V_{min} = \frac{\alpha_A z_A}{\alpha_A - \theta_C} + \frac{\alpha_B z_B}{\alpha_B - \theta_C} + \frac{\alpha_C z_C}{\alpha_C - \theta_C} = \sum_{i=A}^{C} \frac{\alpha_i z_i}{\alpha_i - \theta_C}$$



Ex.: 4-component feed to 4-product "Petlyuk" column

All vapour flows in every Petlyuk column section are found in the V_{min}-diagram

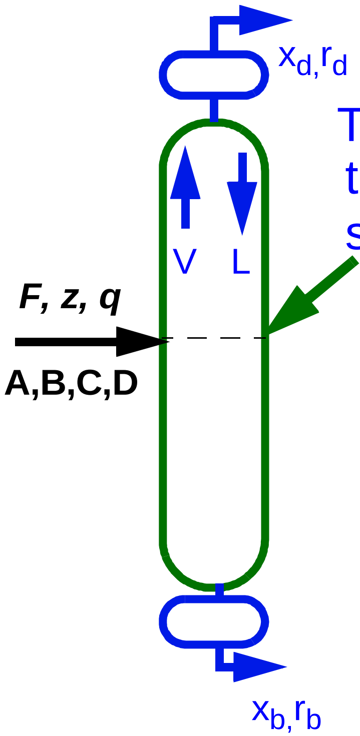




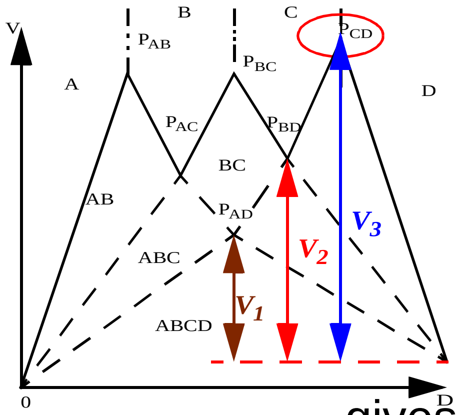
Solution: Operate every "2-product column" at its "preferred split"

Summary of Contributions in Chapter 4 and 5:

The most difficult split in
this standard two-product column..

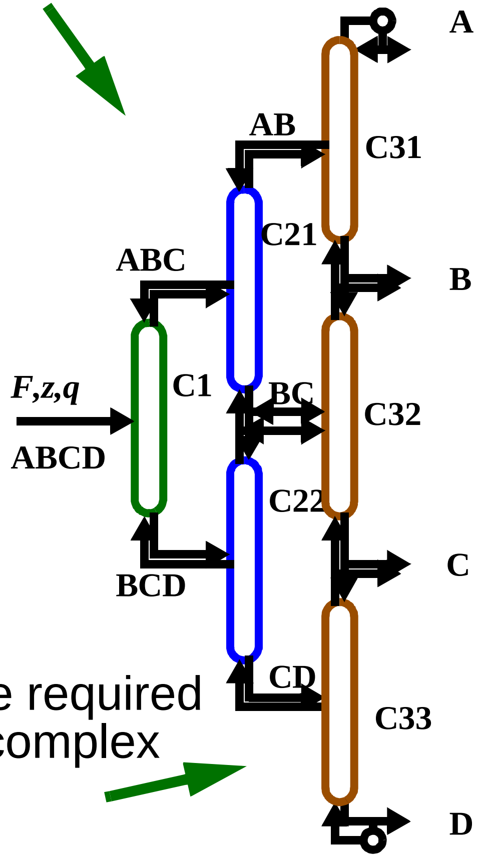


The V_{min}-diagram illustrates
the behaviour in this
simple column and ...



Exact analytical expressions
by the Underwood equations

..gives is the minimum energy
of a directly coupled extended
Petlyuk arrangement



...gives all the required
flows in this complex
arrangement

The new contributions in Chapter 3, 4 and 5 can be listed as:

1. Different and more direct derivation of V_{min} for Petlyuk column
2. Generalize the solution to any liquid fraction (q) and non-sharp splits
3. Generalize to N>3 components and M>3 products
4. Simple visualization in the V_{min}-diagram: ***The highest peak***
5. Simple interpretation: ***The most difficult binary split***

Some more special results

6. Shows that the composition in the recycle stream normally does not affect the computations in reasonable operating regimes.
7. Illustrates the flat optimality region for ternary and quarterly feed
8. Illustrates the relation between composition profile pinch zones and minimum energy operation.
9. Simple design procedure for required number of stages
10. Comparison to some alternative arrangements

Some results from Chapter 6 (2nd Law):

Minimum required external heat supply in an ideal reversible process:

$$Q_{Hmin} = \frac{-\Delta S}{\left(\frac{1}{T_L} - \frac{1}{T_H}\right)}$$

Expressed by vaporization and relative volatility

$$V_{\text{rev,min}} = \frac{-\Delta S}{\lambda\left(\frac{1}{T_L} - \frac{1}{T_H}\right)} = \frac{-\Delta S}{\ln\alpha_{LH} + \ln\frac{P_H}{P_L}}$$

Entropy production in Adiabatic arrangements:

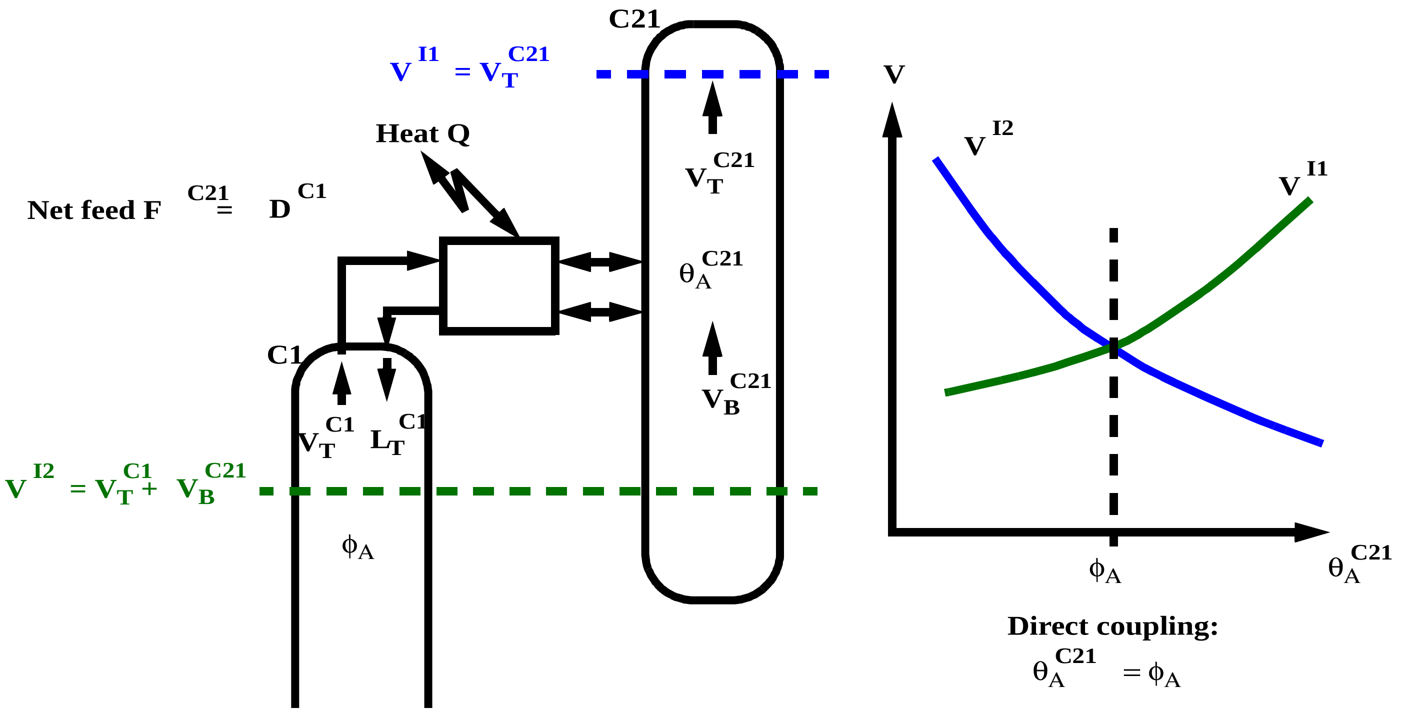
$$\Delta S_{sur} = \lambda V\left(\frac{1}{T_L} - \frac{1}{T_H}\right) = RV\ln\frac{\sum(\alpha_i x_{i,\,T})P_B}{\sum(\alpha_i x_{i,\,B})P_T}$$

which is simplified to $\Delta S_{sur} = RV\ln\alpha_{LH}$ for sharp split

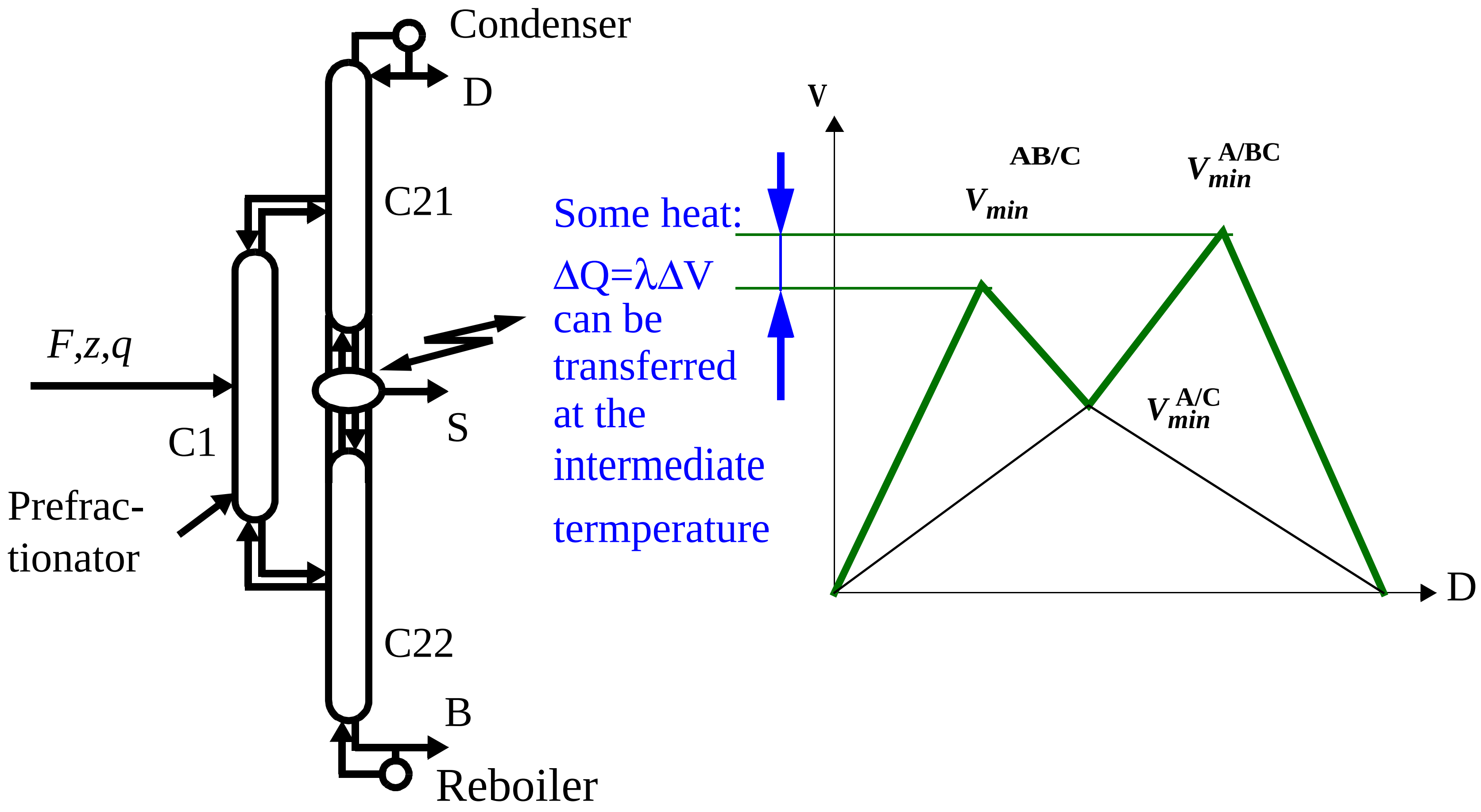
Conjecture:

The adiabatic extended Petlyuk Arrangement require less energy than any other distillation arrangement, when we consider constant pressure and no internal heat integration.

Reason: Direct Coupling Minimize Vapour Flow trough a junction:



Improved 2nd Law performance

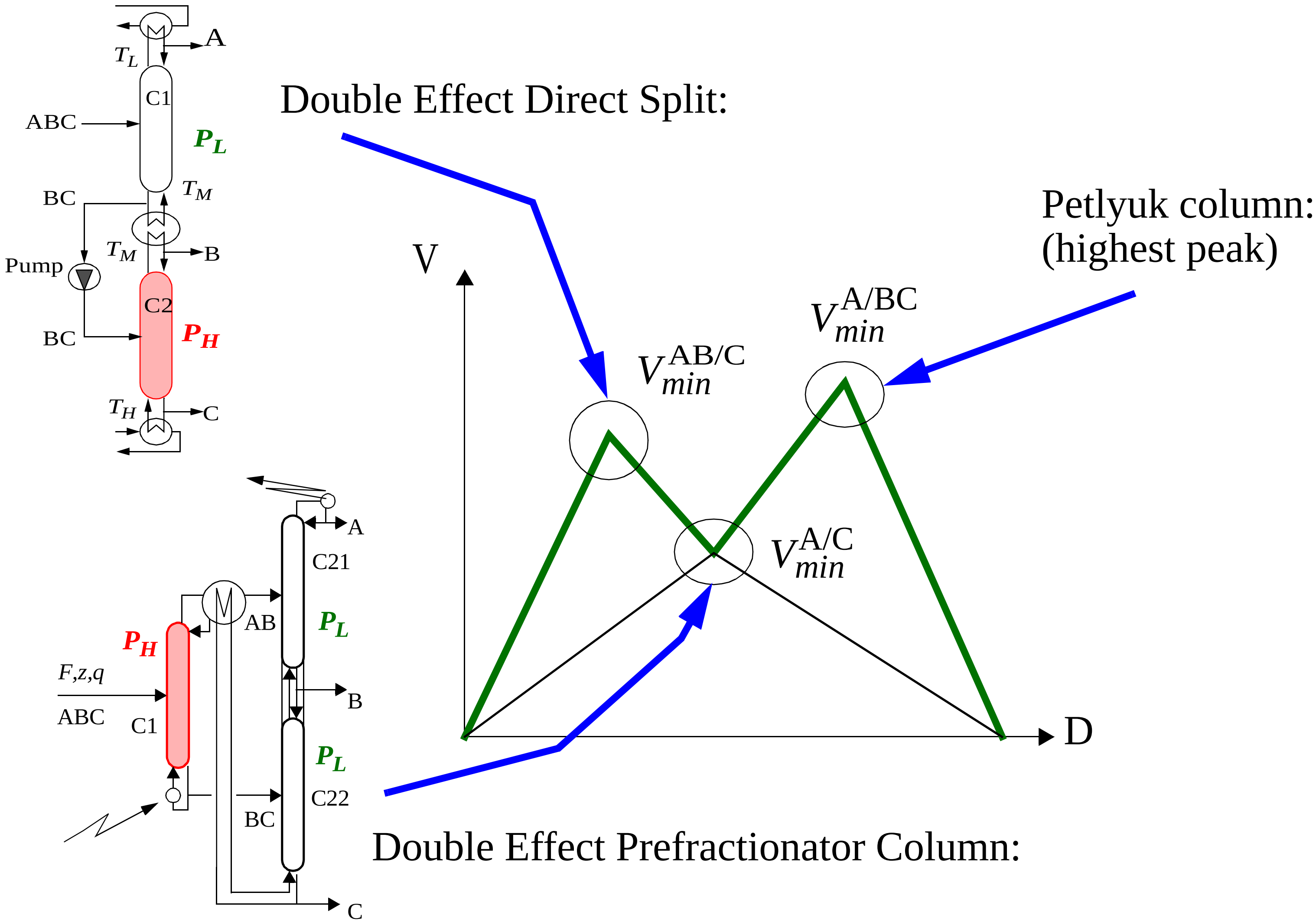


Some heat:
ΔQ=λΔV
can be
transferred
at the
intermediate
termperature

Comparing some selected arrangements

	Configuration (Ad: Adiabatic, Non: Non-ad.) Feed data: α=[4,2,1], z=[1/3,1/3,1/3], q=1		External Energy $V_{min}=\Sigma\Delta Q/\lambda$	Relative Entropy Production $\Delta S_{total}/\lvert\Delta S\rvert$
A	Direct Split, no HE (conventional)	Ad	2.072	0.59
B	Indirect Split, no HE (conventional)	Ad	2.032	1.21
C	Side Rectifier (directly coupled)	Ad	1.882	0.86
D	Side Stripper (directly coupled)	Ad	1.882	1.05
E	Reversible Petlyuk Column	Non	1.667	0.00
F	Conventional prefractionator arrangement	Ad	1.556	0.63
G	Petlyuk Column (typical)	Ad	1.366	0.72
H	Petlyuk Column + side-HE	Ad	1.366	0.54
I	Petlyuk + HE across the dividing wall	Ad+Non	1.222	0.54
J	Petlyuk + HE from sidestream to feed	Ad	1.181	0.49
K	Petlyuk + total middle HE	Ad+Non	1.000	0.26
L	Reversible Petlyuk with internal HE	Non	1.000	0.05
M	Reversible process with only two temperature levels	Non	0.793	0.00

Double Effect Column Arrangements



Note: DE-columns require wider temperature span

Part II: Operation

Control structure selection for on-line optimizing control, with application to the three-product Petlyuk column

- Understanding the Petlyuk column behaviour
- Self-optimizing Control

Can we obtain the potential energy savings in practice?

A basic question in control structure design:

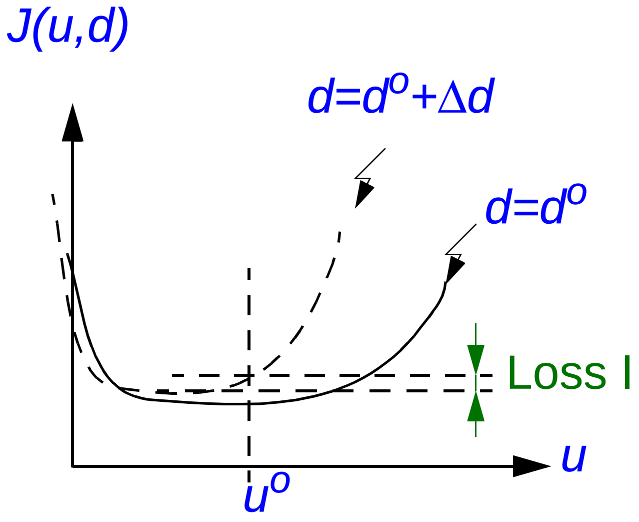
Which variables should we select to control, and why?

The best solution is affected by:

- characteristics of the process model
- available manipulated inputs
- available measurements
- impact from unknown disturbances
- model uncertainties
- measurement noise
- uncertainty in implementation of manipulated inputs

Practical observation: Some choices are better than other.

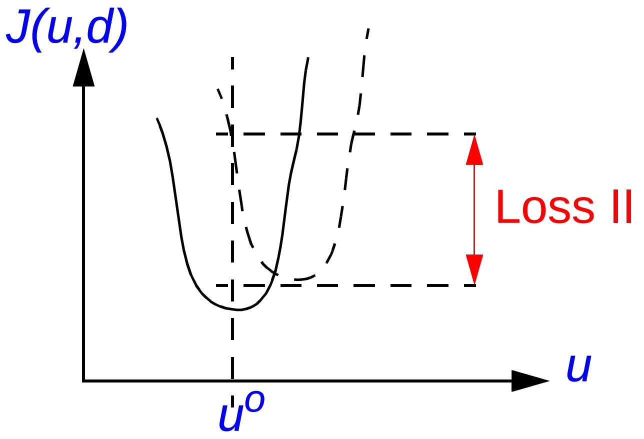
The optimizing control problem:



d: Disturbances and setpoints of other closed loops

I) The trivial case:

Flat optimum, we may keep *u* constant



II) The difficult case:

On-line optimization is required

Question:
CAN WE TURN A CASE II
INTO THE TRIVIAL CASE I ?

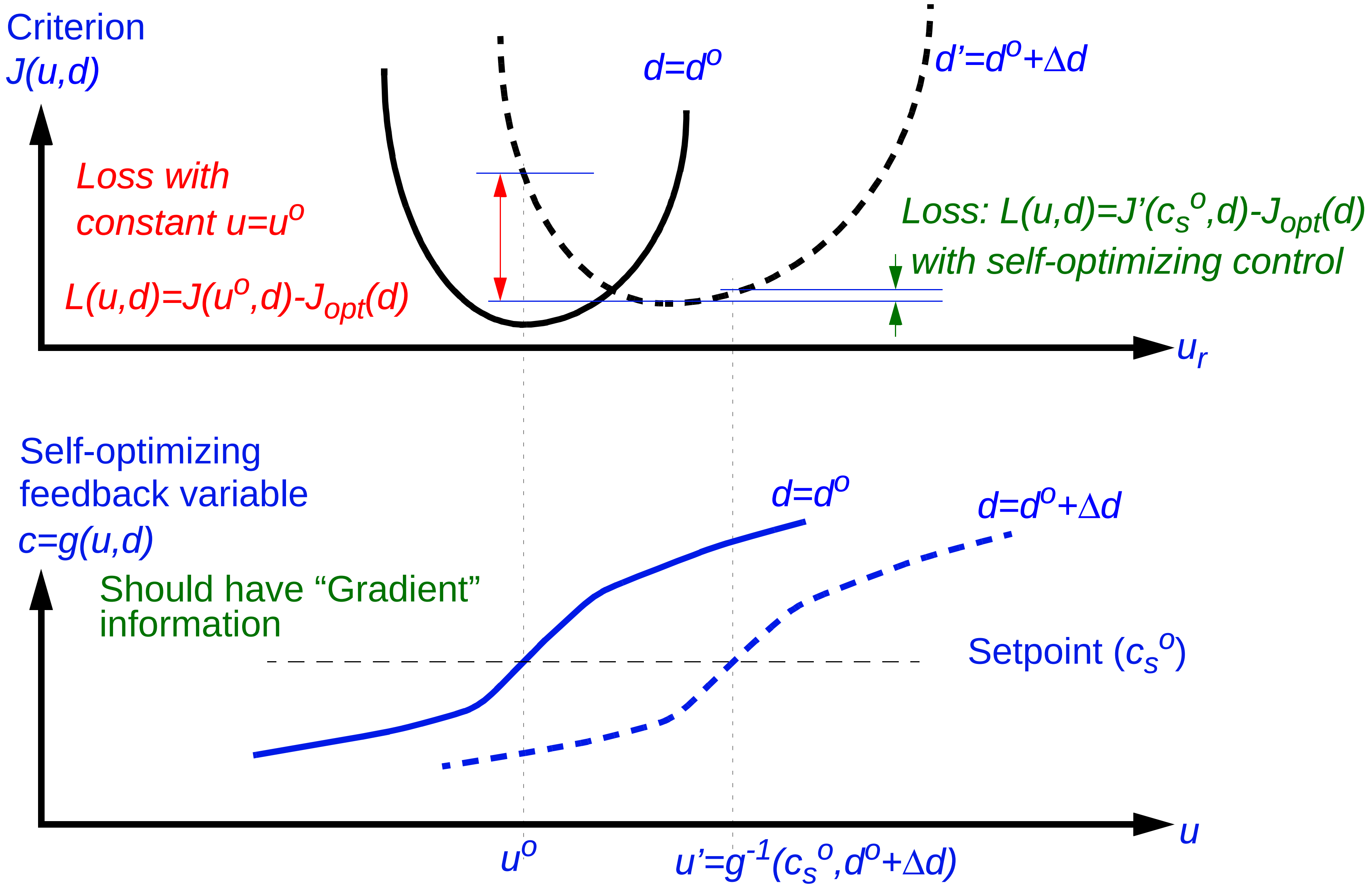
The key idea of self-optimizing control:

Select variables (*c*) which when controlled to a setpoint (c_s) also results in keeping the operation close to optimal.

- Finding the Self-optimizing control variables is a control structure issue (e.g. selecting input and output variables for control)
- The setpoints ($c_s=g(u,d)$) will replace the manipulated inputs (*u*) as the remaining DOFs.

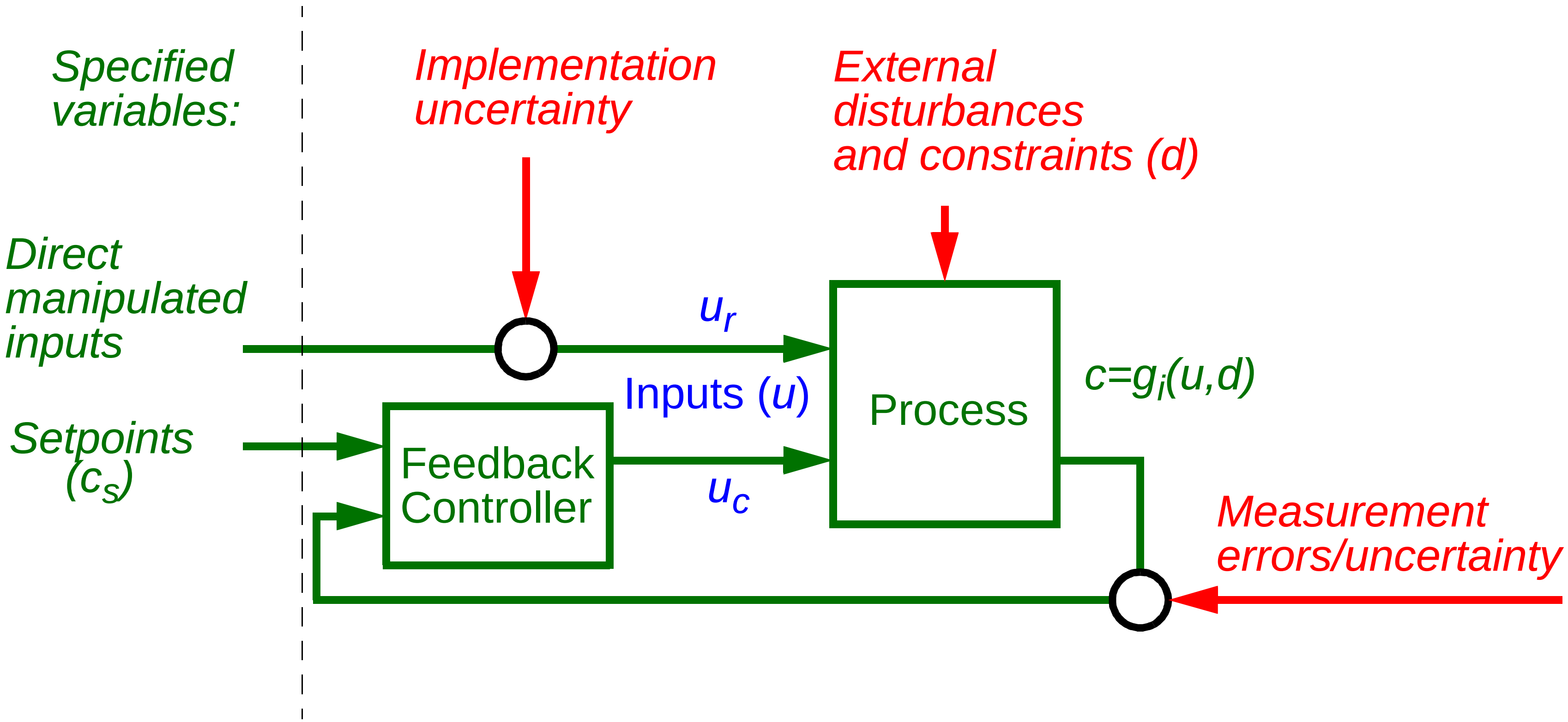
We convert $J(u,d)$ into $J(g^{-1}(c_s,d),d)=J_c(c_s,d)$ *or just* $J_c(d')$ *where* $d'=[d,c_s]$

Illustration of a nice Self-optimizing feedback variable

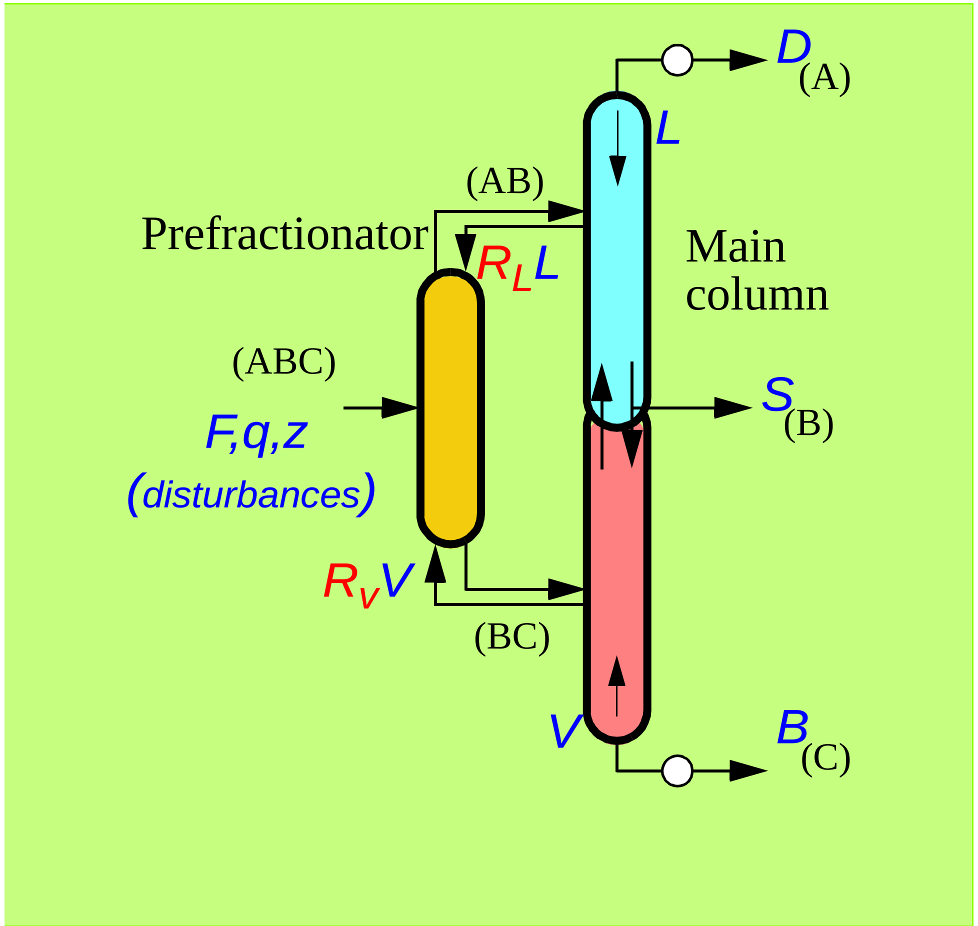


Evaluate the Steady-state Performance:

- Evaluate for expected variations in external disturbances
- Evaluate for expected uncertainty / measurement errors for feedback variables
- Evaluate for uncertainty / implementation error for direct manipulated inputs



Case Study: Evaluate Self-optimizing control structures for an Integrated Petlyuk Distillation Column



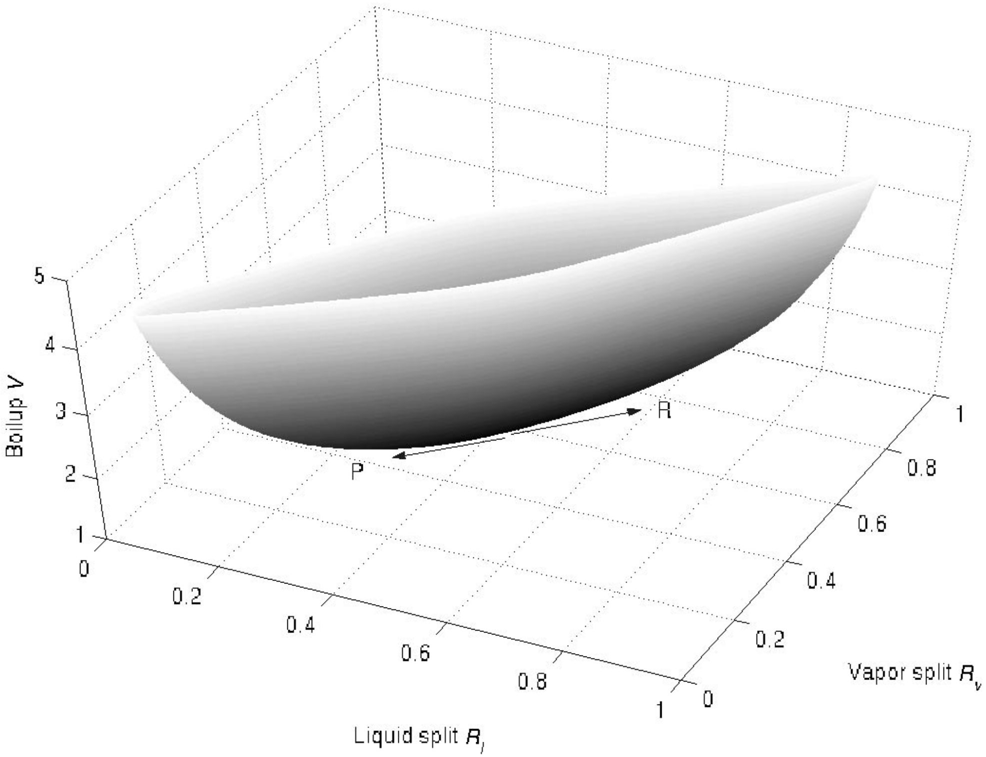
2 extra DOFs (R_l,R_v).

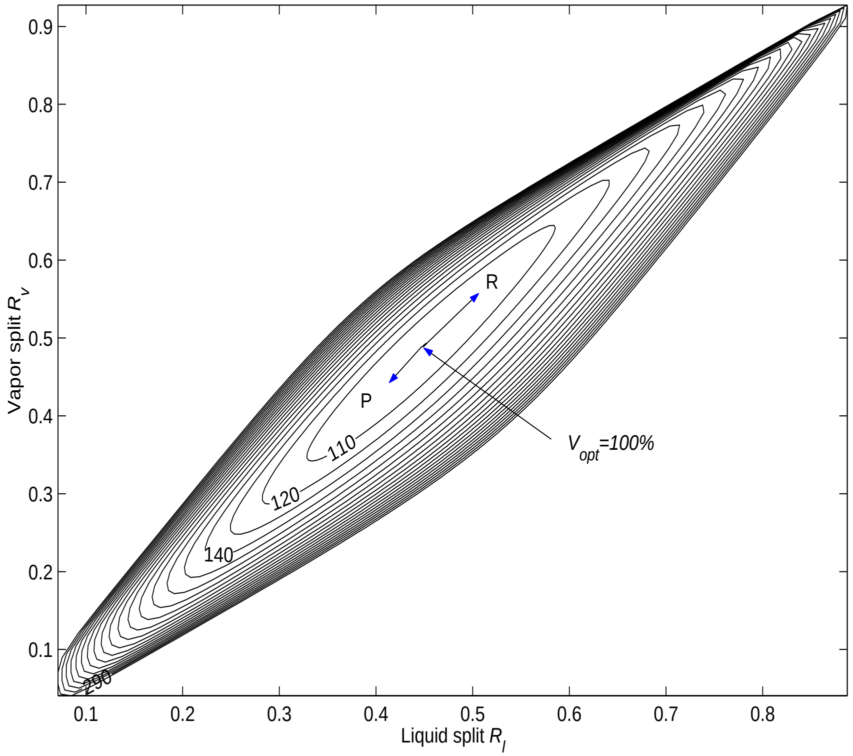
Difficult to operate?

Need for on-line optimization?

Flat or steep optimum?

Cost function: $J=V(R_l,R_V)$ for nominal values of $[x_{DA},x_{SB},x_{BC},z,q,F]$



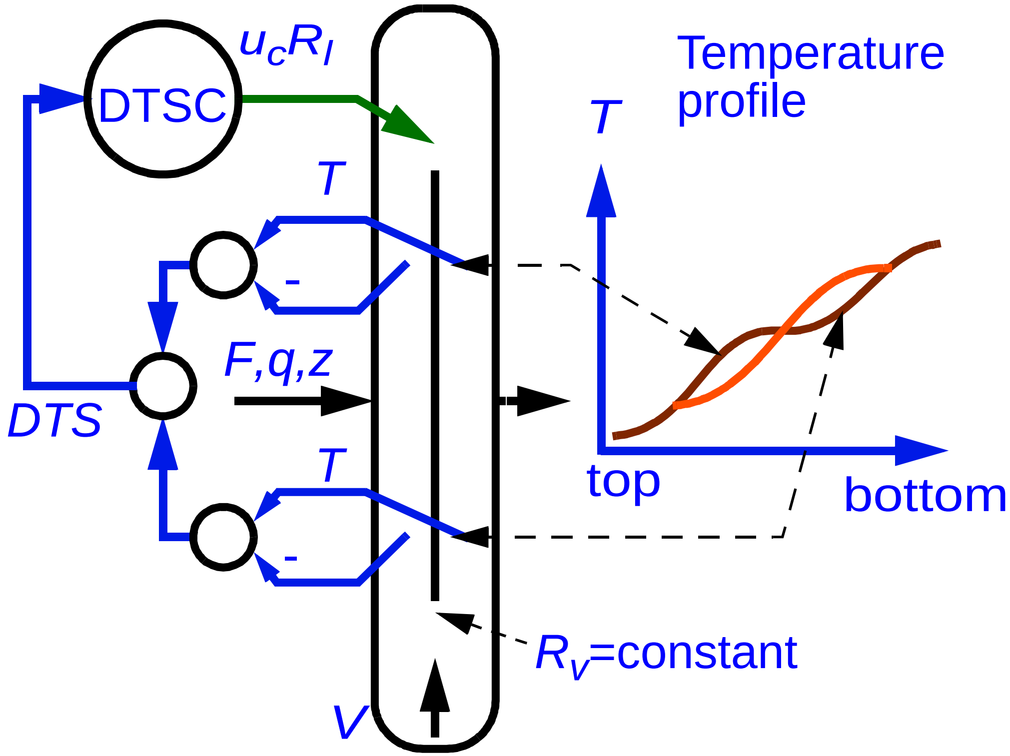


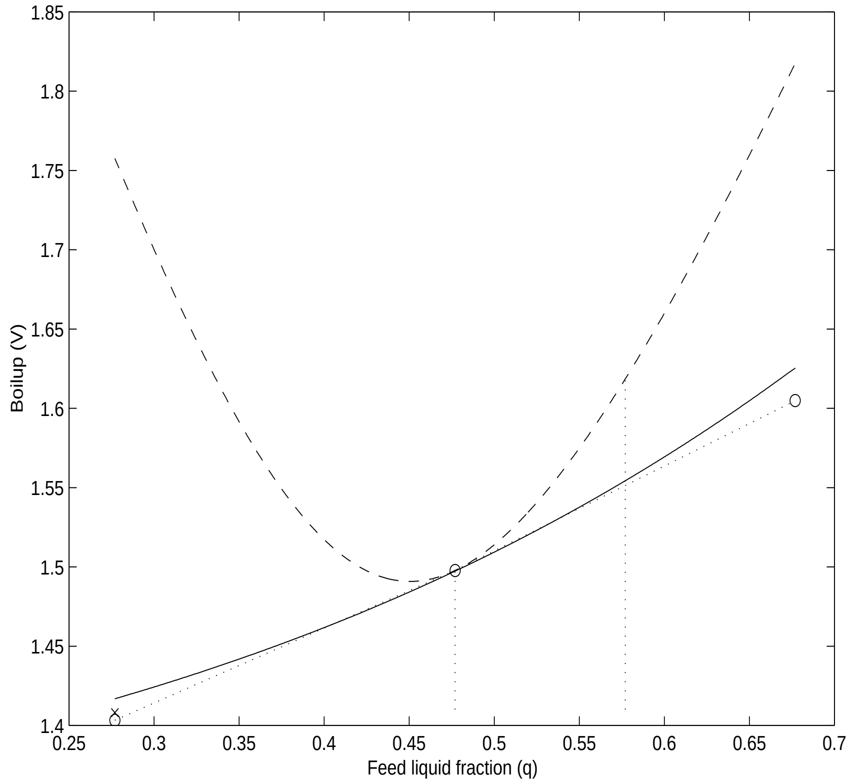
Observe that the surface $V(R_l,R_V)$ is flat along PR and steep normal to PR.

This indicates that one of the remaining DOFs may be kept constant.

We chose to keep the vapour split (R_V) constant, and evaluate self-optimizing control strategies with the liquid split (R_l) as the manipulated variable.

Example: Self-optimizing control by a temperature profile measure. Analyse impact from the feed enthalpy (q)



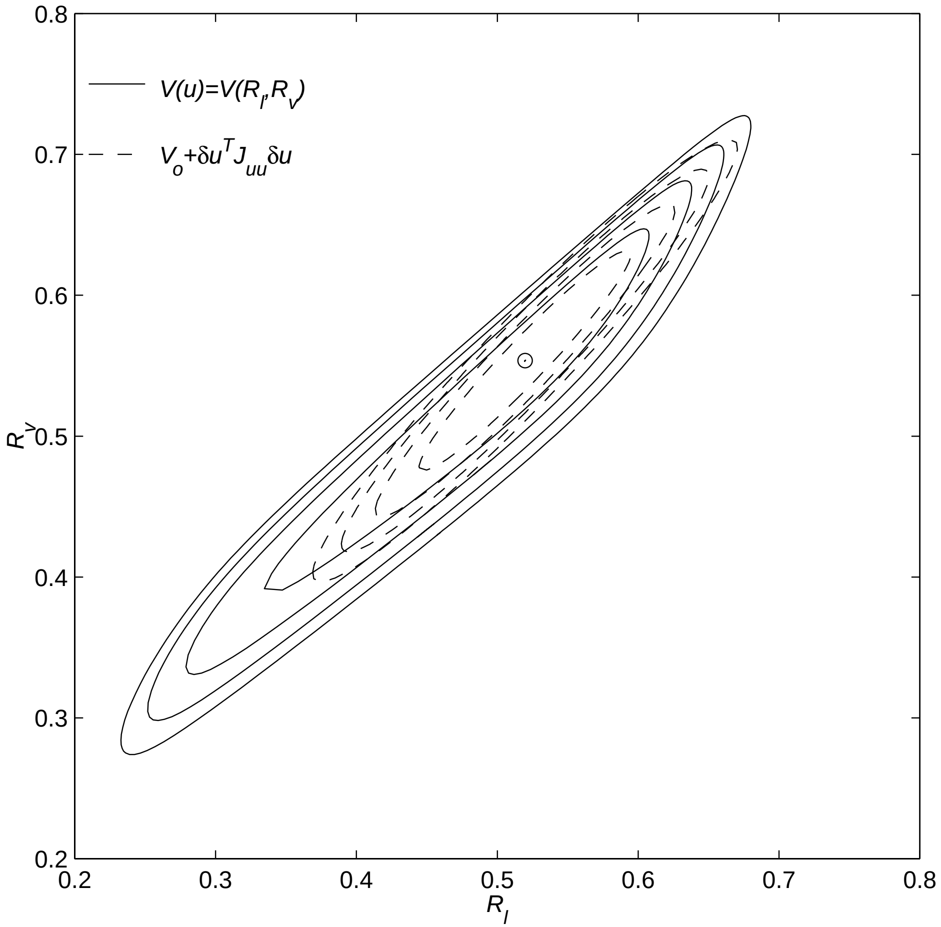


The plot shows the energy usage (V) as a function of a disturbance (q) for:

- No optimizing control: $V(R_l^o, R_V^o, q)$ (R_l and R_V are kept constant) (Dashed)
- Self optimizing control: $V(DTS^o, R_V^o, q)$ (*Manipulate* R_l, keeps DTS const.)(solid)
- Optimal solution $V_{opt}(q)$, where R_l and R_V are optimized for every q. (dotted)

Taylor series method

Effective evaluation by matrix algebra:



$$J(u,d) = J(u_0,d_0) + \begin{bmatrix} J_u^T & J_d^T \end{bmatrix}\begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix} + \frac{1}{2}\begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix}^T H \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix} + O^3$$

The Hessian: $= \begin{bmatrix} J_{uu} & J_{ud} \\ J_{du} & J_{dd} \end{bmatrix}$

Ideal input in case of no noise: $\boxed{u_{opt}(d) = u_0 - J_{uu}^{-1} J_{du}(d - d_0)}$

Candidate variable: $\Delta c = G\Delta u + G_d \Delta d + e$

Select the candidate (given by G and G_d) which minimize:

worst case loss: $L_{max} = \max_{\Delta\tilde{d},\, \Delta\tilde{e}} ?(L) = \frac{1}{2}\bar{\sigma}(M)$

$$M = [M_1, M_2]$$

where

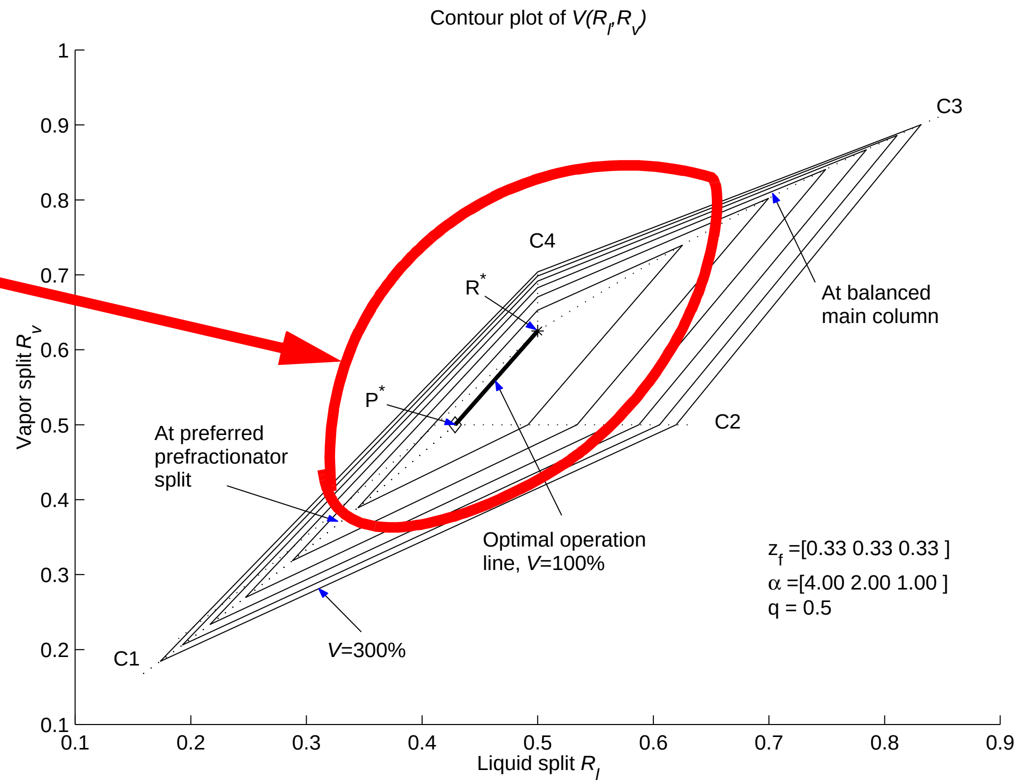
$$M_1 = J_{uu}^{1/2}(J_{uu}^{-1}J_{ud} - G^{-1}G_d)W_d$$

$$M_2 = J_{uu}^{1/2}G^{-1}W_e$$

Understanding the steady-state behaviour of the optimality region and the full solution surface $V(R_l,R_V)$:

Our Contribution:

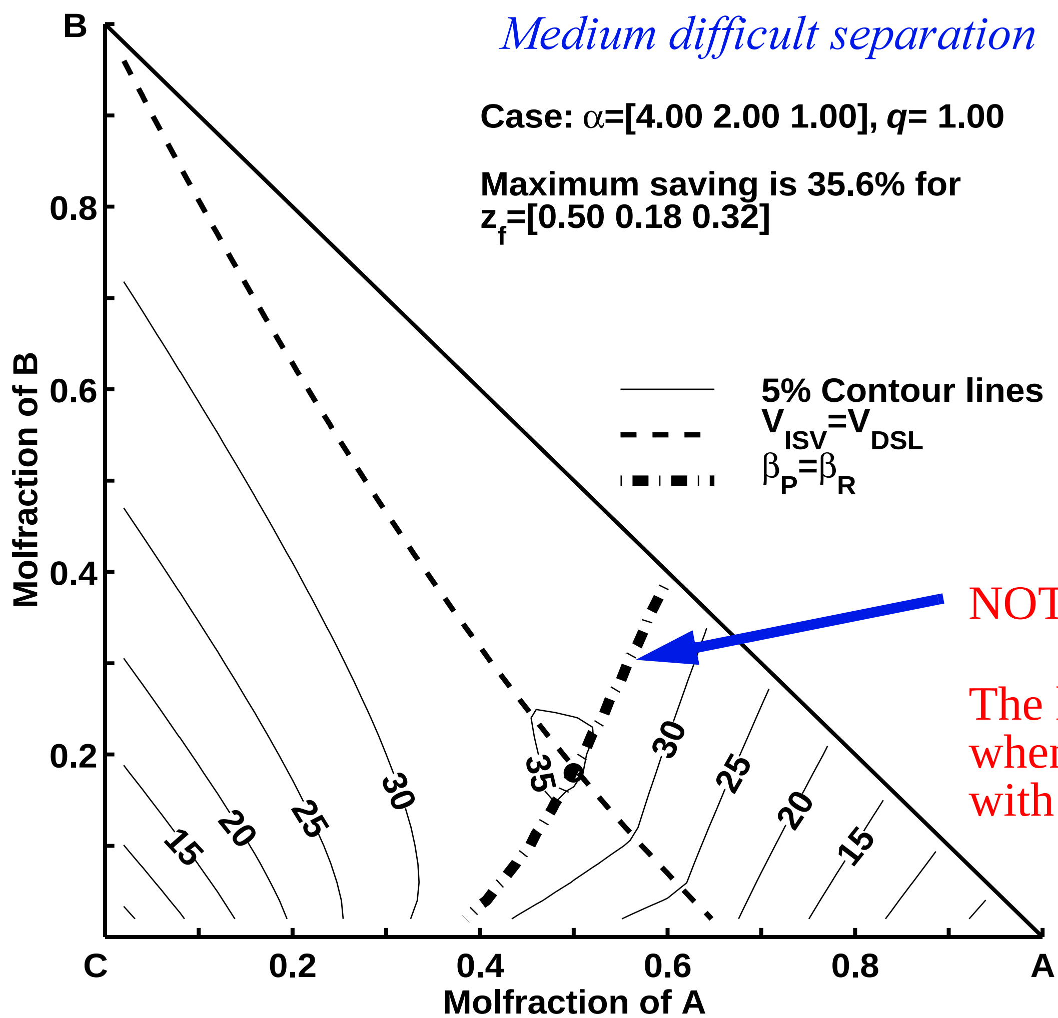
Extended the expression to operation outside the flat region



The energy consumption increase rapidly when the operation is not exactly at the minimum energy region (which is on PR).

Important: When PR is large, one DOF (R_l *or* R_V) may be kept constant!!!

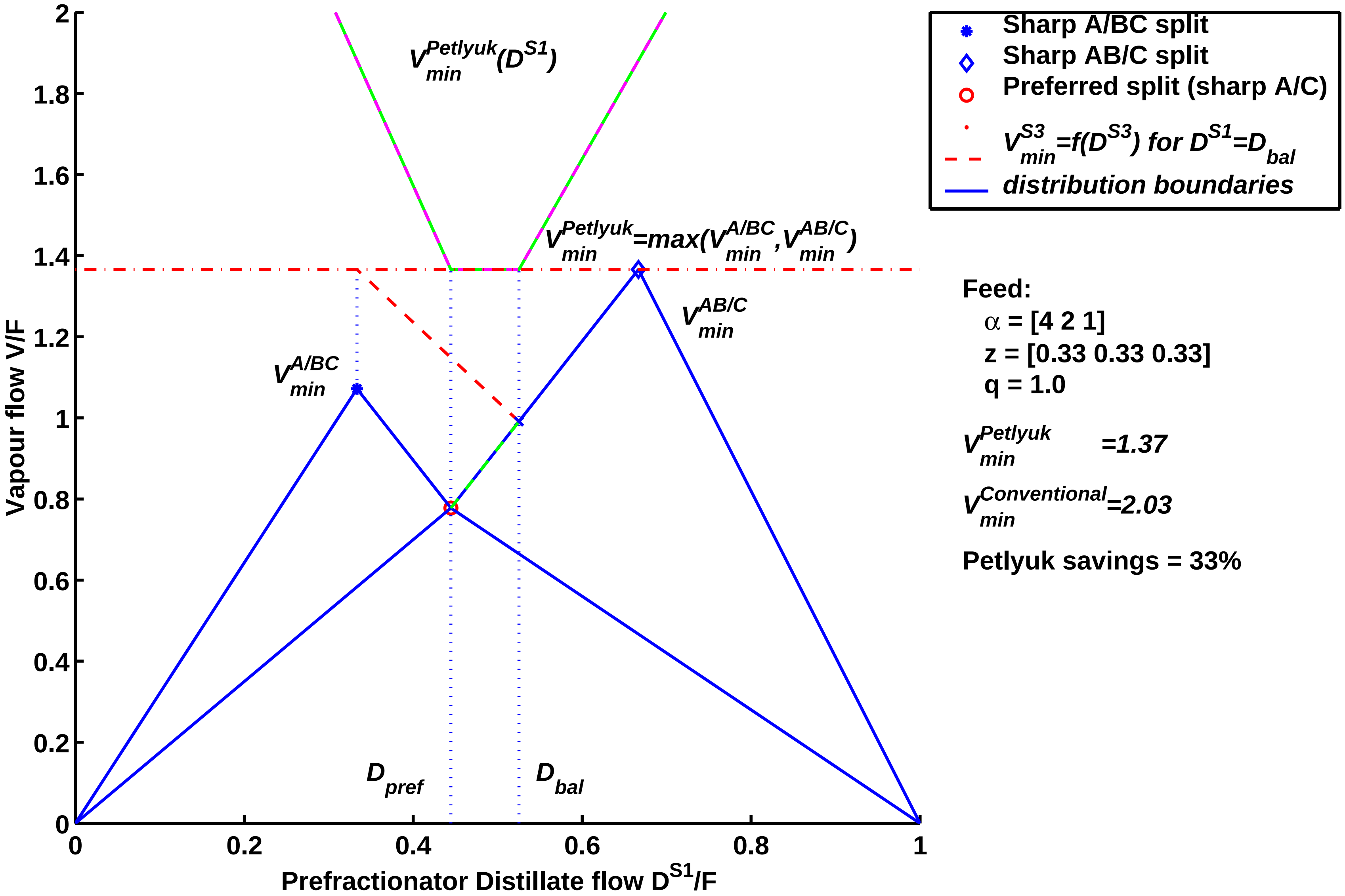
Contour plot of theoretical savings as function of feed composition compared to the best of the conventional configurations.



NOTE!

The largest savings is achieved when the *preferred split* coincide with a *balanced main column*

Example: Relation to the Vmin-diagram:



Feed:

α = [4 2 1]

z = [0.33 0.33 0.33]

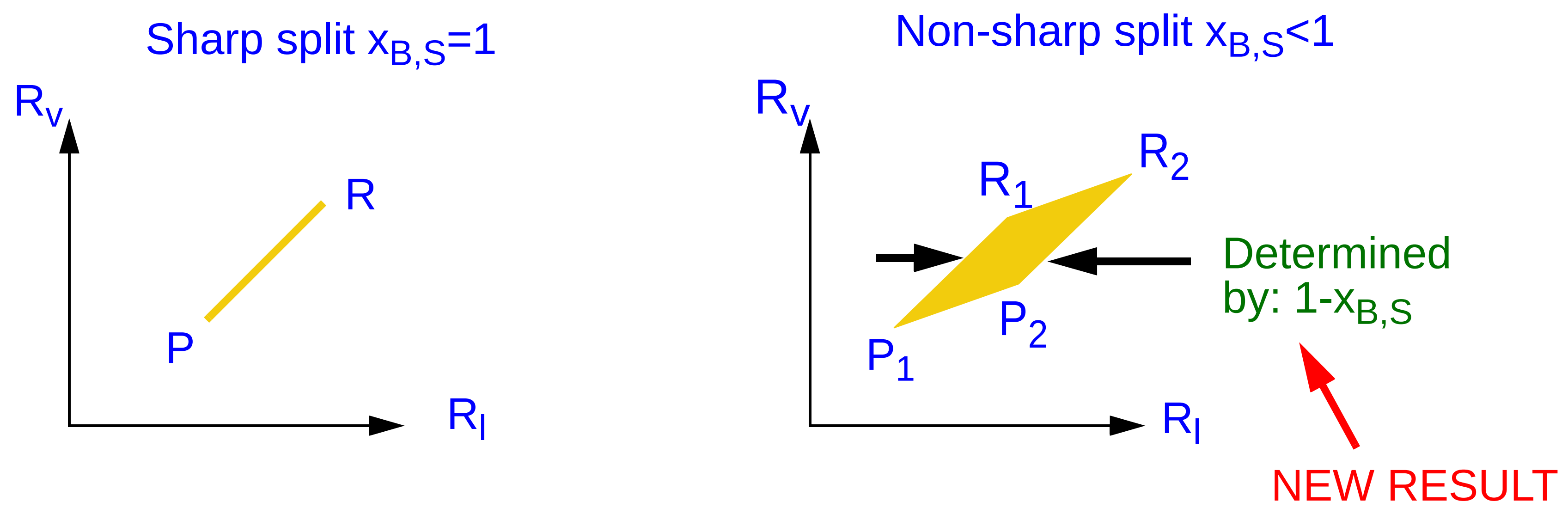
q = 1.0

$V_{min}^{Petlyuk}=1.37$

$V_{min}^{Conventional}=2.03$

Petlyuk savings = 33%

Non-pure side-stream =>
The flat region is extended to a parallelogram



Direction 1 (PR): Depends on “Preferred split” - “Balanced main column”

Direction 2 (12): Depends on side-stream purity ($1-x_{B,S}$)

Summary of contributions in Part II

- Computation of the full solution surface for infinite number of stages, and explanation of the characteristic “corners”.
- Understanding of how the flat optimum and the whole solution surface is affected by feed properties and feed composition
- The boundary curve where there is no flat optimum and its implications
- Analytical description of the optimality region for non-sharp product splits, and in particular the relation to the sidestream impurity.
- Analysis of Self-optimizing control for the Petlyuk column. Qualitative analysis based on process insight and quantitative analysis based on a stage-by-stage model show that there are available self-optimizing control variables.
- The Taylor-series method for self-optimizing control analysis.
- The solution surface is quite steep, so the available degrees of freedom must be set properly at their optimal values and on-line adjustment is required due to the presence of process disturbances and model uncertainties.

- Conclusion: The main control problem of the Petlyuk Column is a control structure problem, and Self-optimizing Control can be applied to find simple practical solutions for a given separation task.

Conclusions and further work

- Better understanding of the characteristics of directly coupled distillation arrangements has been obtained.
- The energy consumption in the process industry can be reduced
- The new insight can be used to develop better engineering procedures
- The methods should be applied to industrial cases