MINLP Optimization of Staged Separation Processes

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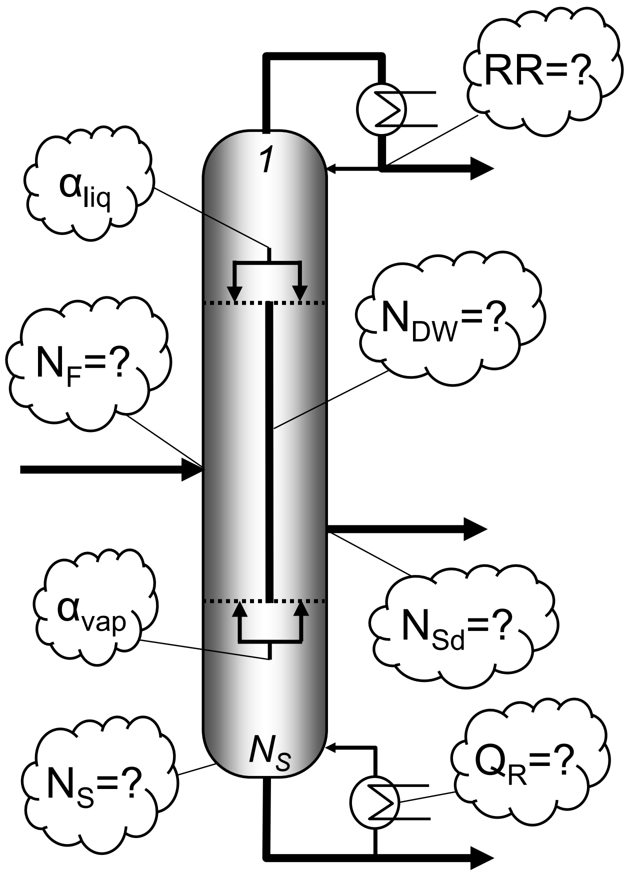
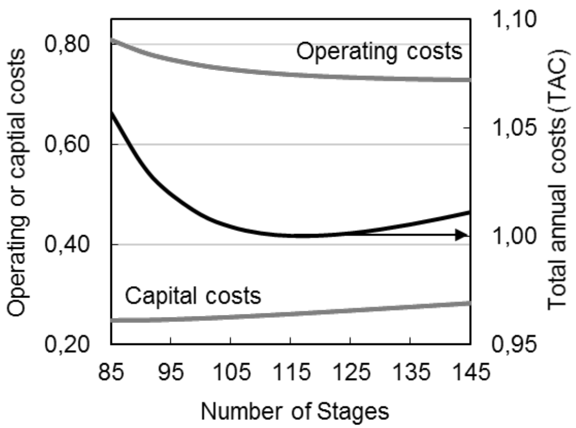
For a DWC, many degrees of freedom must be fixed…



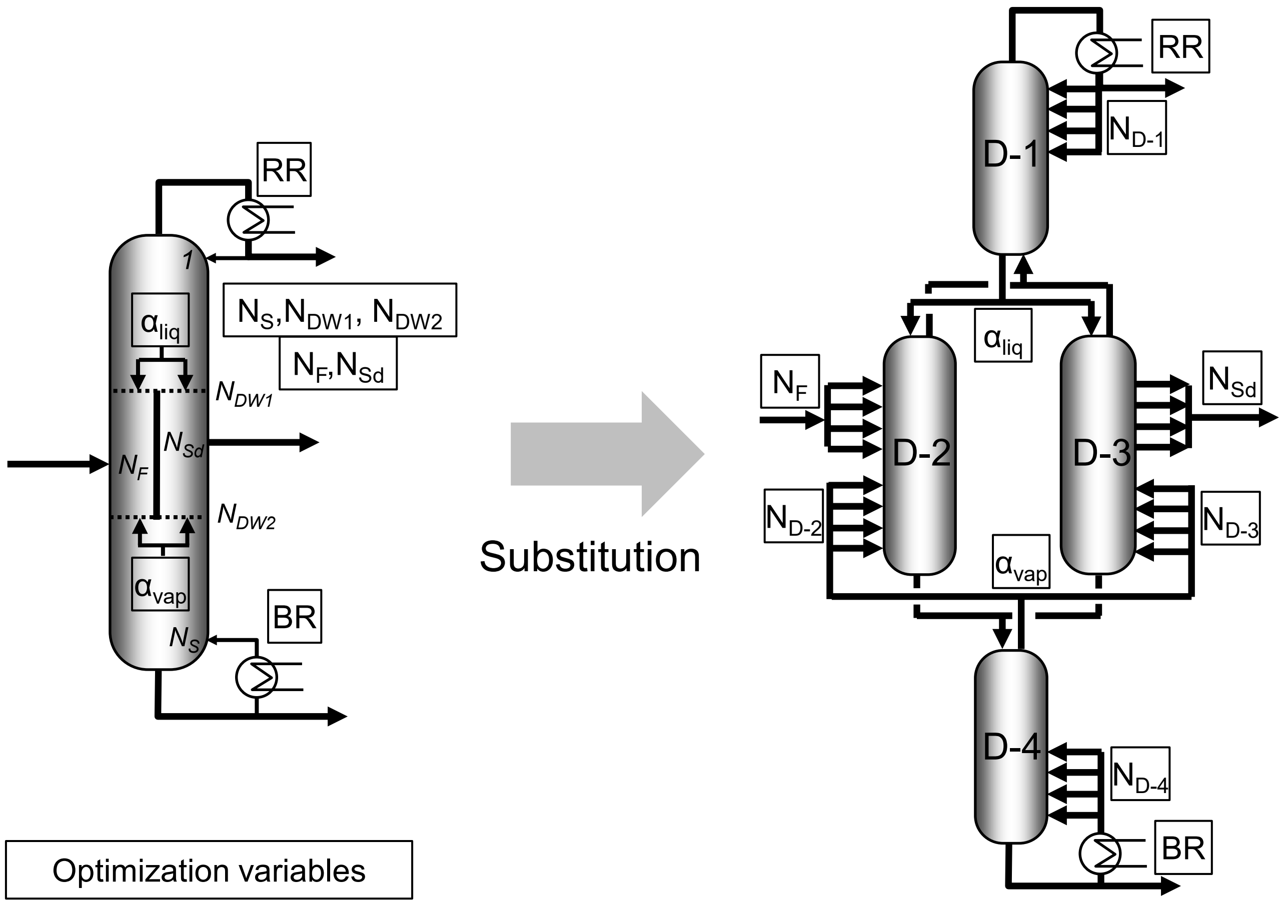


Bayer MaterialScience: Neue TDI-Anlage in Dormagen eröffnet (plasticker.de)

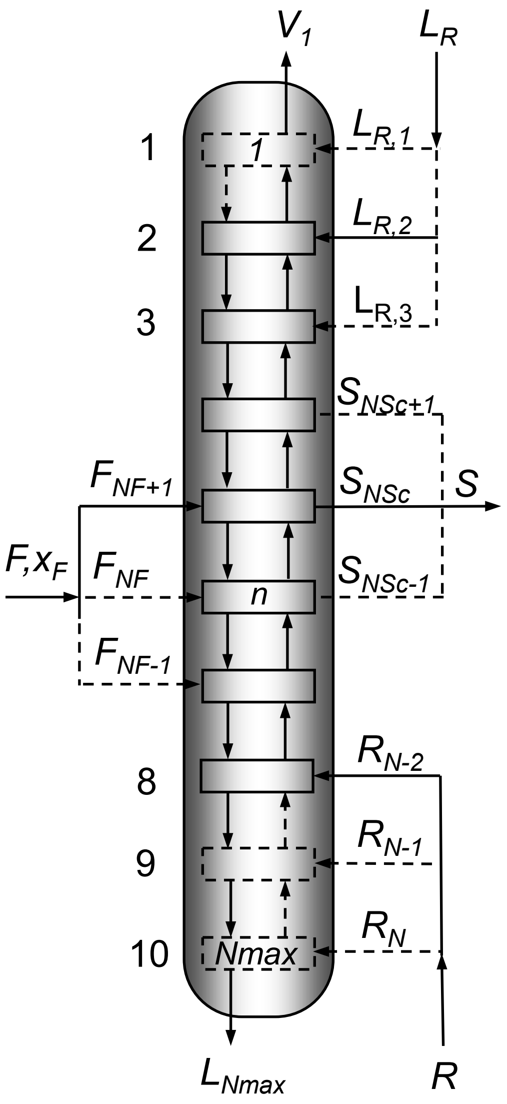
Cost optimal design requires the determination of **continuous** and **integer** optimization variables
Mixed-**i**nteger **N**on**l**inear **P**roblem => **MINLP**

… a suitable model structure must be chosen …

- Thermodynamic equivalent representation of DWC by 4-section column model



… the model equations must be written …



- MESH equations for $n = 1 \dots Nmax$ stages:

$$V_{n+1}x_{Vn+1} + L_{n-1}x_{Ln-1} + F_n x_{Fn} + L_{Rn}x_{LRn} + R_n x_{Rn} = V_n x_{Vn} + L_n x_{Ln} + S_n x_{Sn}$$

$$x_{Vn} = K_n x_{Ln}$$

$$\sum x_{Vn} = 1 \quad \text{and} \quad \sum x_{Ln} = 1$$

$$V_{n+1}h_{Vn+1} + L_{n-1}h_{Ln-1} + F_n h_{Fn} + L_{Rn}h_{LRn} + R_n h_{Rn} = V_n h_{Vn} + L_n h_{Ln} + S_n h_{Sn}$$

- Mixed-integer and pure integer constraints:

$$F_n \le F \cdot y_{F,n} \quad \text{and} \quad \sum y_{F,n} = 1$$

$$L_{R,n} \le L_R \cdot y_{R,n} \quad \text{and} \quad \sum y_{LR,n} = 1$$

$$R_n \le R \cdot y_{R,n} \quad \text{and} \quad \sum y_{R,n} = 1$$

$$S_n \le S \cdot y_{R,n} \quad \text{and} \quad \sum y_{S,n} = 1$$

- Auxiliary model equations:

$$N_S = \sum y_{R,n} \cdot n - \sum y_{LR,n} \cdot n + 1$$

Extended model of Viswanathan and Grossmann (1993), Ind. Eng. Chem. Res., 32, 2942-2949

… and finally, the optimization problem must be set up

- Objective function ***f(x,y)***:
  - ***f(x,y)*** = *Total Annual Costs (**TAC**)*
  - ***TAC*** = C_{op} + 5 * C_{eqp} * 0.2
- Constraints:
  - Equality constraints (model equations) **h**
  - Inequality constraints (design specs) **g**
  - Mixed-integer constraints **x** - **My <= 0**
  - Pure integer constraints **yE** = **e**
- Optimization variables:
  - Continuous variables **d**
  - Binary (integer) variables **y**

$$Z = \min_{\mathbf{d},\mathbf{y}} f(\mathbf{x},\mathbf{y})$$

subject to

$$\mathbf{h}(\mathbf{x},\mathbf{y}) = \mathbf{0}$$

$$\mathbf{g}(\mathbf{x},\mathbf{y}) \leq \mathbf{0}$$

$$\mathbf{x} - \mathbf{M}\mathbf{y} \leq \mathbf{0}$$

$$\mathbf{y}\mathbf{E} = \mathbf{e}$$

$$\mathbf{x} \in R^{nx}, \mathbf{y} \in \{0,1\}^{ny}$$

Remark:
d is the vector of optimization variables and a subset of all cont. **x**

How to Solve It: The Search for the Global Optimum

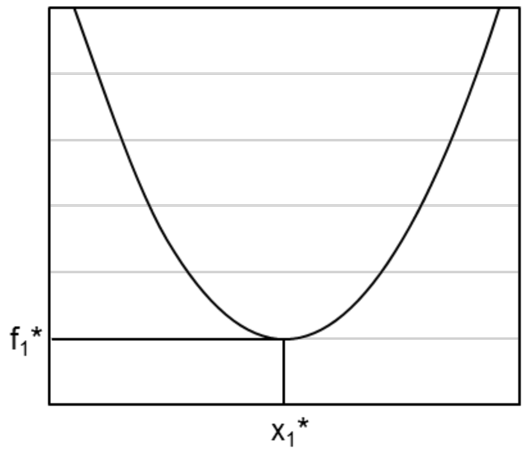
MINLP

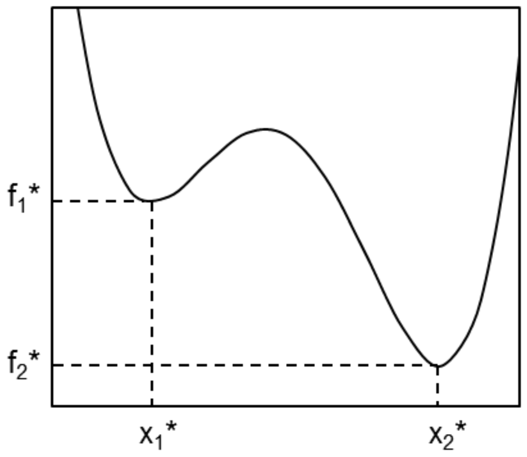
- Local MINLP
  - Deterministic
  - Stochastic
- Global MINLP*

Reformulation M.
- Relaxation
- Smooth Approximation [LB02]
- Successive Relaxed-MINLP [KKM06]

Explicit Methods
- Branch-and-Bound [GR85]
- <u>Generalized Benders Decomposition [Geo72]</u>
- Outer Approximation [DG86]
- Extended Cutting Planes [WSHP98]

Stochastic Methods
- Simulated Annealing [CSFB00]
- Tabu Search [LK03]
- Evolutionary Algorithms [GR98]
- Particle Swarm Optimization [JRC13]

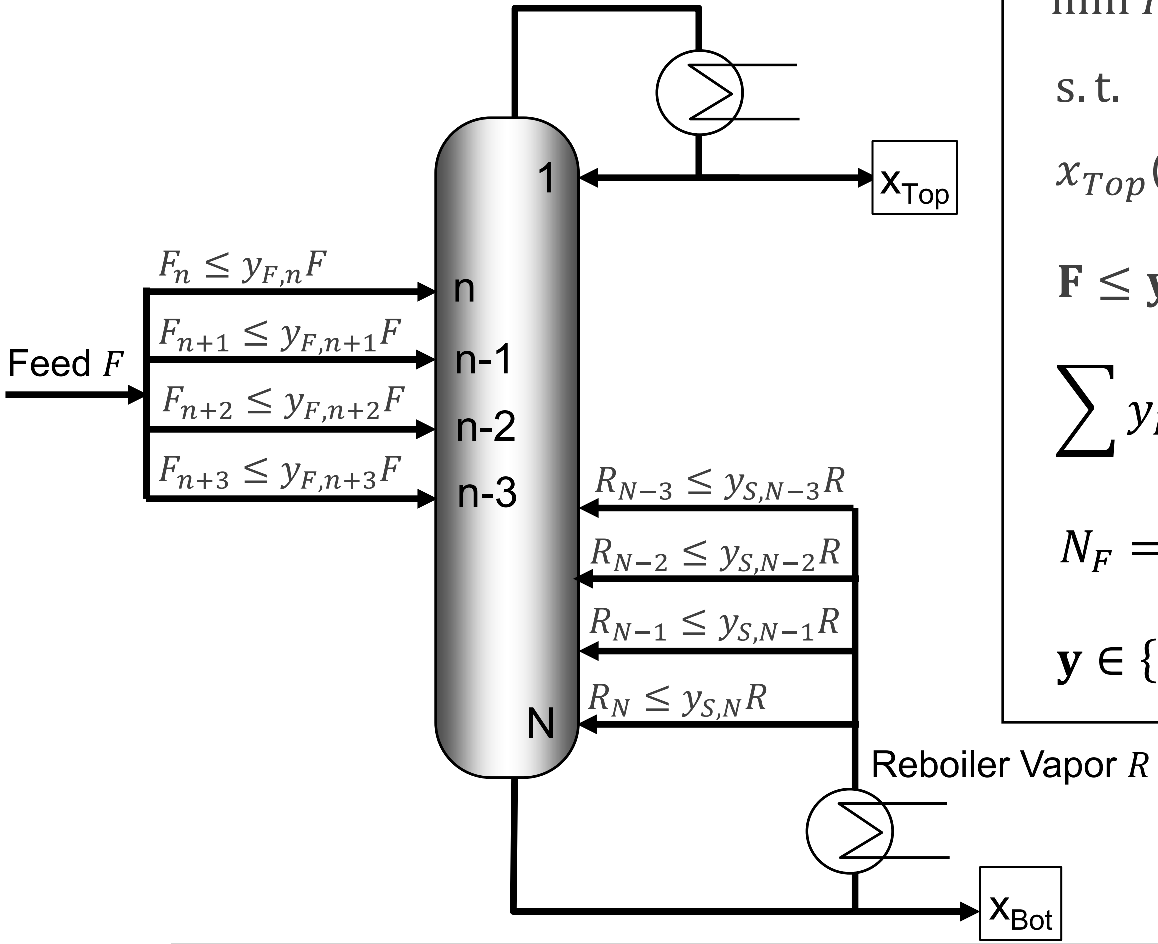




*guaranteed global optimum in finite number of steps

Optimization with Discrete Variables

Example: Distillation column
for n = 1 … N stages:



Optimization problem:

$$\min TAC = f\left(x_{Top}(RR), x_{Bot}(R), N_F, N_S\right)$$

s.t.

$$x_{Top}(RR) \geq x_{Top}^* \quad \text{and} \quad x_{Bot}(R) \geq x_{Bot}^*$$

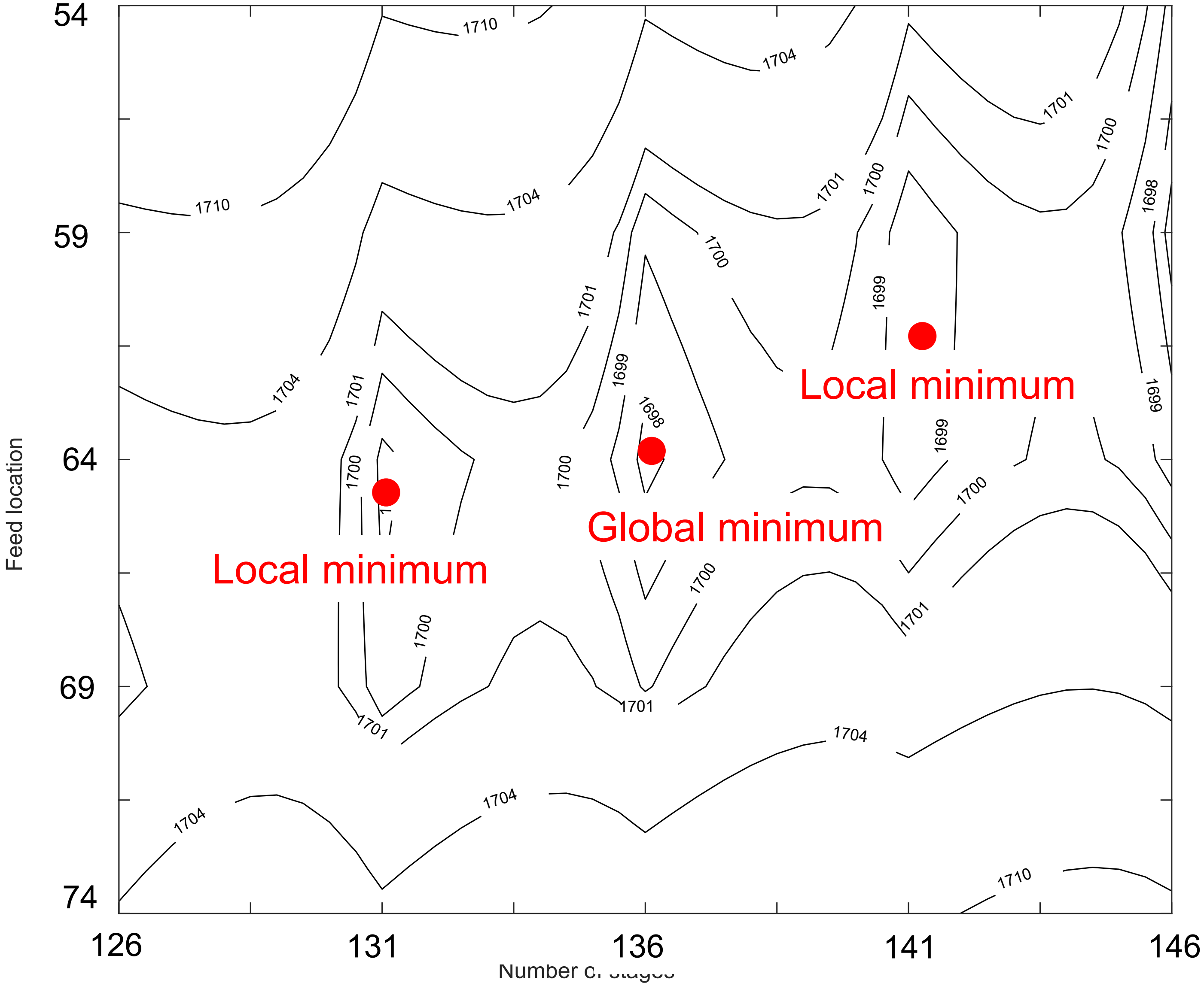
$$\mathbf{F} \leq \mathbf{y}_F F \quad \text{and} \quad \mathbf{R} \leq \mathbf{y}_S R$$ Mixed-integer constraints

$$\sum y_{F,n} = 1 \quad \text{and} \quad \sum y_{S,n} = 1$$ Pure integer constraints

$$N_F = \sum n \cdot y_{F,n} \quad \text{and} \quad N_S = \sum n \cdot y_{S,n}$$ Pure integer constraints

$$\mathbf{y} \in \{0,1\}^{ny} \quad \text{and} \quad N \in \mathbb{N}$$ Definition of stets

Contour Plot with Quasi-continuous Variables



Case study: Hybrid separation process

$$\min TAC = f\left(x^*_{Top}, x^*_{Bot}, N_F, N_S\right)$$

Quasi-continuous binary variables:

$$\mathbf{y}_F \in [0,1]^{ny} \quad \text{and} \quad \mathbf{y}_S \in [0,1]^{ny}$$

Additional integer constraints:

$$y_{F,n} + y_{F,n+5} = 1 \text{ and } y_{S,n} + y_{S,n+5} = 1$$

Converting binary in integer variables:

$$N_F = n + 5\left(1 - y_{F,n}\right) \text{ and } N_S = n + 5\left(1 - y_{S,n}\right)$$

Discrete-continuous problems
- in quasi-continuous representation -
are often **nonconvex**!

Generalized Benders Decomposition (GBD)[1]

- Key principle of GBD: Decomposition

NLP Subproblem
(Upper bound)

Cont. Variable Values, Lagrange Multipliers →

← New Binary Values

MILP Master Problem
(Lower Bound)

NLP Subproblem:

$$Z_{UB}^{k} = v(\mathbf{y}^{k}) = \min_{\mathbf{d}} f(\mathbf{x}, \mathbf{y}^{k})$$

subject to

$$\mathbf{h}(\mathbf{x}, \mathbf{y}^{k}) = \mathbf{0}$$
$$\mathbf{g}(\mathbf{x}, \mathbf{y}^{k}) \le \mathbf{0}$$
$$\mathbf{x} - \mathbf{M}\mathbf{y}^{k} \le \mathbf{0}$$
$$\mathbf{x} \in R^{nx}$$

$\mathbf{x}^{k}, \boldsymbol{\lambda}^{k}$ →

← $\mathbf{y}^{k}$

MILP Master Problem:

$$Z_{LB}^{k} = \min_{\mu, \mathbf{y}} \mu$$

subject to

$$\mu \ge L^{k} = f(\mathbf{x}^{k}, \mathbf{y}) + (\boldsymbol{\lambda}^{k})^{T} (\mathbf{x}^{k} - \mathbf{M}\mathbf{y})$$
$$\mathbf{y}\mathbf{E} = \mathbf{e}$$
$$\mathbf{y} \in \{0,1\}^{ny}$$

Benders Cuts
= Lagrange functions
= Linear underestimators

[1] Geoffrion (1972), Journal of Optimization Theory and Applications, 10(4), 237-262

How Non-convexity May Prevent the Global Optimum

$$Z_{UB}^{k} = v(\mathbf{y}^{k}) = \min_{\mathbf{d}} f(\mathbf{x}, \mathbf{y}^{k})$$

subject to

$$\mathbf{h}(\mathbf{x}, \mathbf{y}^{k}) = \mathbf{0}$$
$$\mathbf{g}(\mathbf{x}, \mathbf{y}^{k}) \leq \mathbf{0}$$
$$\mathbf{x} - \mathbf{M}\mathbf{y}^{k} \leq \mathbf{0}$$
$$\mathbf{x} \in R^{nx}$$

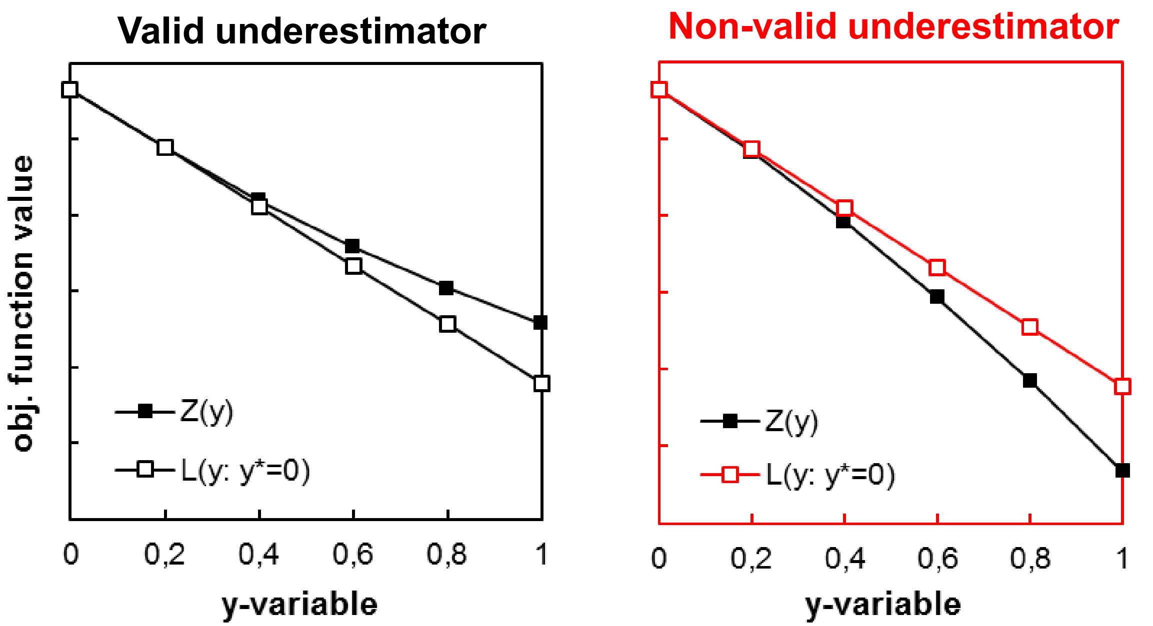
$\mathbf{x}^{k}, \boldsymbol{\lambda}^{k}$

$\mathbf{y}^{k}$

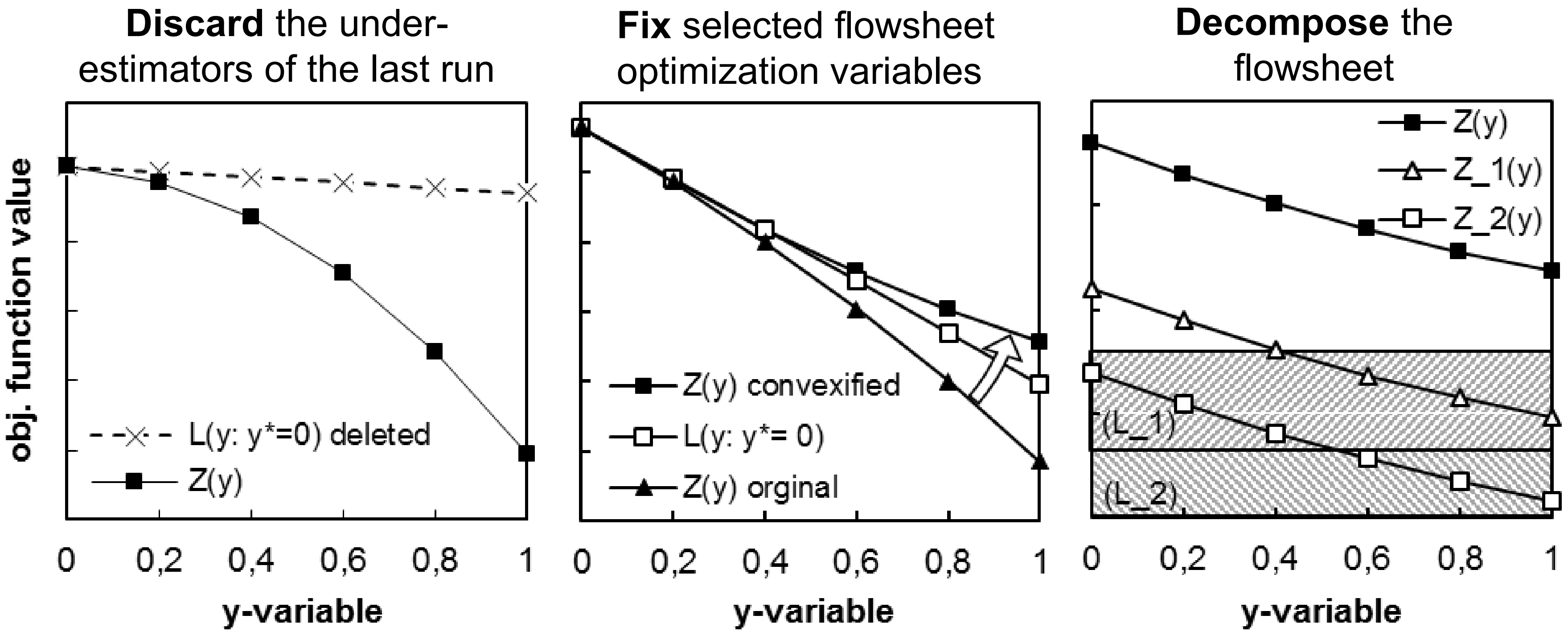
$$Z_{LB}^{k} = \min_{\mu, \mathbf{y}} \mu$$

subject to

$$\mu \geq L^{k} = f(\mathbf{x}^{k}, \mathbf{y}) + (\boldsymbol{\lambda}^{k})^{T} (\mathbf{x}^{k} - \mathbf{M}\mathbf{y})$$
$$\mathbf{y}\mathbf{E} = \mathbf{e}$$
$$\mathbf{y} \in \{0,1\}^{ny}$$



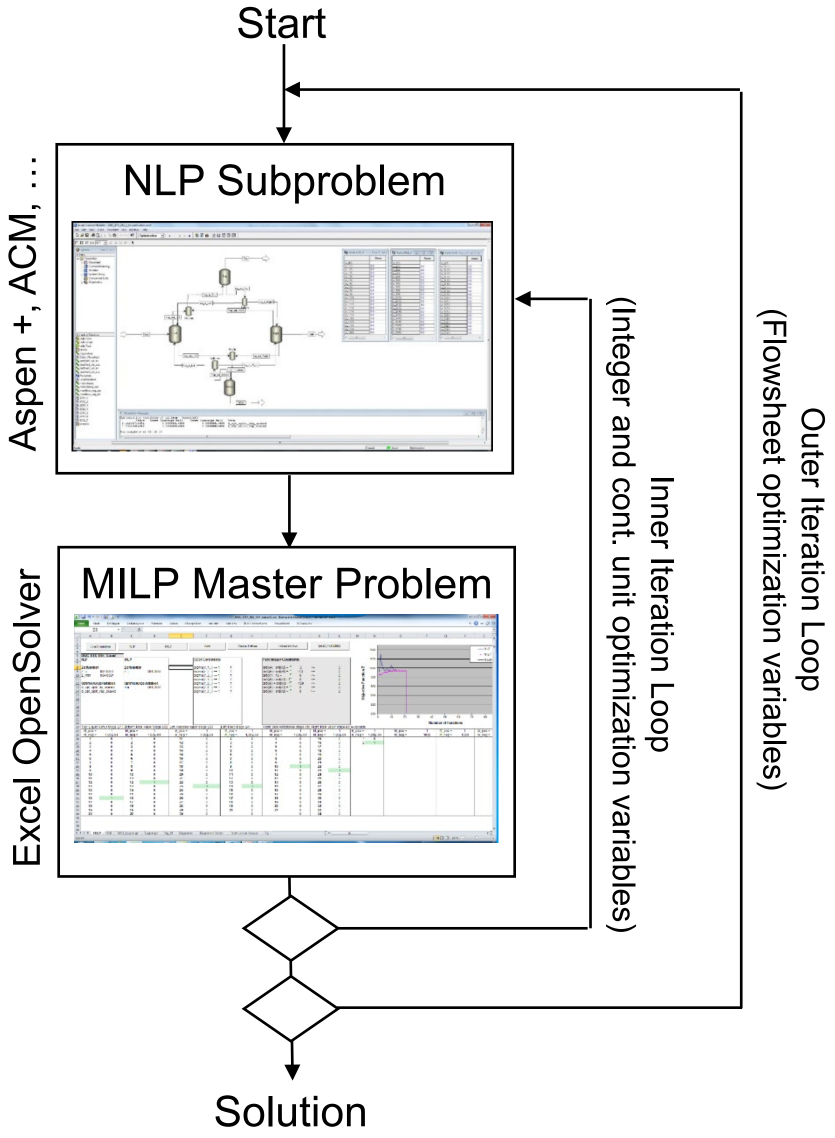
How to Cope With Non-convexity

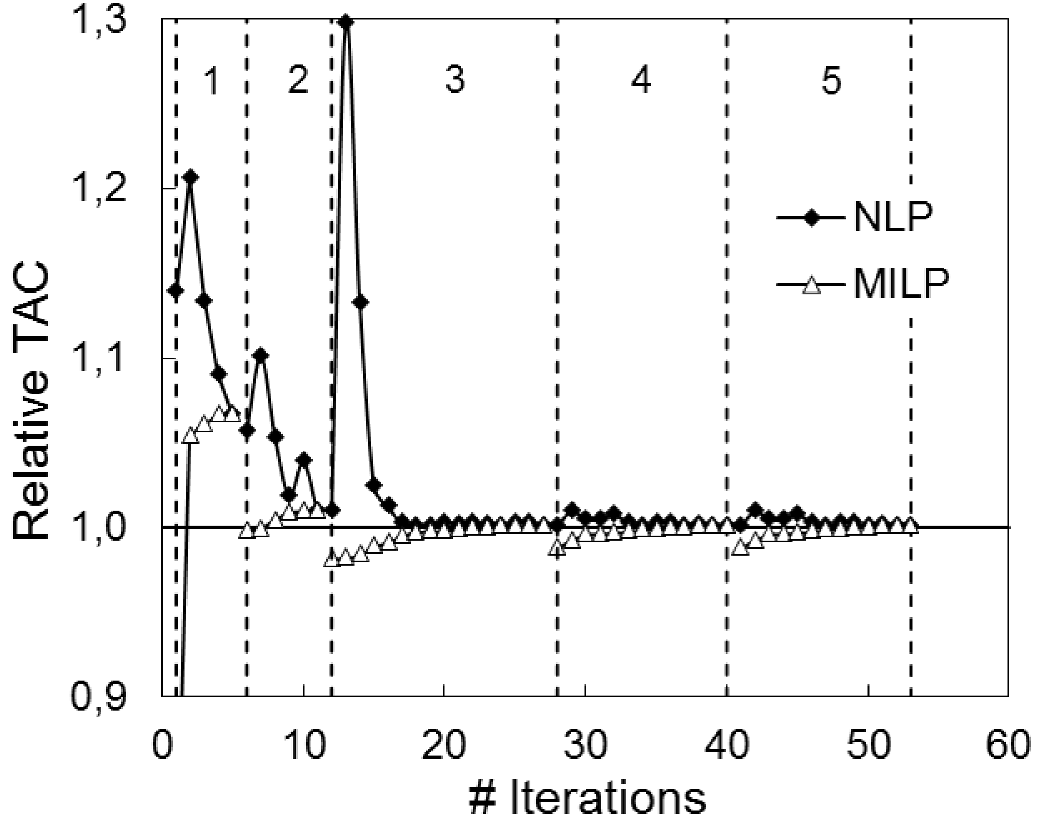


- With the Discard-Fix-and-Decompose[1] strategy, the likelihood of getting trapped into local optima is reduced

[1]Franke (2019), Comp. Chem. Eng., 131, 106583

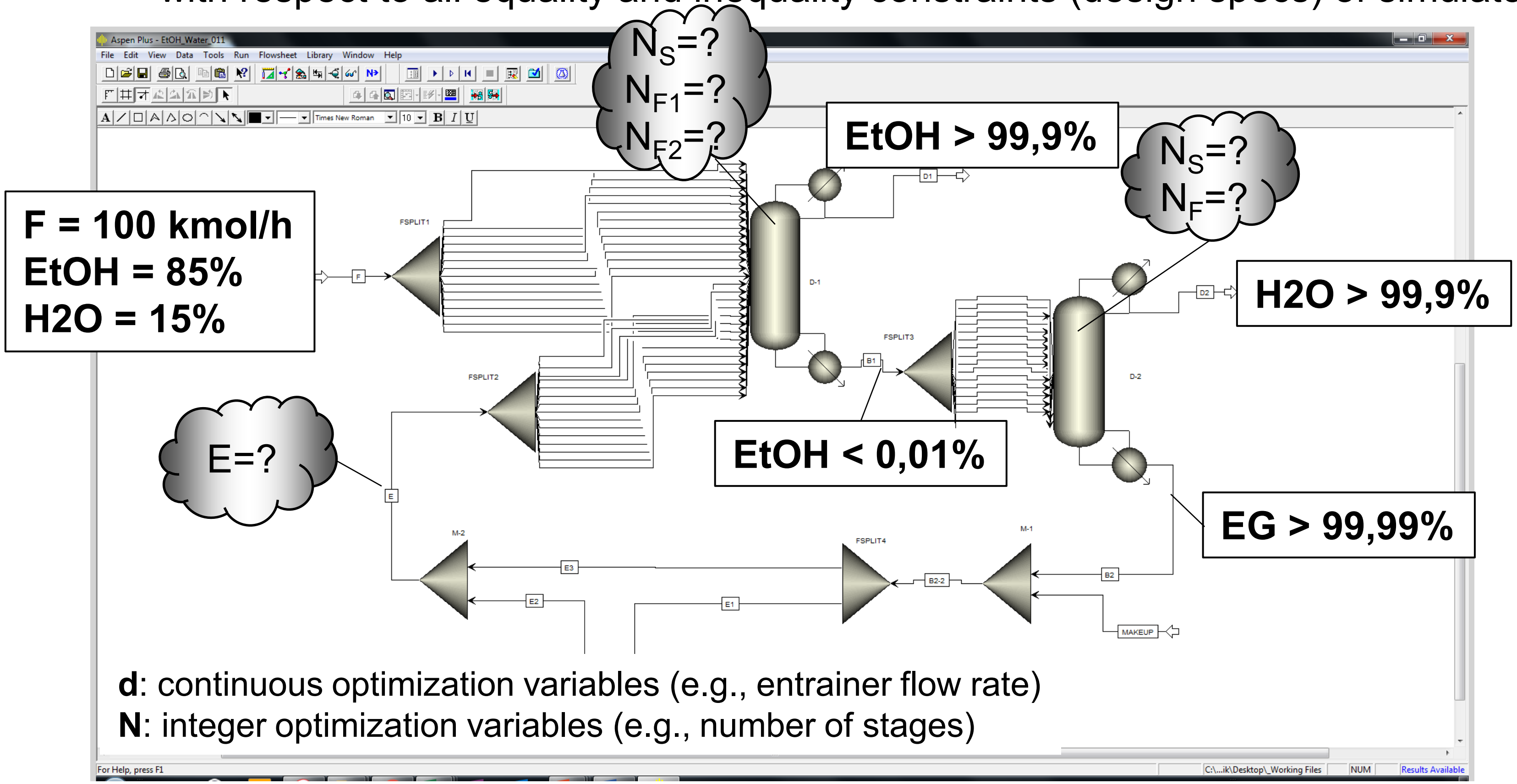
Implementation of mGBD





Implementation in Sequential-modular Flowsheet Simulator

- Extractive distillation process optimization problem (Ethanol/water with ethylene glycol as entrainer):
  - Minimize objective function $TAC = C_{op}(d) + 5 * C_{eqp}(d,N) * 0.2$
  - with respect to all equality and inequality constraints (design specs) of simulator



d: continuous optimization variables (e.g., entrainer flow rate)
N: integer optimization variables (e.g., number of stages)

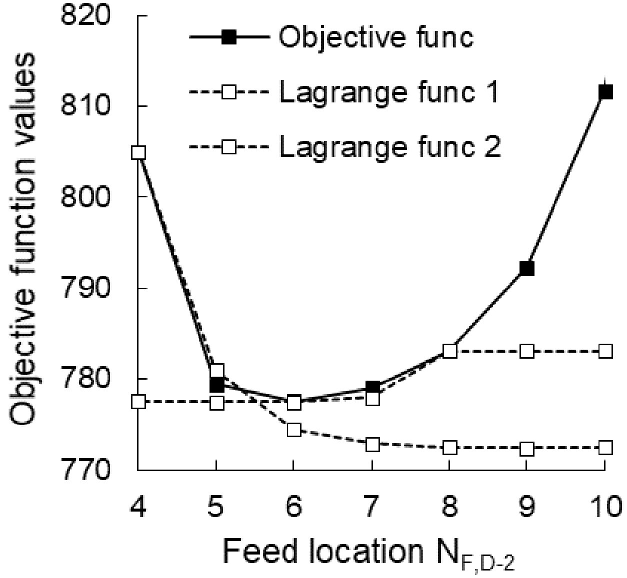
Construction of Linear Underestimators

For calculation of the linear underestimators, the sensitivity information (= Lagrange multipliers) is crucial: $L = f_0(y_0, N_0) + \lambda_{NF}(y_0 - y) + \lambda_{NS}(N_0 - N)$

Feed stage

- Feed is distributed over several stages; lambda is calculated by perturbation of every feed stream

$$\lambda_{NF} = -\frac{\Delta f}{\Delta \varepsilon} = -\frac{(f_0 - f_\varepsilon)}{\Delta \varepsilon}$$

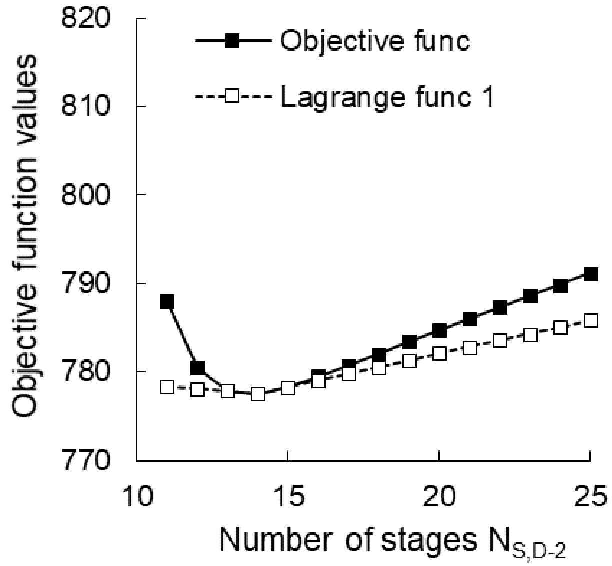


Number of stages

- Expansion and shrinking of column by 1 stage; different for left and right side with respect to actual stage

Left: $\lambda_{NS} = (f_0 - f_{NS-1})$

Right: $\lambda_{NS} = -(f_0 - f_{NS+1})$



Several Case Studies Successfully Accomplished

Separation problems solved by mGBD

	Simulator	Customer	Year
Isomer Mixture 1	ACM	Company	2005
Isomer Mixture 2	ACM	Company	2008
Isocyanate Dividing-Wall Column	ACM	Company	2010
EtOH/H2O Heteroazeotropic Dist.	ACM	Literature	2016
DWC for EtOH/H2O Separation	ACM	Literature	2017
Acetic Acid Recovery	A+	Company	2017
EtOH/H2O Extractive Distillation	A+	Literature	2018

Currently working on

- Reactive distillation (homogeneous)
- Membrane cascades (gas separation)

Other examples

- There are several other examples in literature, most of them rely on GAMS (“self-written models”) and OA (“likely to get trapped in local optima”).
- With more computational power and parallelization, it is likely the stochastic as well global optimization methods will gain more importance.