Minimum Energy for Separation of Multicomponent Mixtures in *Directly Coupled Distillation Arrangements*

by

Ivar J. Halvorsen and Sigurd Skogestad

Norwegian University of Science and Technology (NTNU)
Department of Chemical Engineering

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email: Ivar.J.Halvorsen@ecy.sintef.no, Sigurd.Skogestad@chembio.ntnu.no

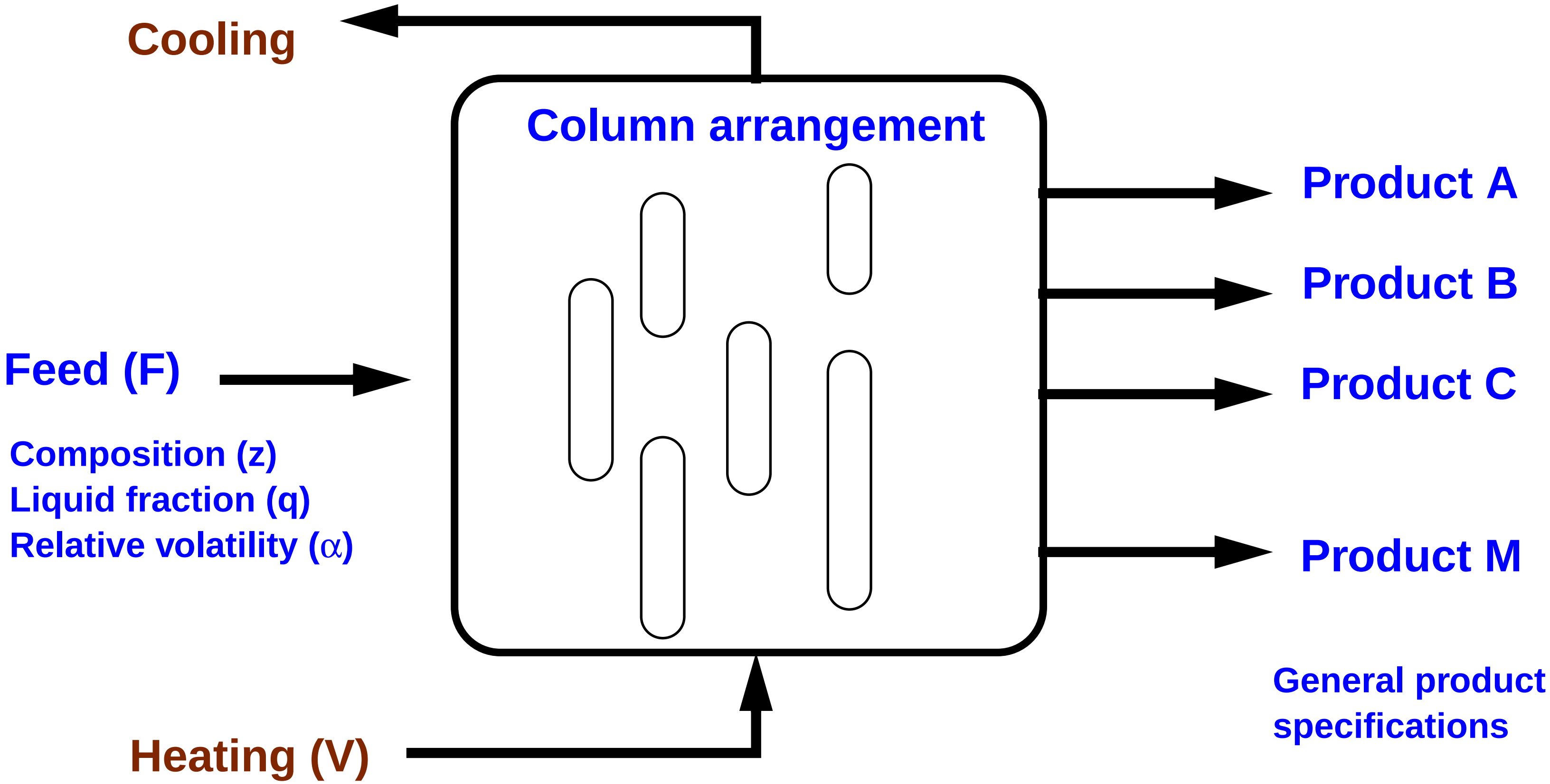
Motivation

1. Need for quick determination of energy requiremen in complex distillation configurations, e.g for Petlyuk columns.
2. Need for better understanding of how to operate complex column arrangements.

Main results:

1. Exact analytical solution for minimum energy in directly coupled distillation arrangements
2. Simple graphical visualization in the V_{min}-diagram.
3. Handle N components and M products.
4. Detailed solution for all internal flows is also obtained

The General Problem



Minimum energy (V_{min}) ?

Internal flows ?

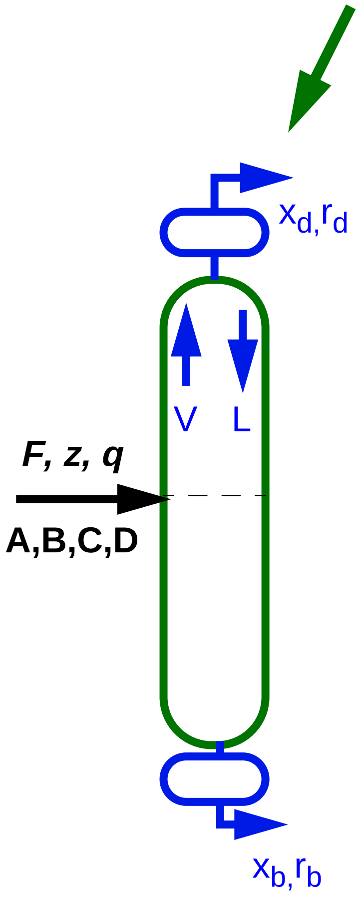
Intermediate recoveries ?

Some simplifying assumptions:

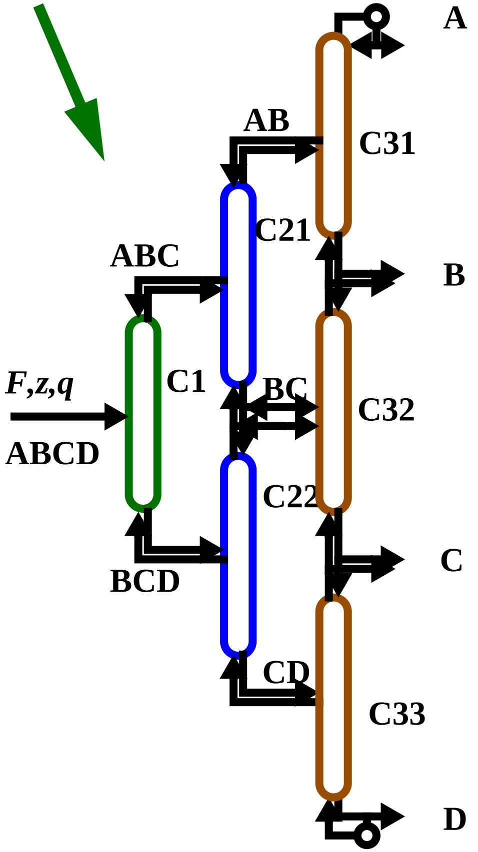
- constant relative volatilities (α)
- constant molar flows
- constant pressure
- no internal heat exchange

Our Contribution:

We can use the behaviour in this standard two-product column -

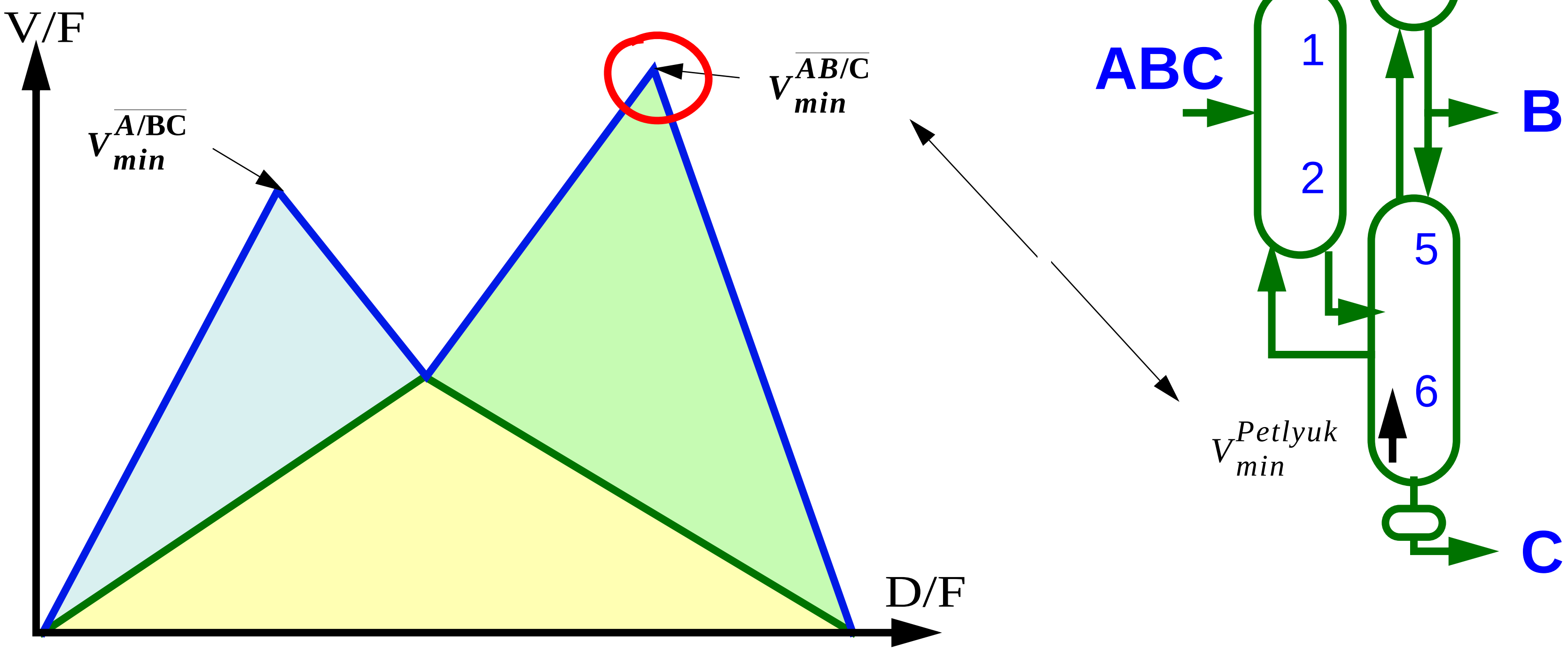


to predict the optimal performance of a directly coupled extended Petlyuk arrangement



V_{min} for the 3-product Petlyuk column is found as the highest peak in the V_{min}-diagram:

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



Selected references:

Classical references for multicomponent distillation

- Underwood (1946, 1948a,b), Fractional distillation of multicomponent mixtures
- Shiras (1950), Calculation of Minimum Reflux in Distillation Columns
- Franklin, Forsyth (1953), The interpretation of minimum reflux conditions in multicomponent distillation
- King (1980), Separation Processes.(book)
- Koehler (1995), A review of minimum energy calculations
- Stichlmair (1998), Distillation: Principles and Practice. (book)

Minimum energy expressions for Petlyuk arrangements:

- Fidkowski, Krolikowski (1986), Thermally Coupled Columns: Optimization proc.
- Carlberg, Westerberg (1989) Temperature-Heat Diagrams for Complex Columns. 3. Underwood's Method for the Petlyuk Column.

Revisit of Underwood's Equations

Starting points:

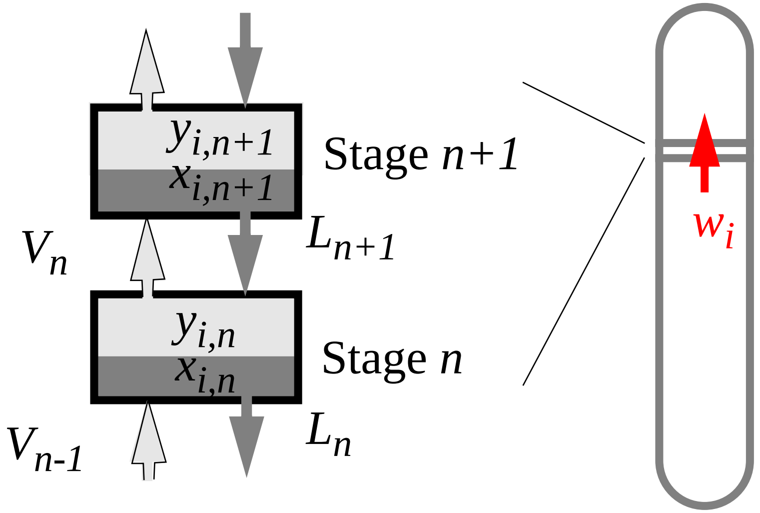
1. Net component flow (w) through a stage

$$w_i = V_n y_{i,n} - L_{n+1} x_{i,n+1} \quad (1)$$

(w is defined positive upwards)

w_i is constant in a section:

$w_{i,D} = r_{i,D} z_i F$



2. Vapour liquid equilibrium (VLE):

$$y_i = \frac{\alpha_i x_i}{\sum_i \alpha_i x_i}$$

Summary of Underwood's Equations for Minimum Energy Calculations

Feed equation gives common "V_{min}"-roots θ

$V^T - V^B = (1-q)F$

Component i

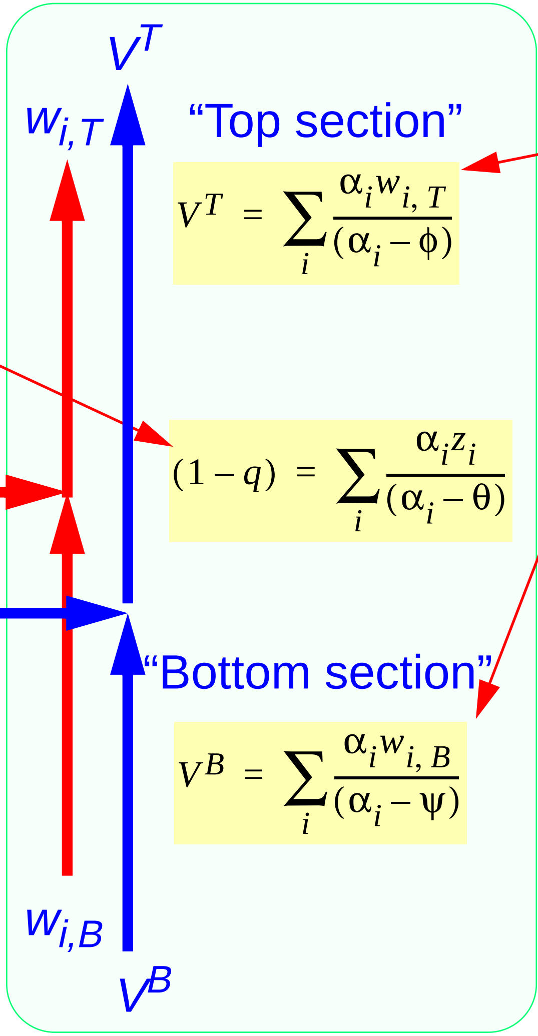
$w_{i,F}$

$(1-q)F$

Vapour

$w_{i,F} = F z_{i,F}$

$w_{i,B} = w_{i,T} - F z_{i,F}$



Top and bottom equations gives "real" - roots ϕ and ψ

Underwood's V_{min}-result:
When one or more pairs ϕ_i, ψ_{i+1} coincide, then
$\phi_i = \psi_{i+1} = \theta_i$, and
$V = V_{min}$

How to compute:
- $V=?$
- $D=?$
- $w_{i,T}=?$

KEY: *DISTRIBUTION*

How to use Underwood's minimum energy results:

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

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

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

$$\bullet$$

$$\bullet$$

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

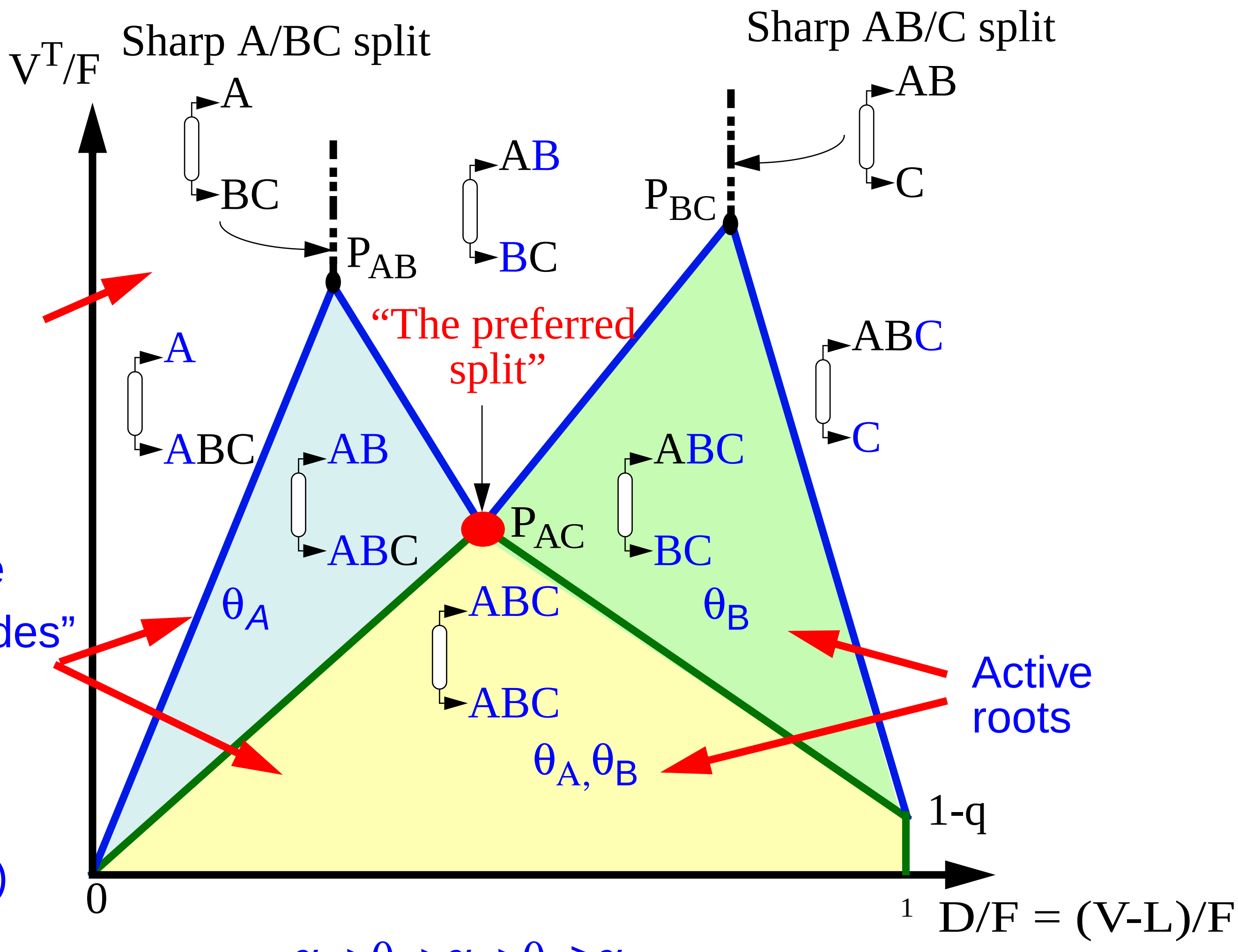
This procedure particularly simple for sharp component splits (*r_i=1 and r_j=0*)

Visualisation of minimum energy and component distribution for the ternary example (feed components ABC)

$V > V_{min}$
above the "mountains"

$V = V_{min}$ in the "mountain-sides" and below

Note:
$V_{min} = f(\text{spec.})$

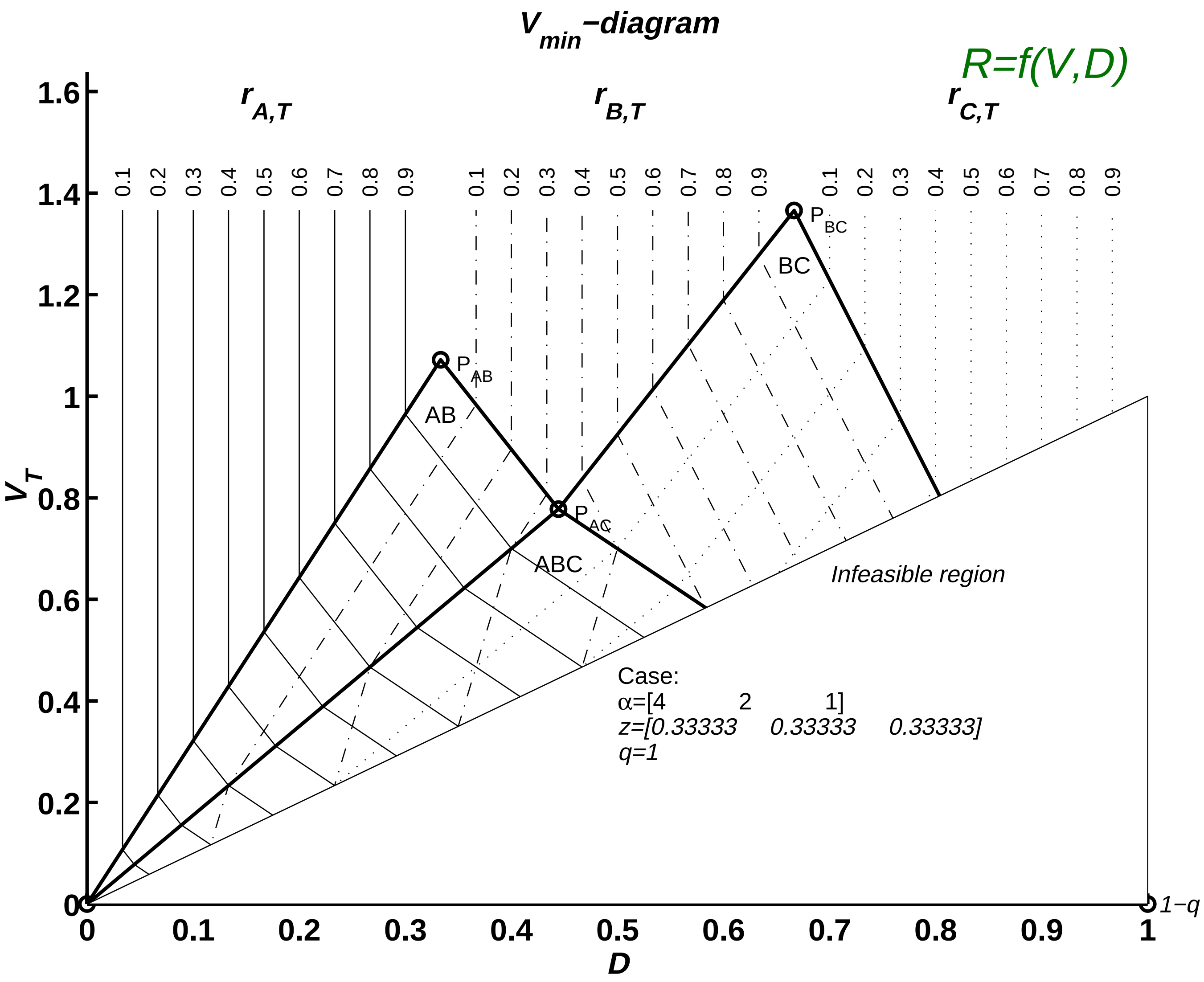


$\alpha_A > \theta_A > \alpha_B > \theta_B > \alpha_C$

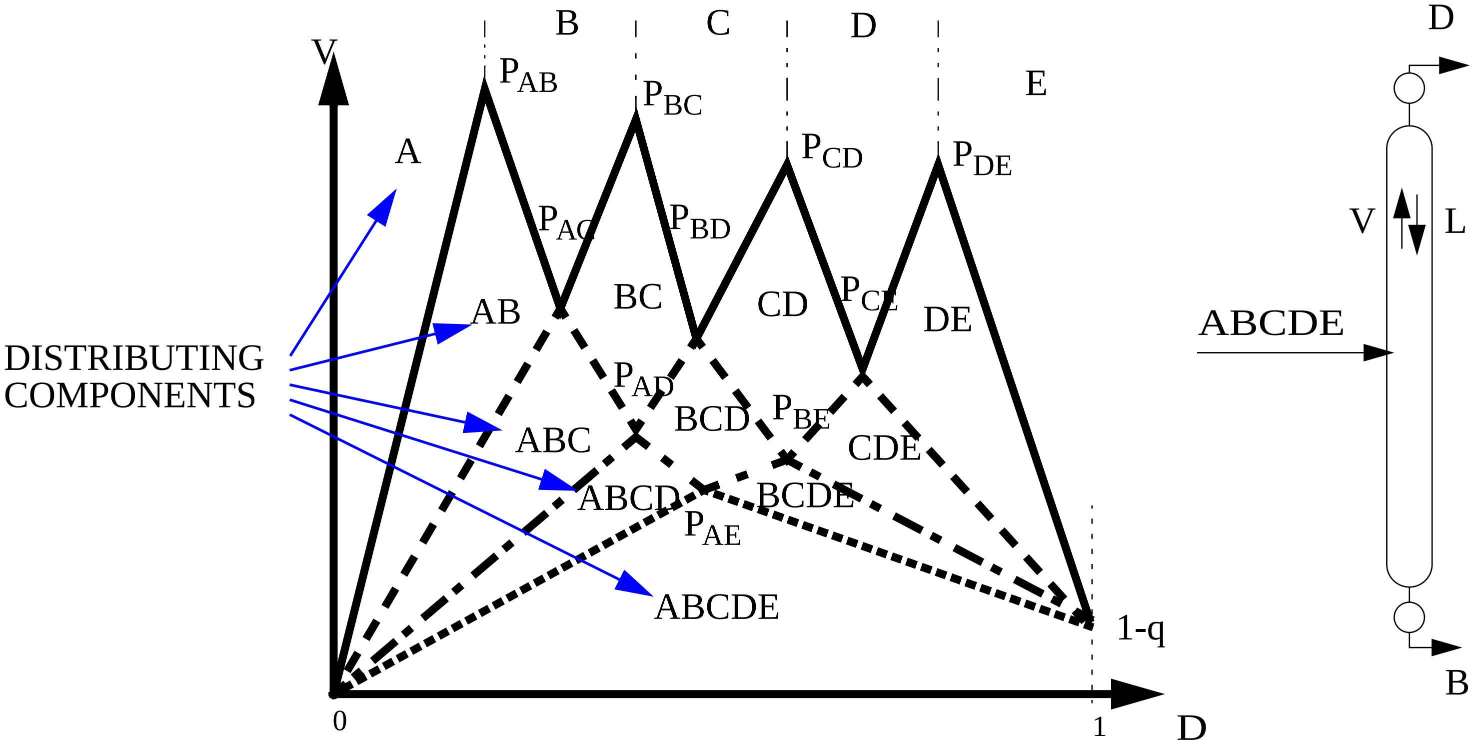
Visualization of the operation in the D-V plane

- Any feasible point in the 2-dimensional plane spanned by 2 independent DOFs (here D,V) determines the operation completely.
- In every polygon region, a particular set of components distribute.
- The "active Underwood roots" are always adjacent, and are in the set laying between the volatilities of the distributed components. Thus each polygon region corresponds to a set of active Underwood roots.
- On the straight line boundaries between the polygon regions, one particular component is at the limit of being distributed to both products.
- The "mountain" tops: Sharp splits between adjacent key components (neighbours i relative volatility)
- Minimum points: "Preferred split", or optimal distribution of intermediate components.

Ternary 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).

Simple Matlab™ function prototypes

[θ] =UWroots(α,z,q)	Compute the common roots from the feed equation
[Vs,Ds,Rs]=UWmulti(α,z,q)	Compute all the polygon points in the D-V plane
[V,D,R]=UWrspec(α,z,q,ri,rj)	Compute an operation point from specification the recoveries (r) of keys i,j
[V,D,R]=UWxspec(α,z,q,xi,xj)	Compute an operation point from specification the product composition (x) of keys i,j
[R] =UWvdspec(α,z,q,V,D)	Compute all recoveries R as function of V and D

V: Normalized top section vapour flow (F=1)

D: Normalized distillate product flow (F=1)

R: All component recoveries $R=[r_1,r_2,r_3,....r_{Nc}]$ (in the distillate product)

α: Relative volatilities $\alpha=[\alpha_1,\alpha_2,\alpha_3,....\alpha_{Nc}]$

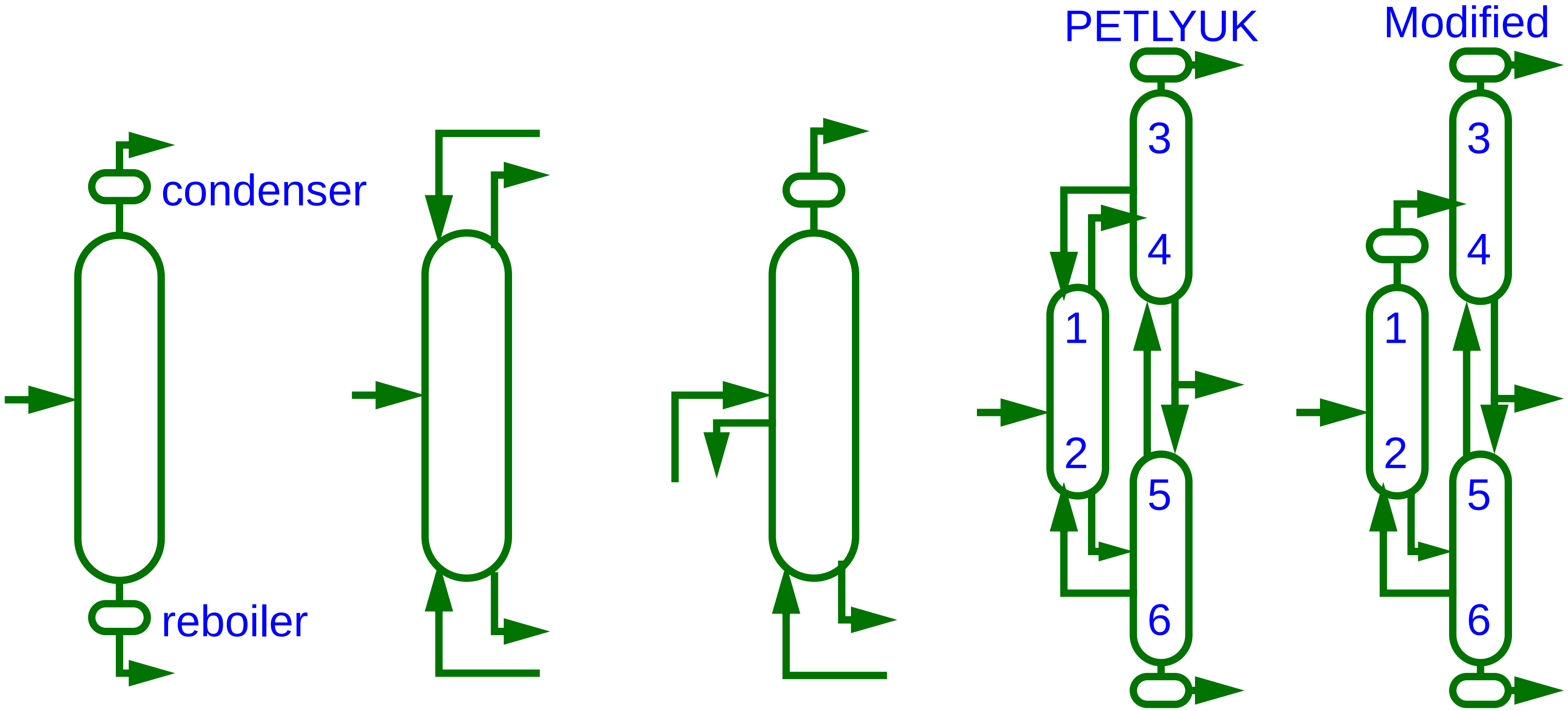
z : Feed composition $z=[z_1,z_2,z_3,....z_{Nc}]$

q : Feed liquid fraction

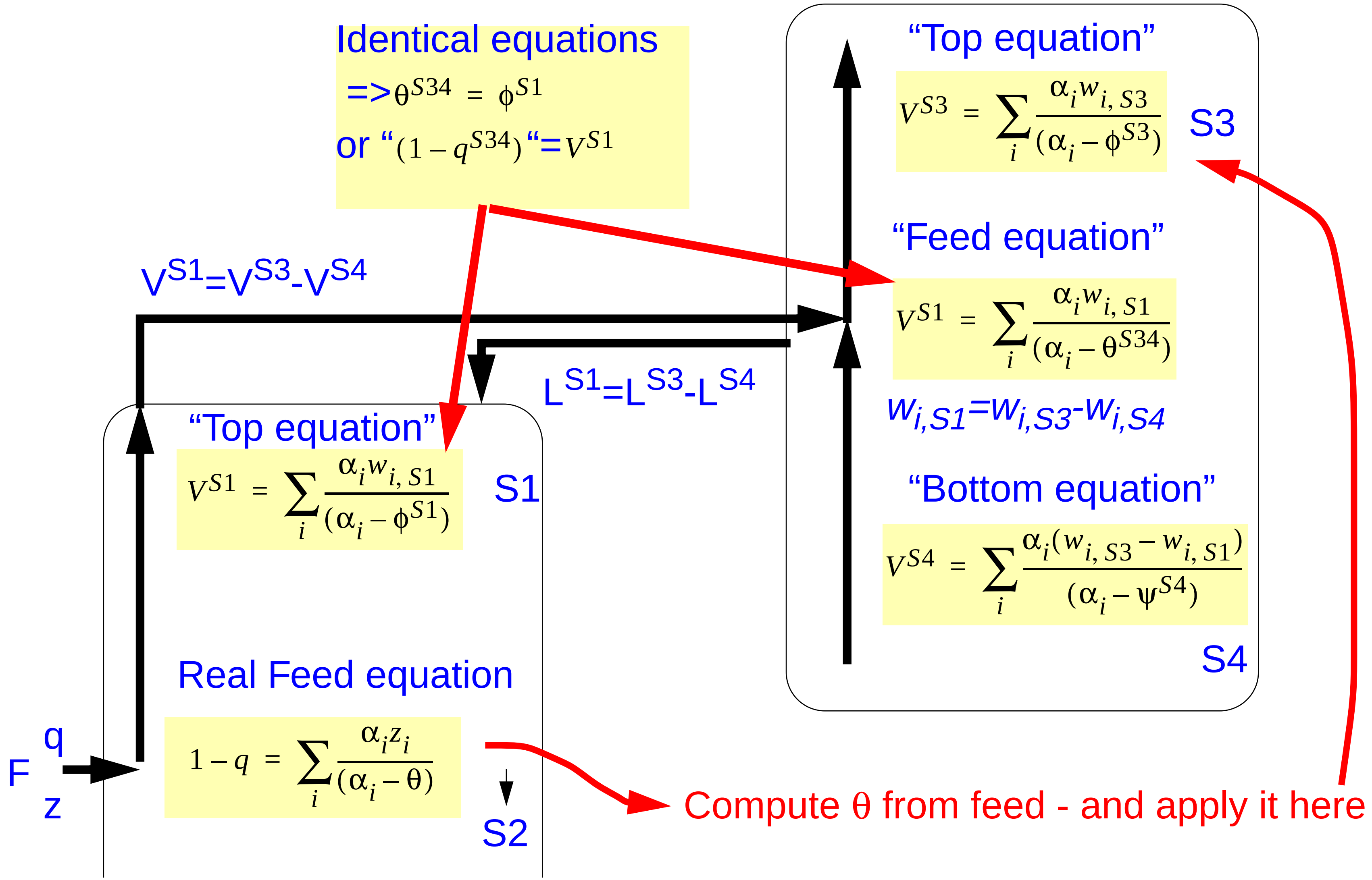
Note that the distillate flow $D=FRz^T$, and the top composition $x_{i,D}=r_i z_i/(D/F)$

Application to directly (fully thermally) coupled columns:

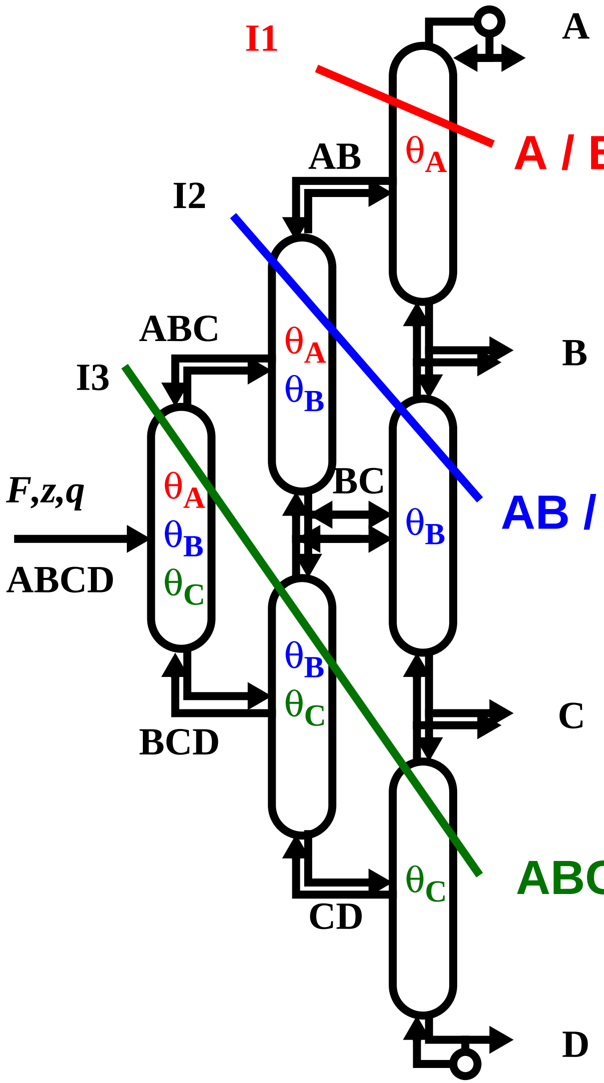
:



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

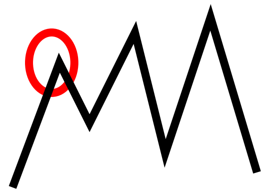


Proof for the general N-component case



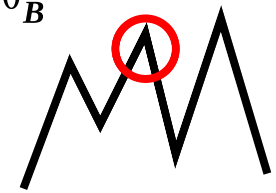
A / BCD - split

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



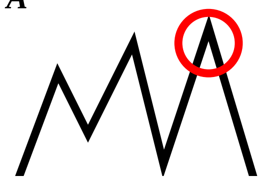
AB / CD - split

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



ABC / D - split

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



Minimum energy for the N-product Petlyuk column:

$$V_{Tmin}^{Petlyuk} = \max_j \sum_{i=1}^{j} \left(\frac{\alpha_i w_{i,T}}{\alpha_i - \theta_j} \right) \quad (2)$$

In the ternary case, our general approach gives the same results as the analytical solution by Fidkowski and Krolikowski (1986) (valid for q=1 and sharp splits):

$$V_{Tmin}^{Petlyuk} = \max\left(\frac{\alpha_A z_A}{\alpha_1 - \theta_A}, -\frac{\alpha_C z_C}{\alpha_C - \theta_B} \right) \quad (3)$$

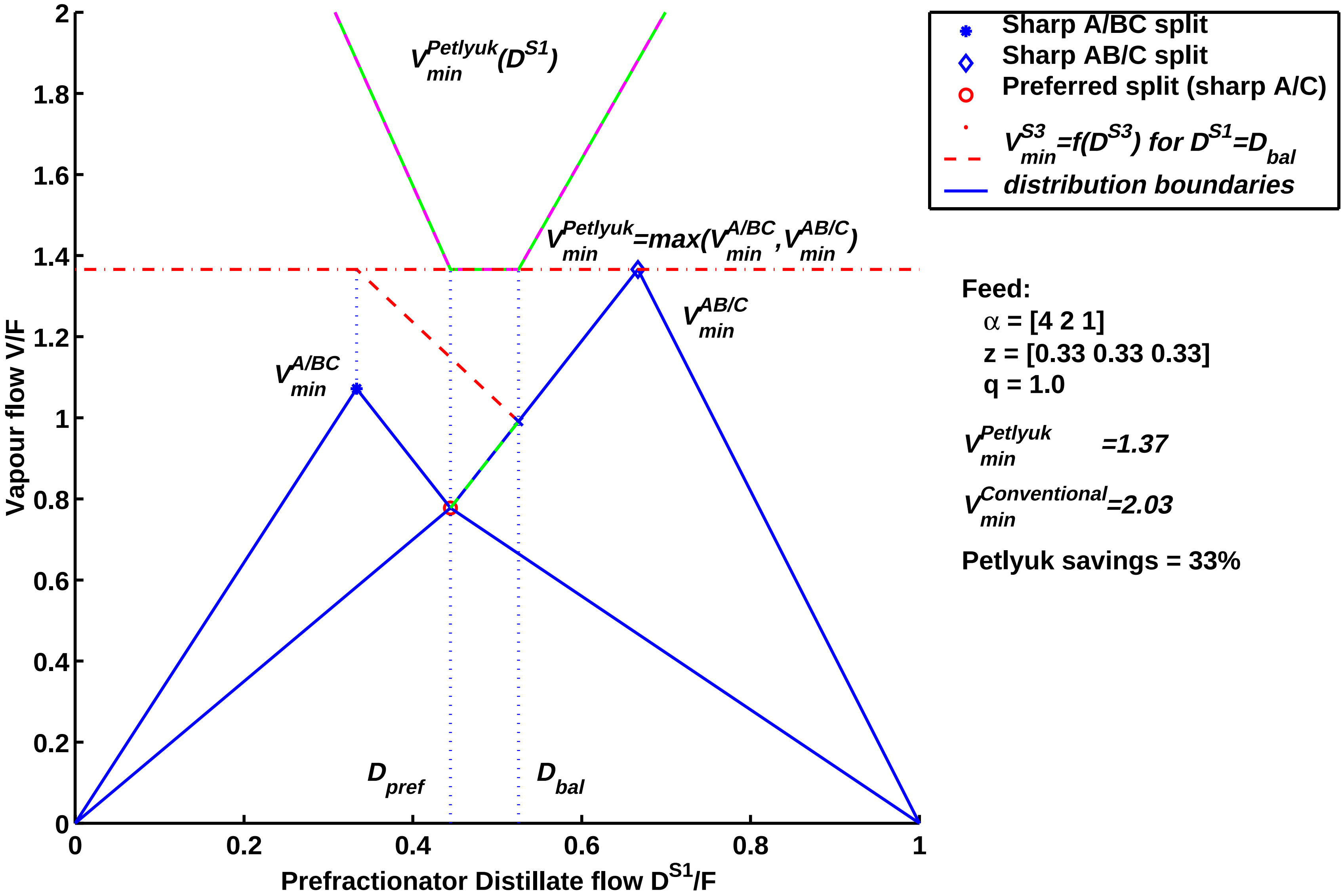
Our contributions can be listed as:

1. Different and more direct deduction
2. Generalize the solution to any liquid fraction and nonsharp splits
3. Handle N>3 components and M>3 products
4. Simple visualization in the V_{min}-diagram: ***The highest peak***!

Super-simple procedure for the minimum energy requirement for 3 product Petlyuk Column

1. Compute the V_{min}-diagram for the feed:
2. Compute the energy requirement to produce the Petlyuk top product specification in a single column, and plot it into the diagram ($V_{min}^{A/BC}$)
3. Compute the energy requirement to produce the Petlyuk bottom product specification in a single column and plot it into the diagram ($V_{min}^{AB/C}$)
4. Operate the prefractioantor at the preferred split: $V_{min}^{A/C}$
5. The minimum energy requirement for the Petlyuk column is simply the maximum value of 2 and 3 (adjusted for 1-q): $V_{min}^{Petlyuk} = max(V_{min}^{A/BC}, V_{min}^{AB/C})$
6. This also gives us information of the extent of the flat region. If the difference is large, there is a large flat region.

Example: Application to a 3 product Petlyuk Column:



Feed:

α = [4 2 1]
z = [0.33 0.33 0.33]
q = 1.0

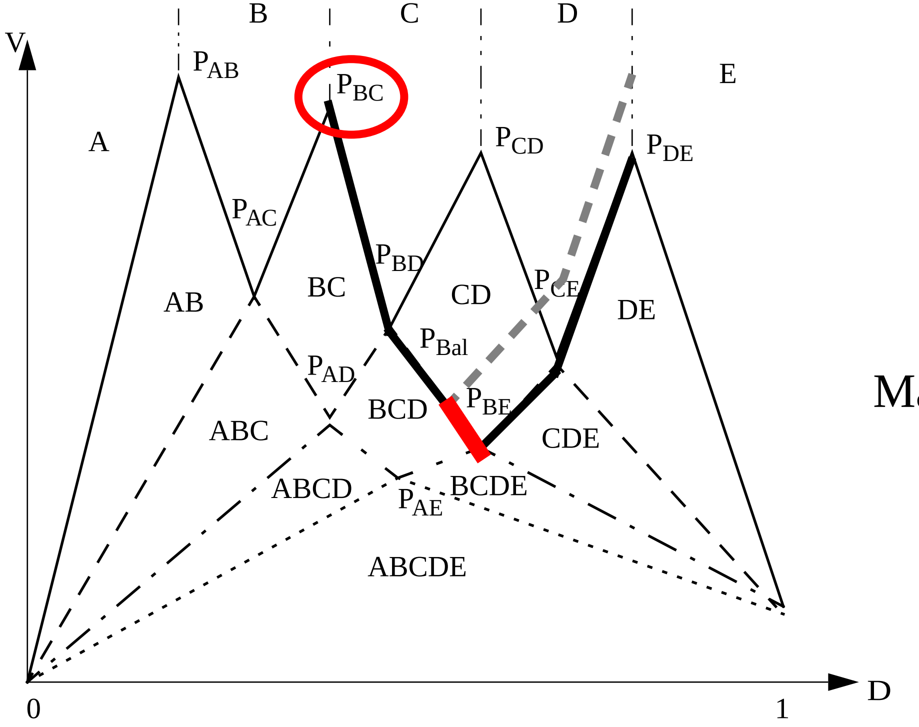
$V_{min}^{Petlyuk}=1.37$

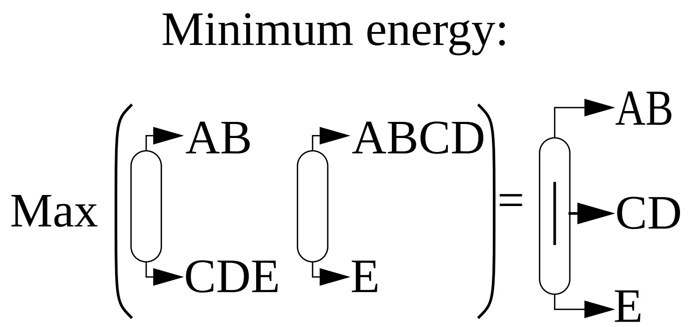
$V_{min}^{Conventional}=2.03$

Petlyuk savings = 33%

Ex.: Application to 3-product Petlyuk arrangement with 5-component feed

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



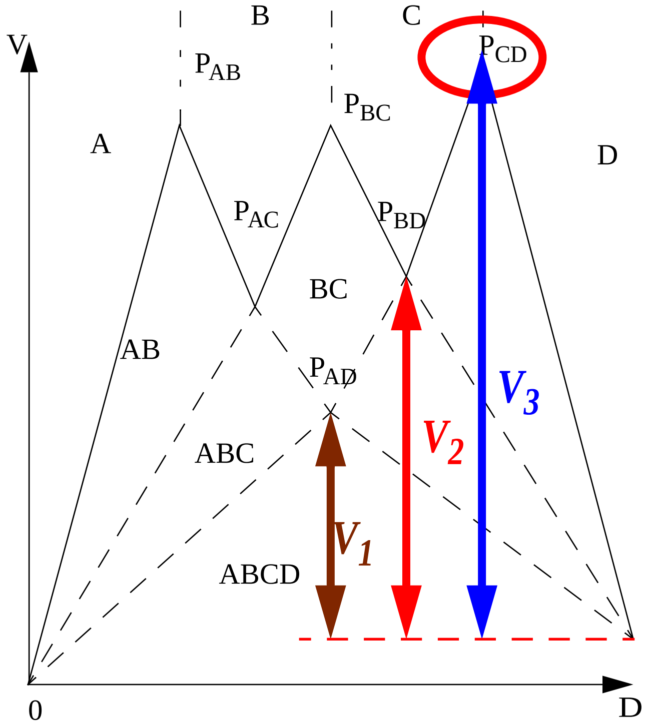


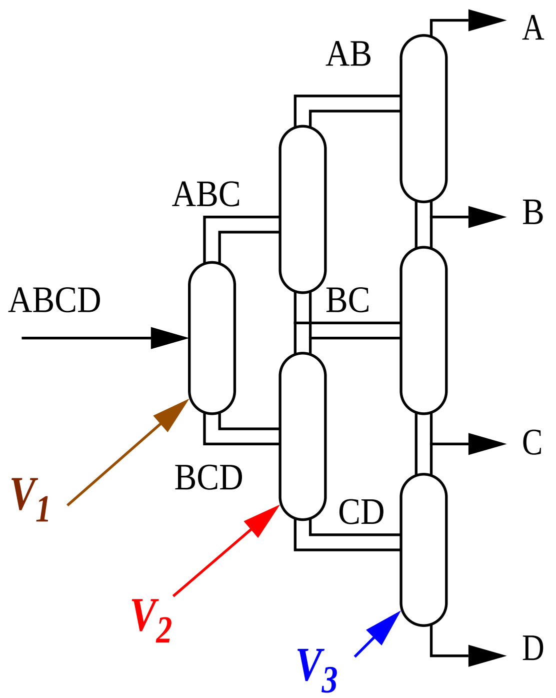
Solution: Operate the prefractionator between P_{Bal} and P_{BE}

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

Ex.: 4-component feed to 4-product “Petlyuk” column

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

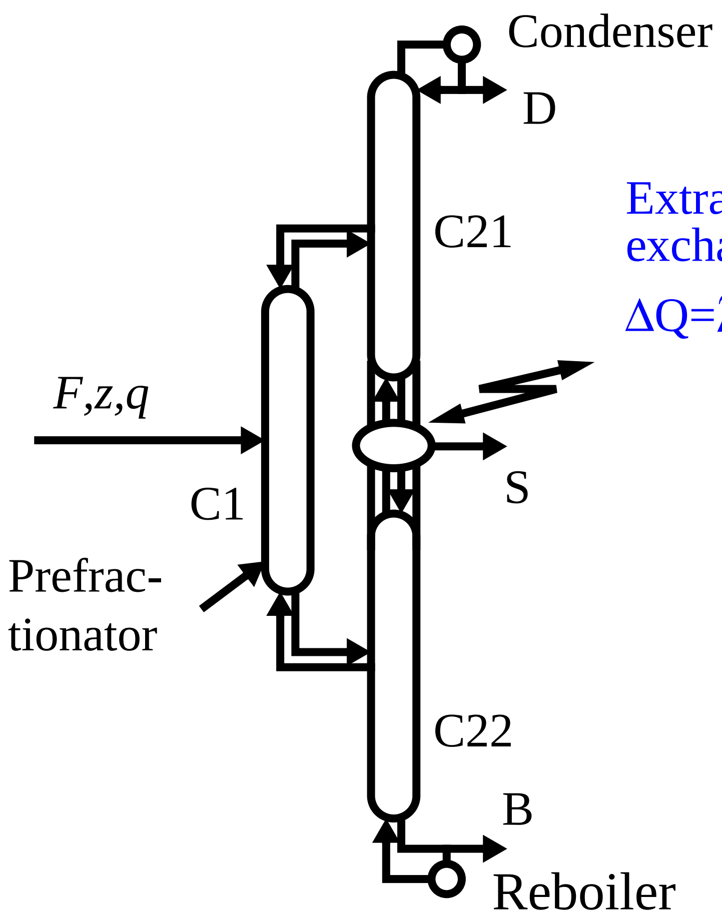


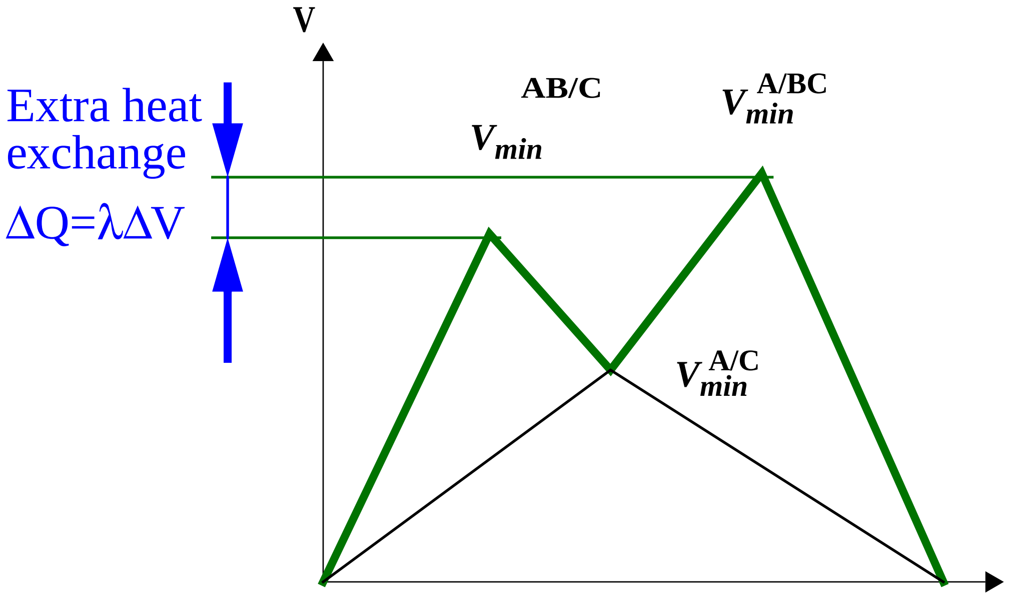


Solution: Operate every “2-product column” at its “preferred split”

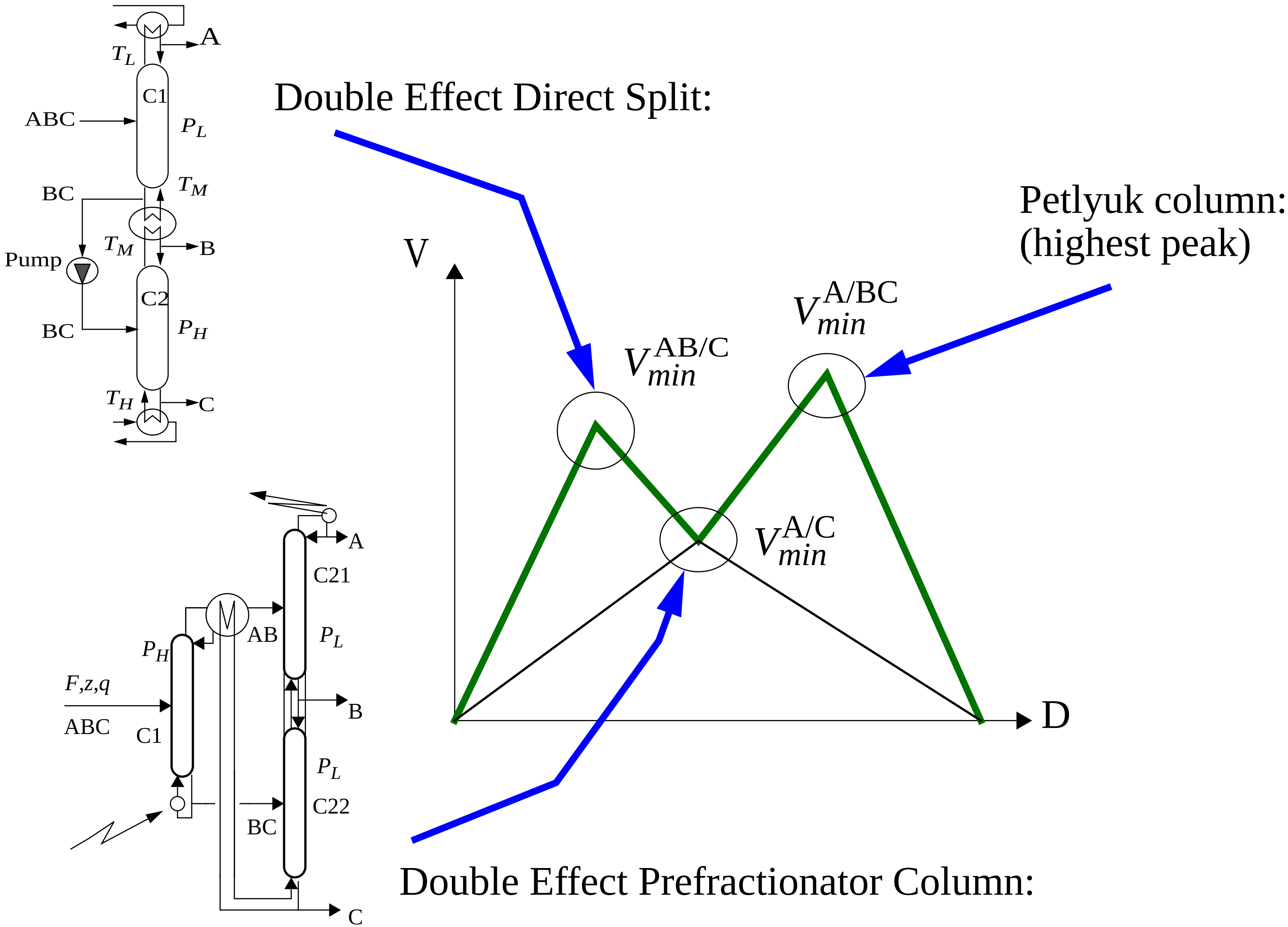
The energy requirement to the Petlyuk column: V_{min}=max(P_{AB},P_{BC},P_{CD})=P_{CD}

Improved 2nd Law performance



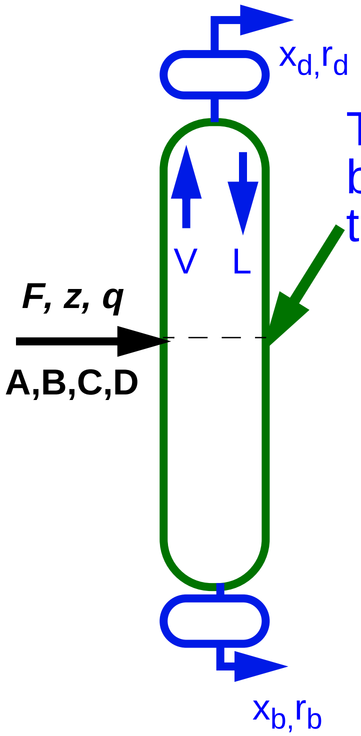


Double Effect Column Arrangements



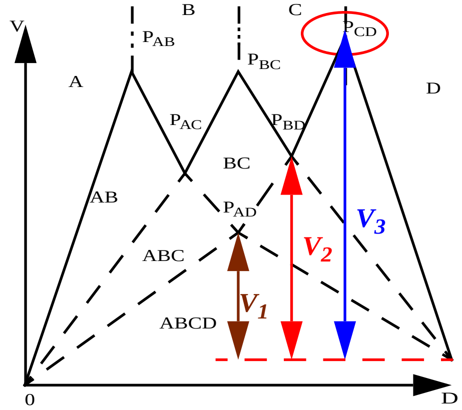
Summary of our Contribution:

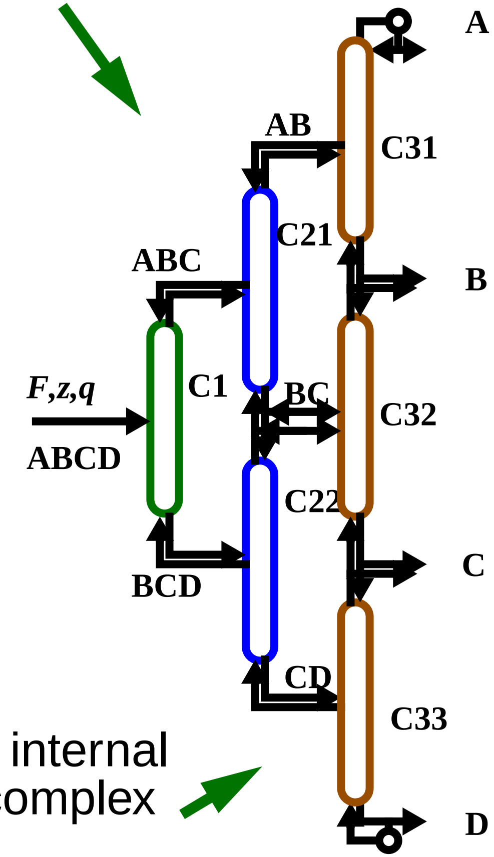
The most difficult split in this standard two-product column..



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

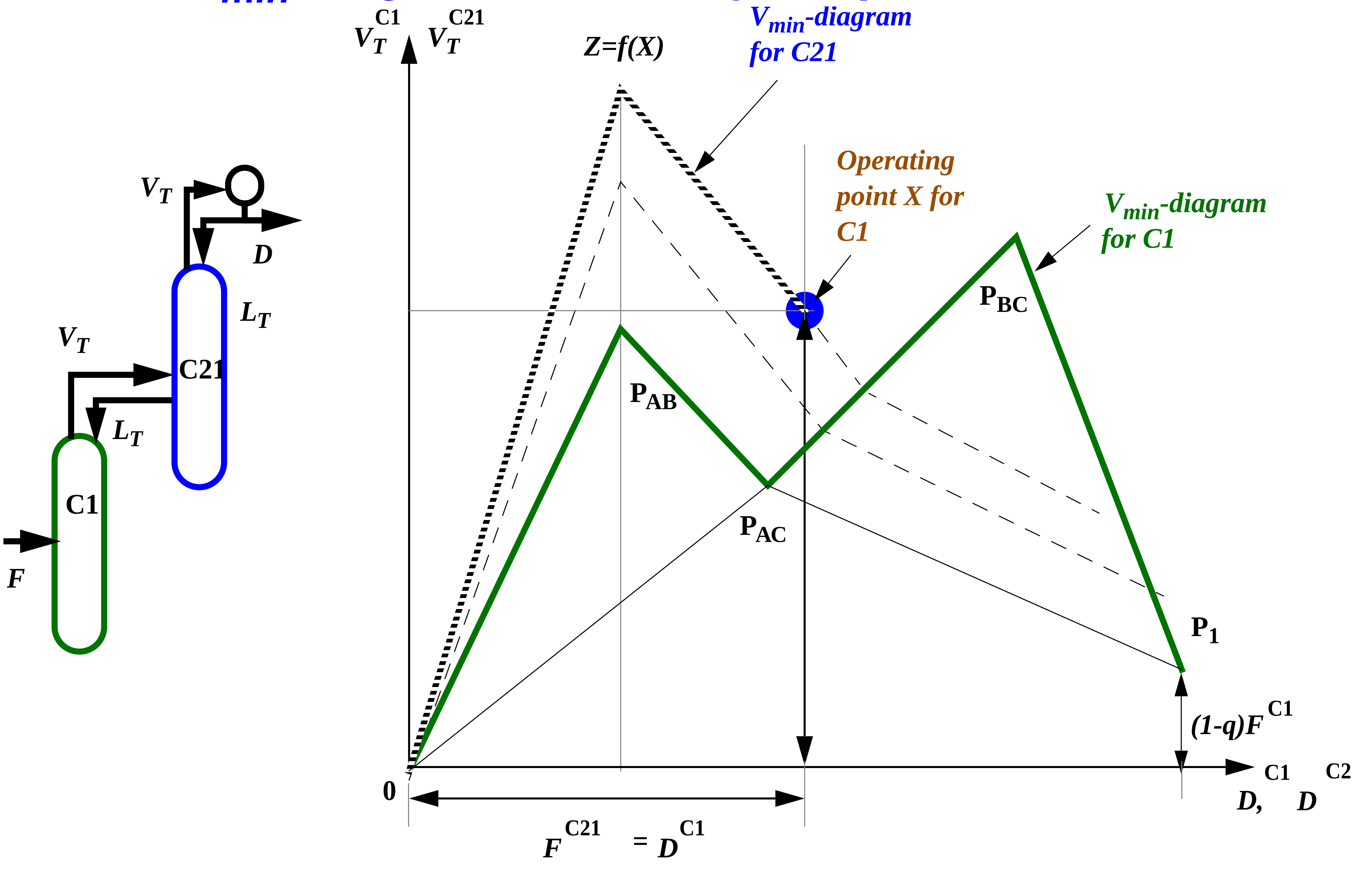
The V_{min}-diagram given by the behaviour in this simple column ....



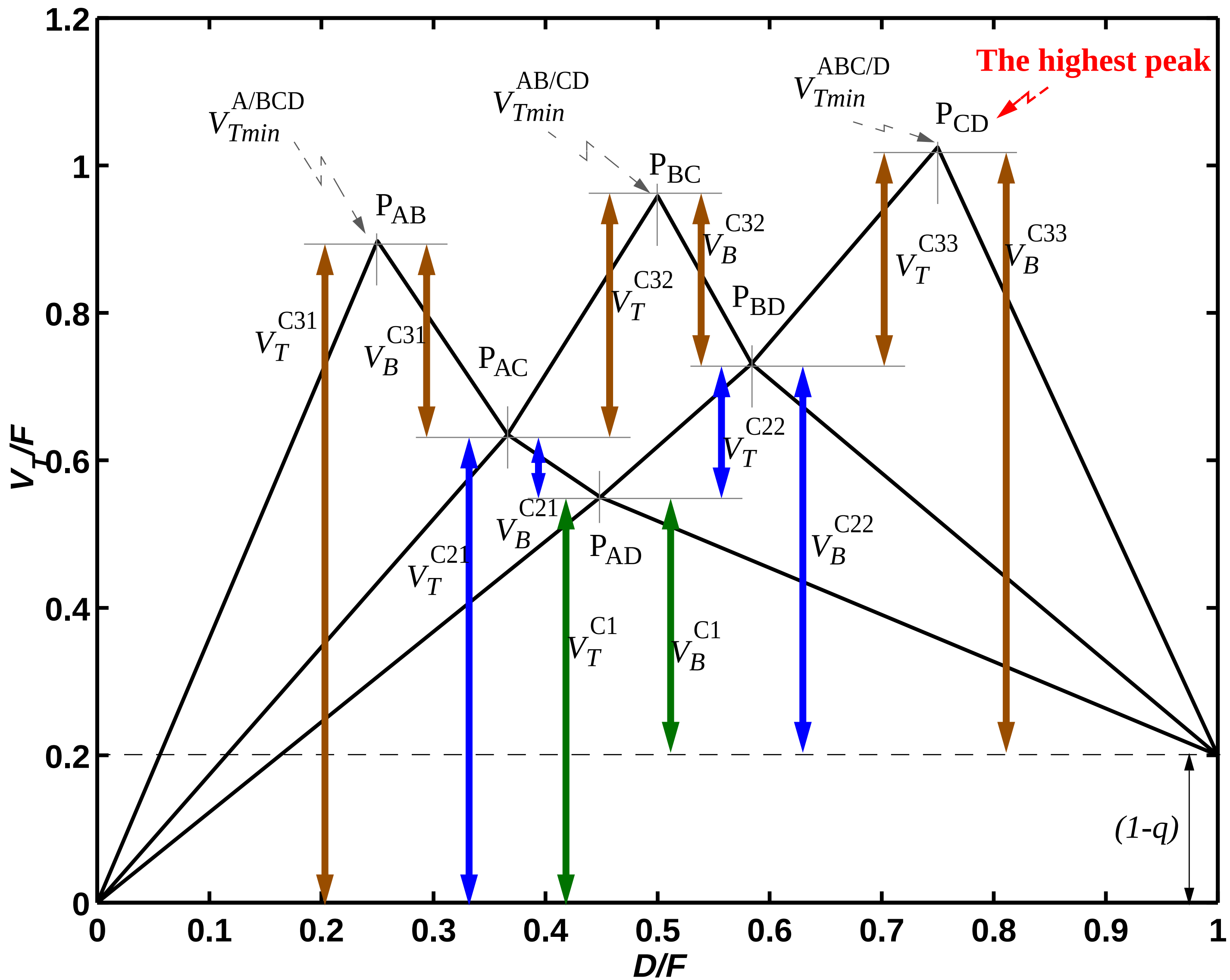


..gives all the internal flows in this complex arrangement

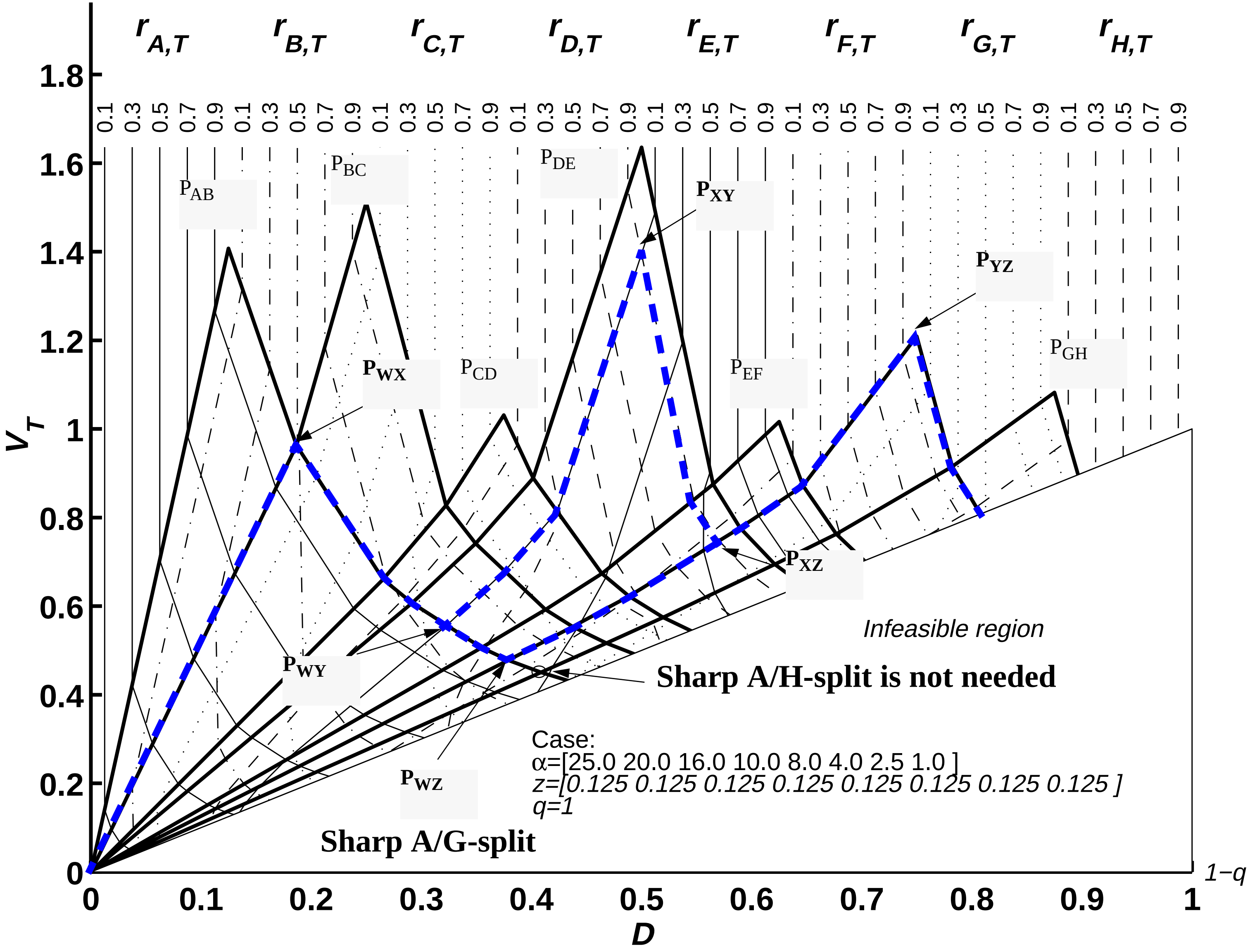
V_{min}-diagram for directly coupled columns



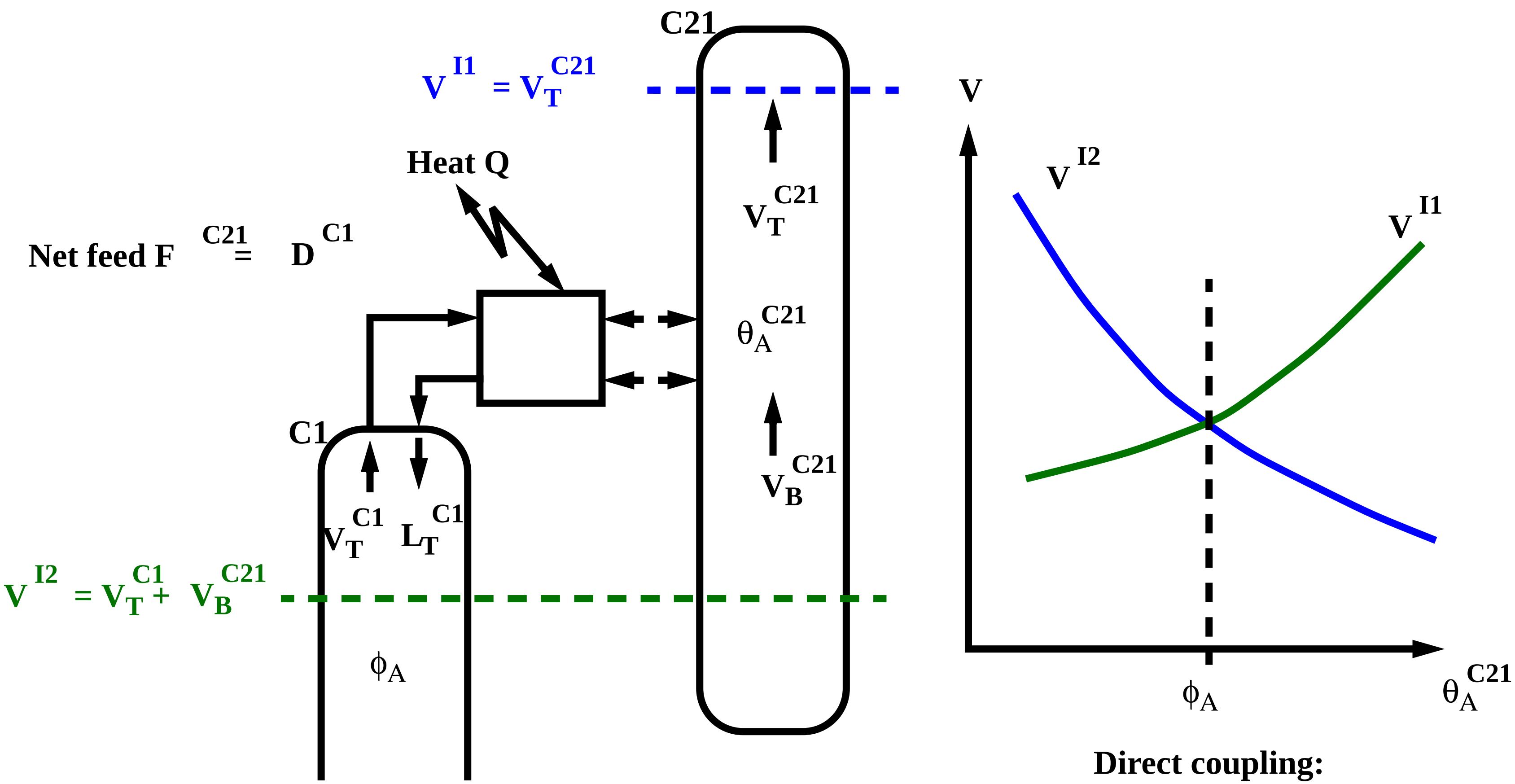
The V_{min}-diagram gives all internal flows



Example: N (9) components and M (4) products



Direct Coupling Minimize Vapour Flow



Direct coupling:

$\theta_A^{C21} = \phi_A$

	Configuration (Ad: AdiabaticNon: 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 $\Delta S_{total}/\|\Delta S\|$
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 prefrac-tionator 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