Towards Systematic Design of Intensified Fluid Separation Processes

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Personal Introduction

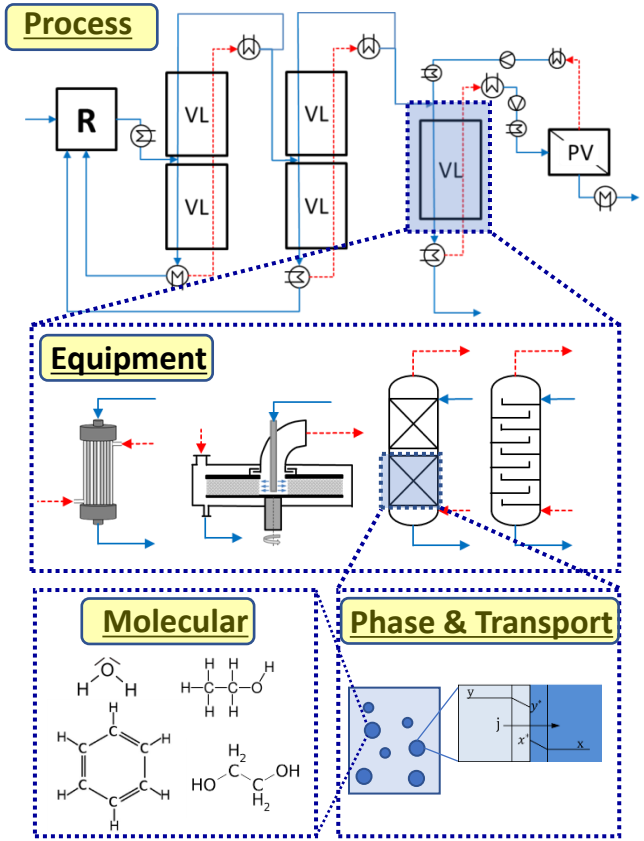
- Dipl.-Ing. Computational Engineering Science

- *Ph.D.* in Process Systems Engineering
  - with Prof. Dr.-Ing. W. Marquardt
  - *"Optimization-based methods for the conceptual design of separation processes for azeotropic mixtures"*

- *Habilitation* in Fluid Separations
  - with Prof. Dr.-Ing. A. Górak
  - "*Towards the systematic design of intensified fluid separation processes*"

- *Prof.* for Process Systems Engineering

Process intensification for fluid separations



PI on <u>process and equipment level</u>

- integration of reaction & separation
  (e.g. reactive distillation, membrane reactor, …)
- integration of separation technologies
  (e.g. hybrid separation processes, …)
- integration of heat and mass
  (e.g. heat integration, DWC, HiDiC, VRC, …)

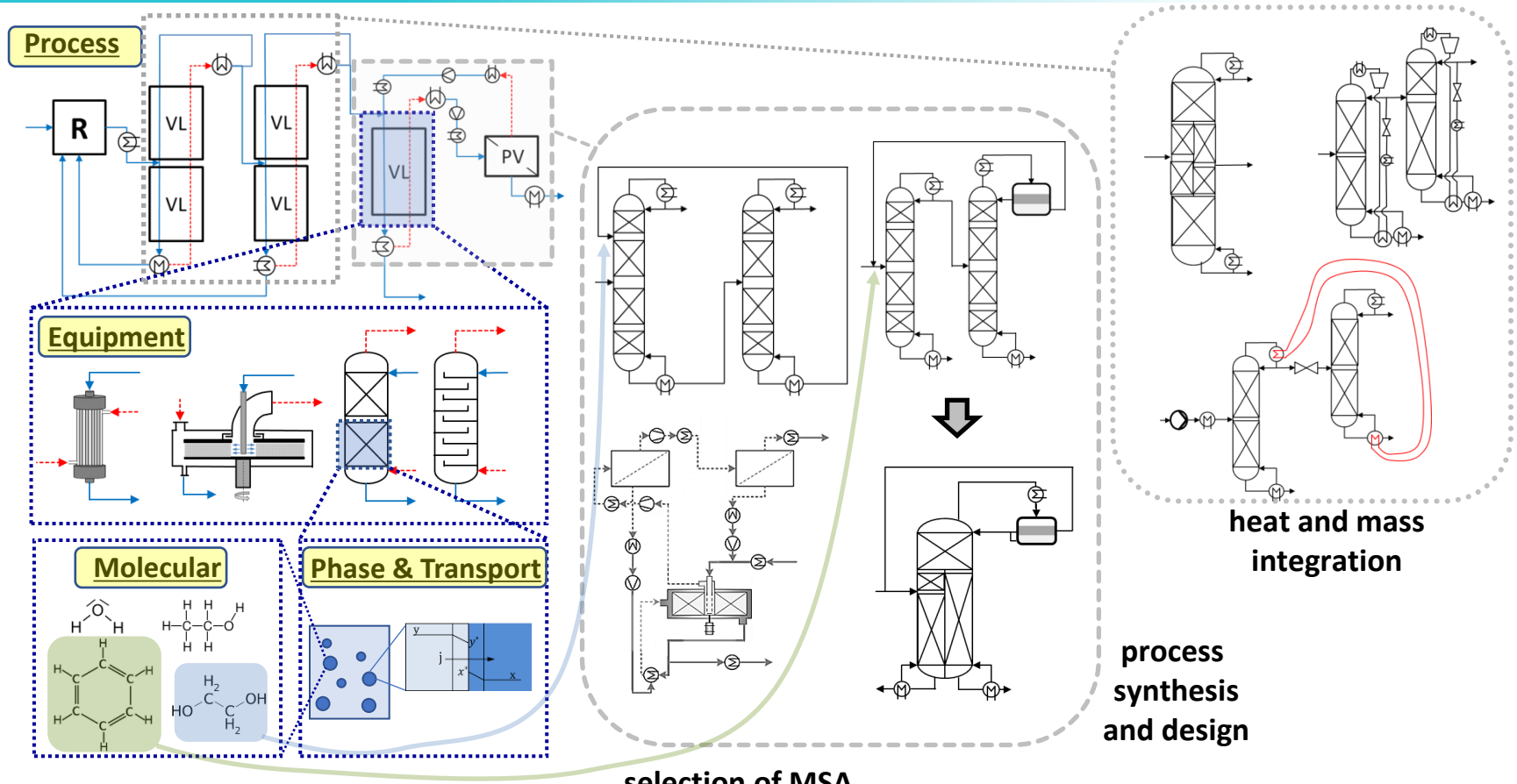
PI on <u>equipment and transport level</u>

- structurization and miniaturization
  (e.g. hollow fibre memebranes modules …)
- enhancement of transport phenomena
  (e.g. mass transfer machines, ultrasound, …)

PI on <u>phase and molecular level</u>

- innovative solvents (e.g. organics, IL, DES, …)
- innovative catalysts and their immobilization
  (e.g. enzyme beads, BDS, …)

Process intensification for fluid separations



A need for a systematic approach to PI

- *"Not only the process has to be intensified, but also the process design methodology"* Gourdon et al., Oil & Gas Science Technology, 2015. 70 (3) 463-473
- *Exploiting the symbiosis between*

Process Intensification

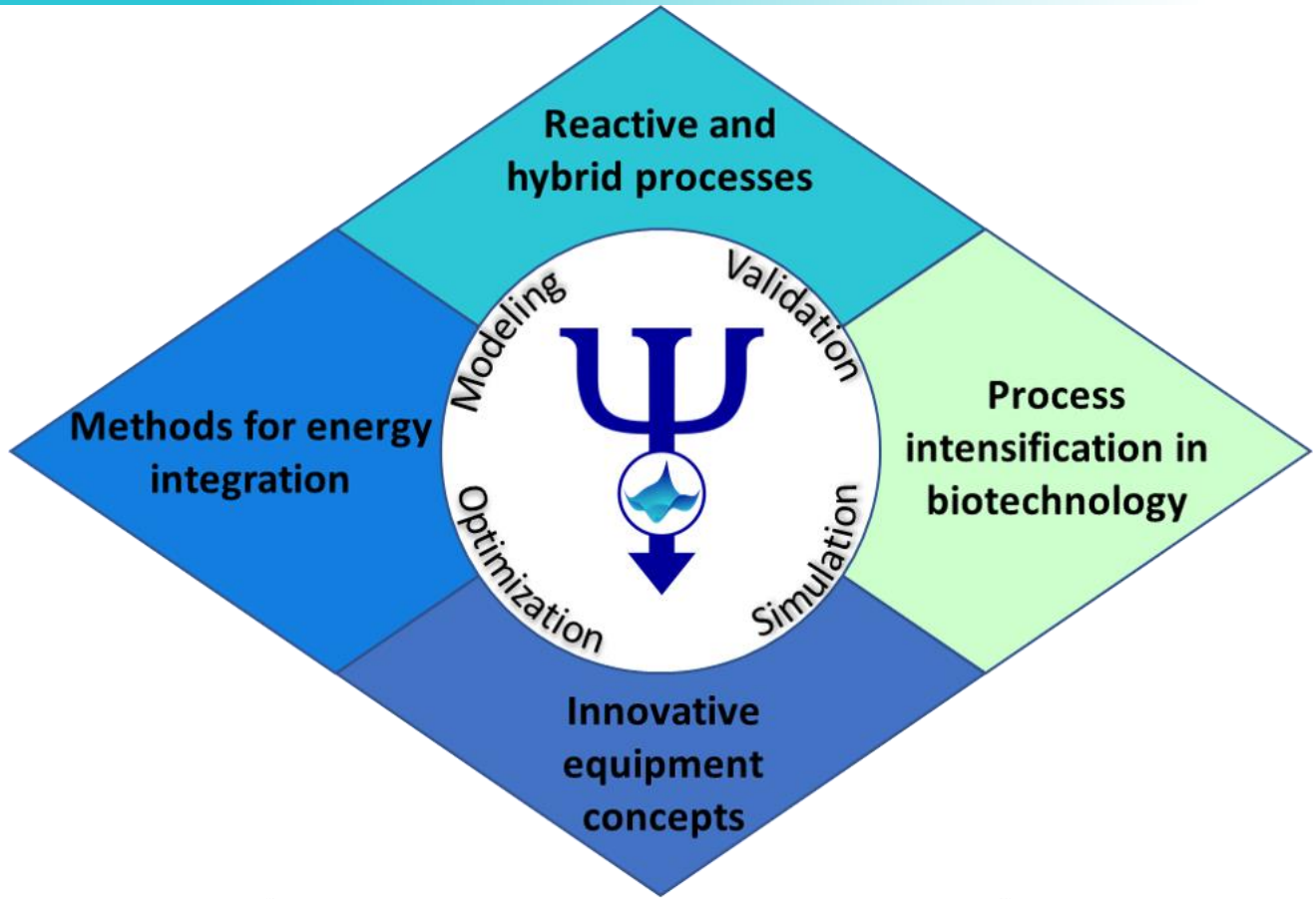
PI skill area
– Effective use of resources
– Equipment and materials oriented
– Experimental techniques enable
– Experiments and modeling
– New processing methods
– Development of processing devices, catalysts, integrated unit operations
– Creation of spatial structures
– Compact and robust structures
– Resolution at microscales and nanoscales
– Bottom-up, phenomena driven, model based

Process Systems Engineering

PSE skill area
– Efficient use of resources
– Information and software oriented
– Computing technology enables
– Modeling as key approach
– New simulation methods and decision making tools
– Functional, integrated design of product and process
– Control over time events
– Optimization of performance
– Multi-scale integration
– Top-down, system's view, model based

Moulijn et al.. Comput Chem Eng 2008; 32: 3–11
Keil, Rev Chem Eng 2018; 34(2): 135–200.

Institute for Process Systems EngineerIng



Improving energy efficiency of distillation

Process Systems Engineering TUHH

2013

Review

SCI

Received: 30 July 2013 Revised: 31 October 2013 Accepted article published: 6 November 2013 Published online in Wiley Online Library: 3 December 2013

(wileyonlinelibrary.com) DOI 10.1002/jctb.4262

Distillation technology – still young and full of breakthrough opportunities

Anton A. Kiss*

2020

DOI: 10.1002/aic.16294

Check for updates

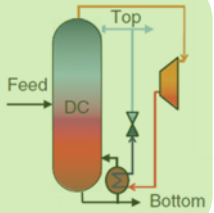
PERSPECTIVE

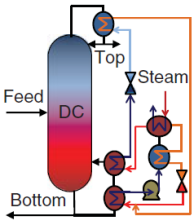
AIChE JOURNAL

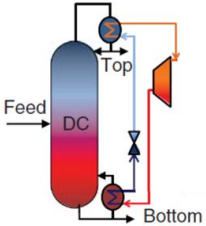
Misconceptions about efficiency and maturity of distillation

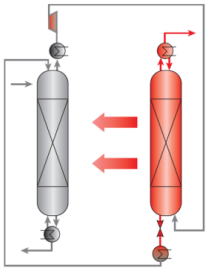
Rakesh Agrawal | Radhakrishna Tumbalam Gooty

heat pumps









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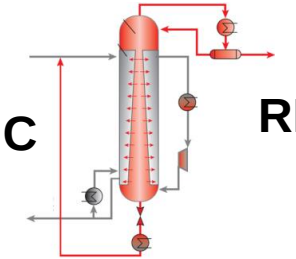
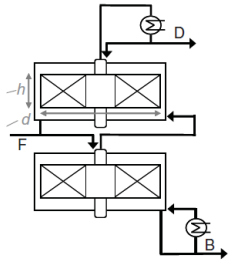
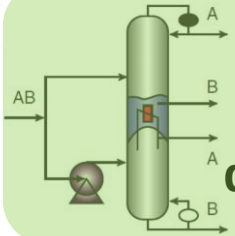
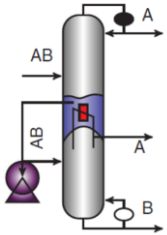


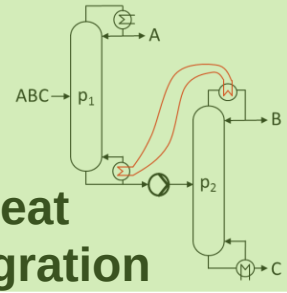
RPBs



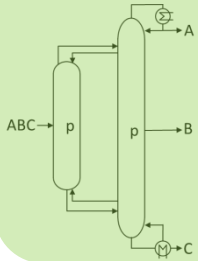


multi effect distillation

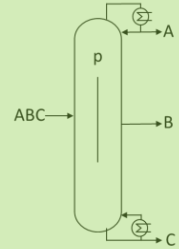




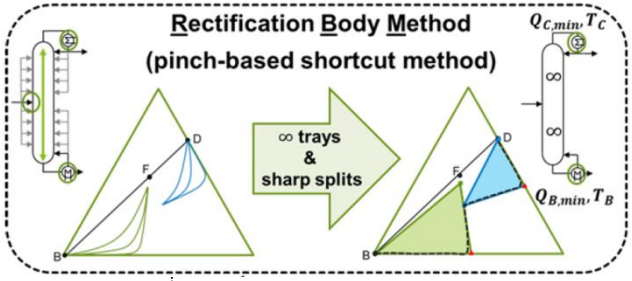
heat integration



thermal coupling - DWC



Shortcut-based screening of options



RBM*

Code

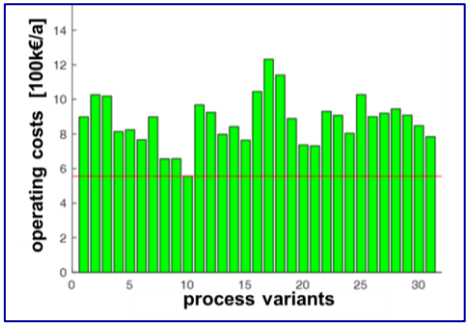
property data

*open source version from AVT.PT/AVT.SVT

report file parser

aspentech property model parameters

MATLAB-based framework



automatic evaluation

process variant evaluation

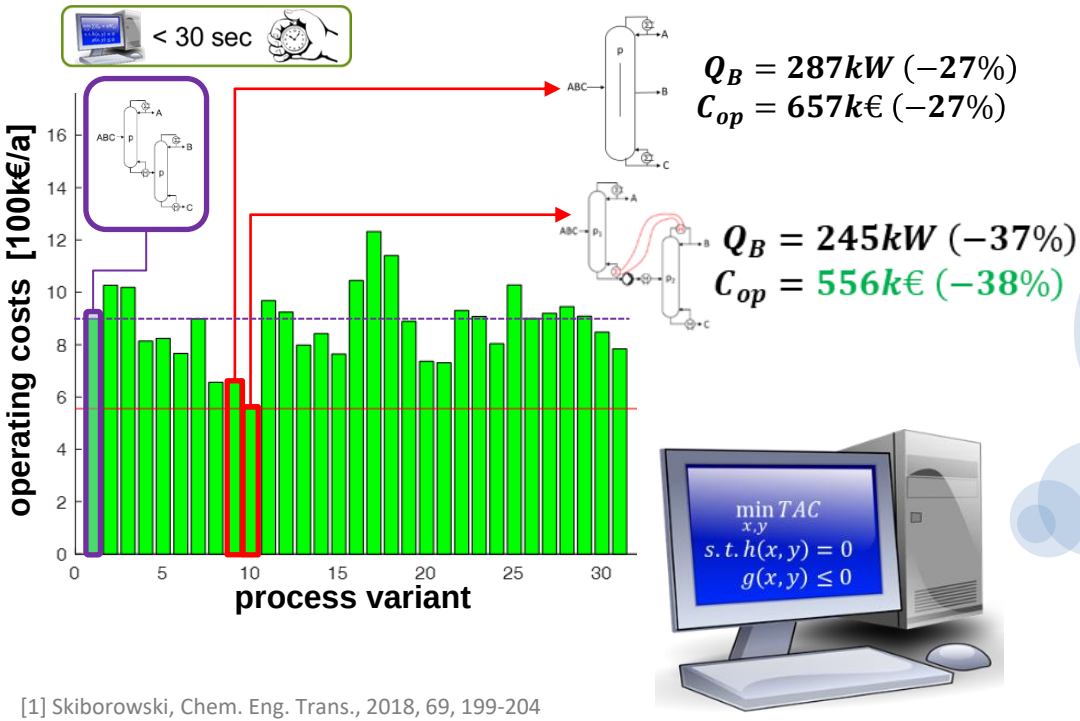
economic evaluation

easy to set up a problem & good comparability

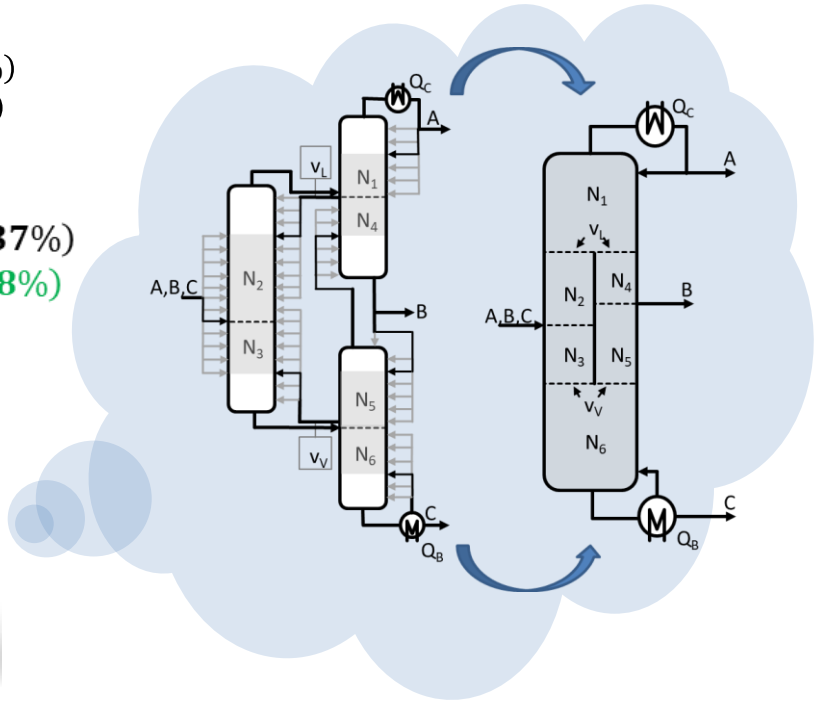
Skiborowski, 2018, Chem. Eng. Trans., 69, 199-204

Shortcut-based screening of options

- Shortcut Screening[1]



- Economic Optimization[2,3]



[1] Skiborowski, Chem. Eng. Trans., 2018, 69, 199-204
[2] Waltermann & Skiborowski, Chem. Ing. Tech., 2017, , 89(5), 562–581
[3] Waltermann & Skiborowski, Comp. Chem. Eng., 2019, 129, 106520

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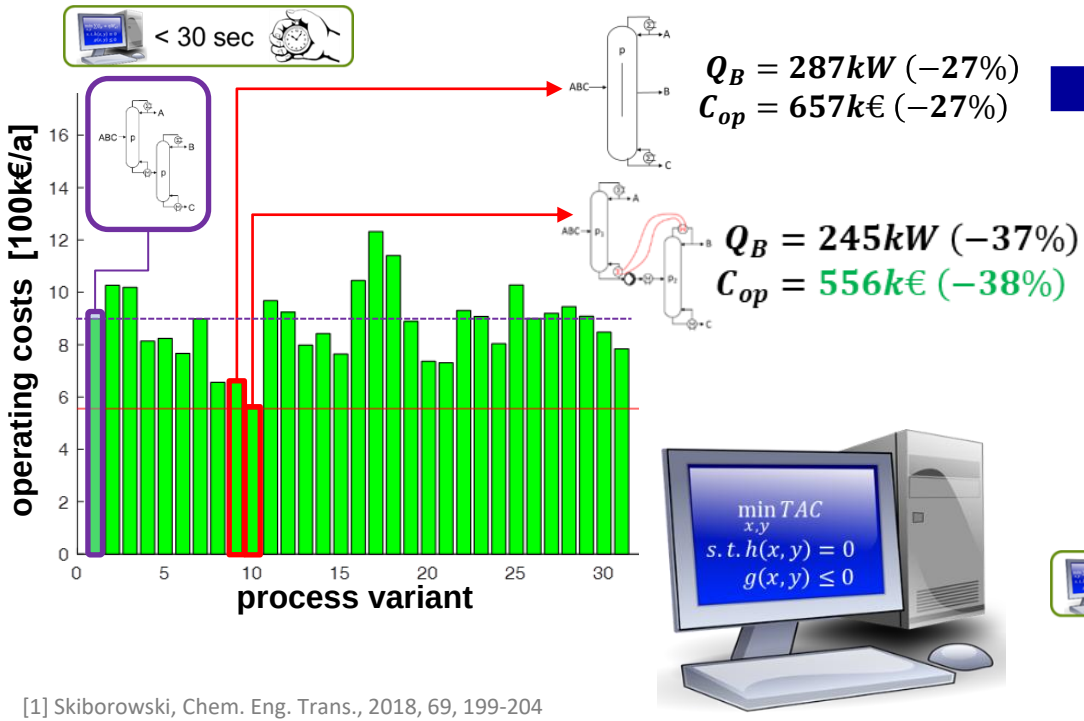

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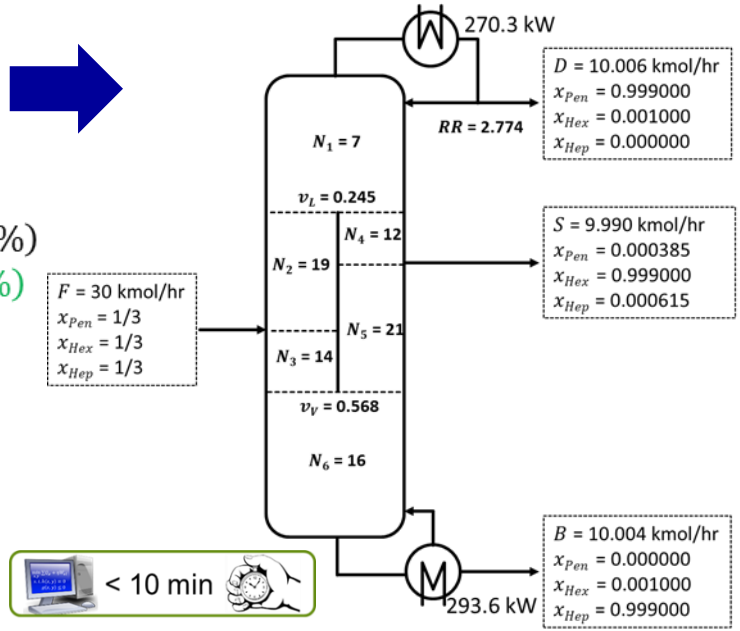

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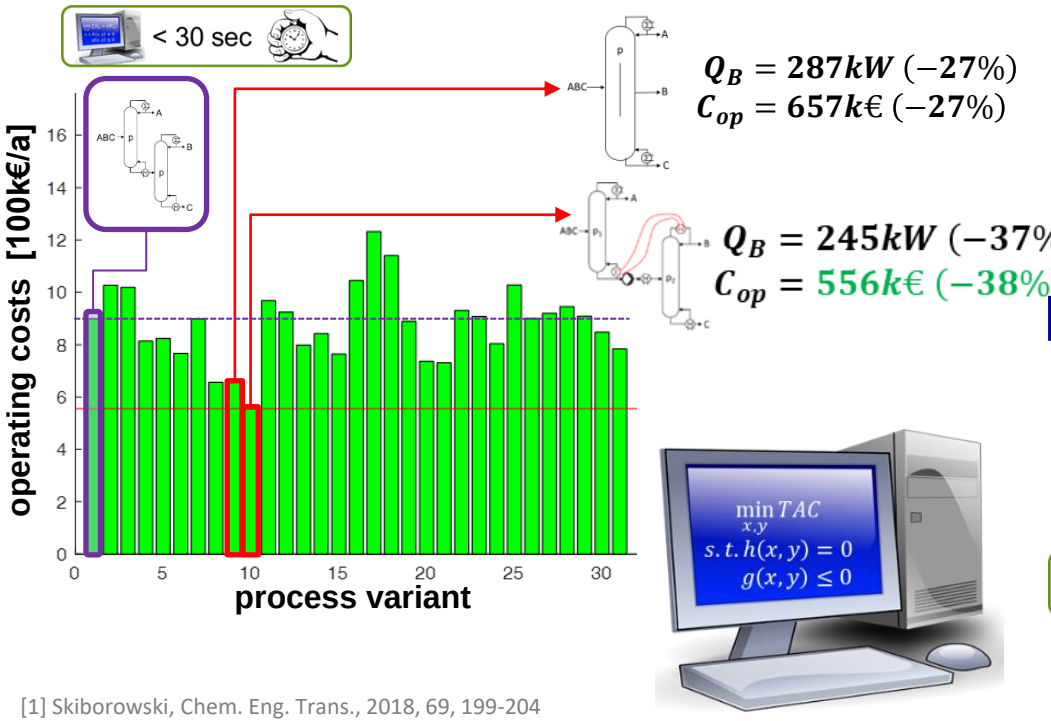

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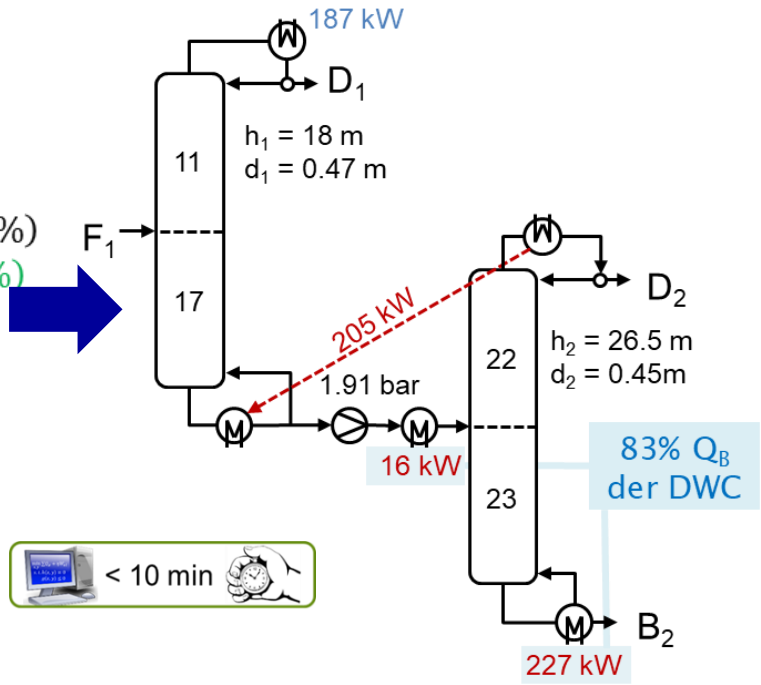

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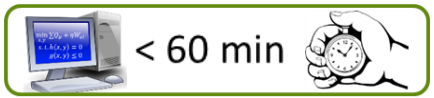
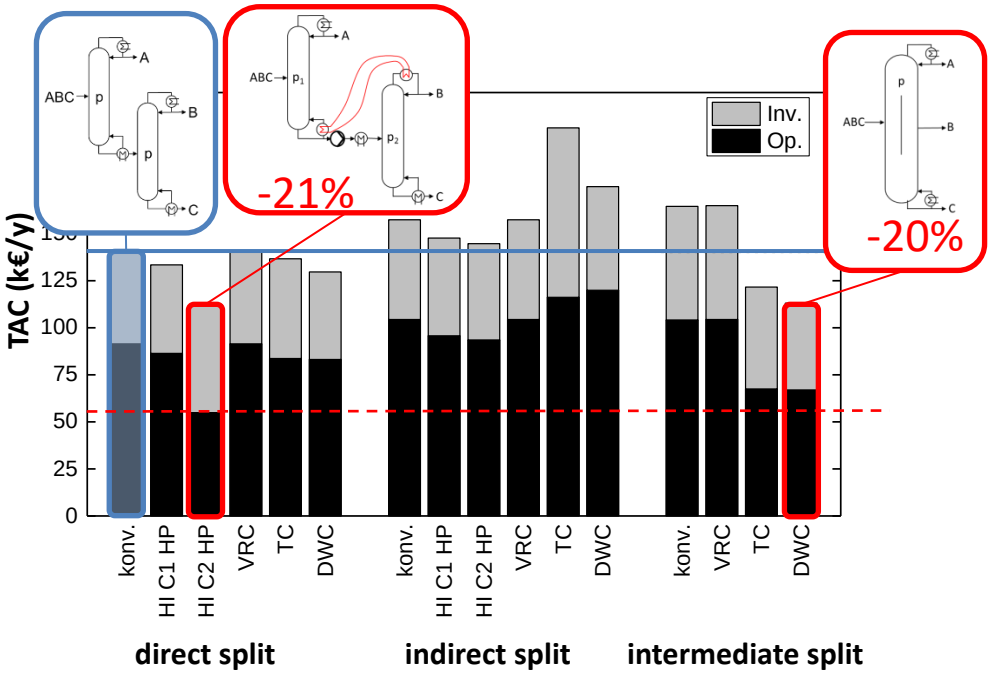
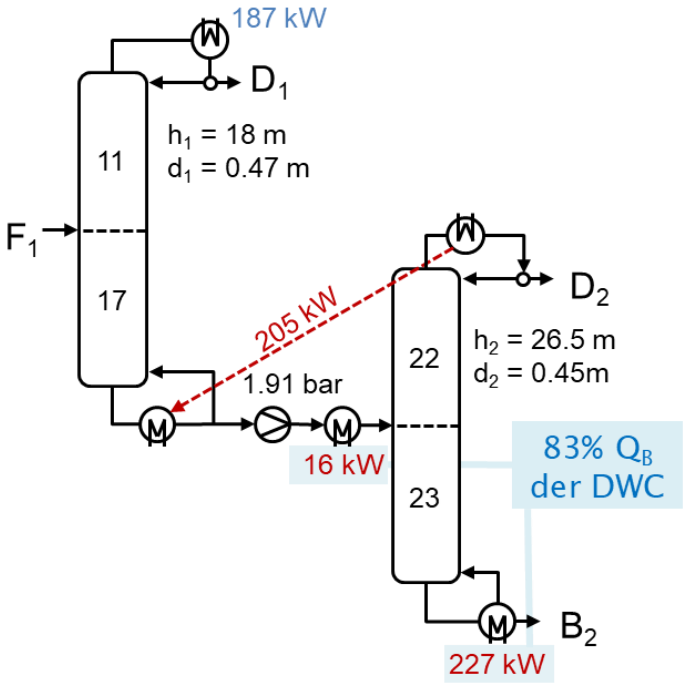
[2] Waltermann & Skiborowski, Chem. Ing. Tech., 2017, , 89(5), 562–581
[3] Waltermann & Skiborowski, Comp. Chem. Eng., 2019, 129, 106520

Rigorous optimization-based design

- Computationally efficient evaluation





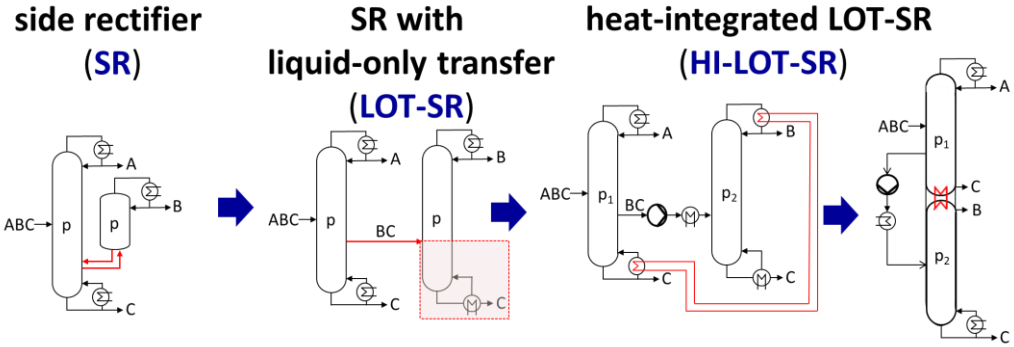


Waltermann & Skiborowski, Comp. Chem. Eng., 2019, 129, 106520

Evaluation of innovative configurations

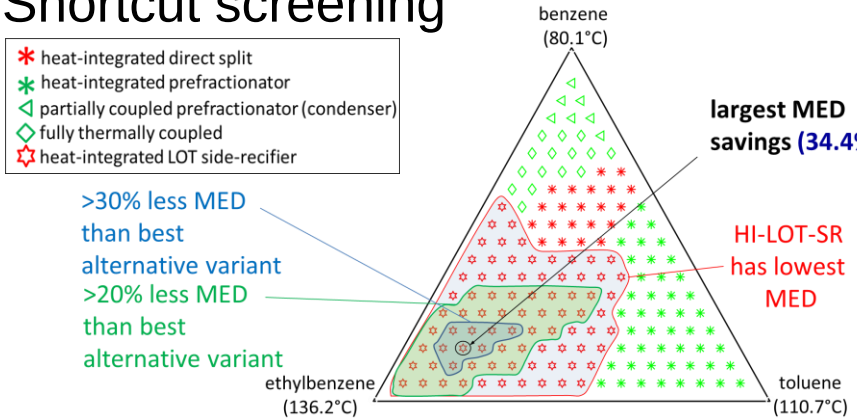
- Combination of thermal coupling and heat integration

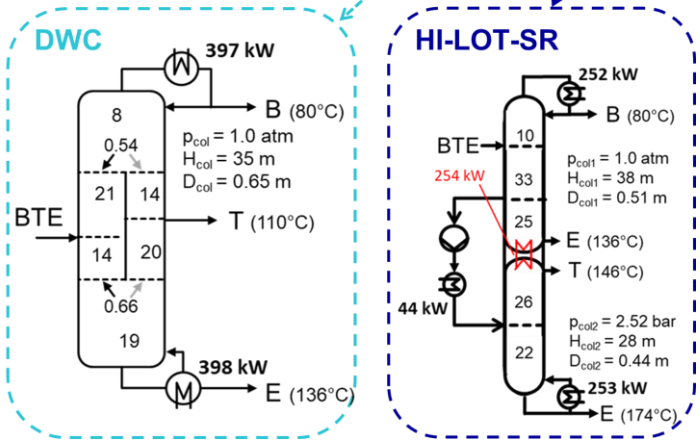
R. Agrawal, AIChE J 46 (11), 2211–2224, 2000
Z. Jiang & R. Agrawal, Chem. Eng. Res. Des., 147,122-145, 2019.



	DWC		HI-LOT-SR
TAC (k€/a)	203.4	(-14%)	236.1
AOC (k€/a)	92.2	(+10%)	83.8
AIC (k€/a)	111.2	(-27%)	152.8
$\sum Q_B$ (kW)	397.0	**(+37%)**	252.0
$\sum Q_C$ (kW)	398.0	(+34%)	297.0

- Shortcut screening

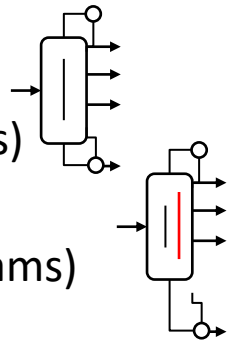




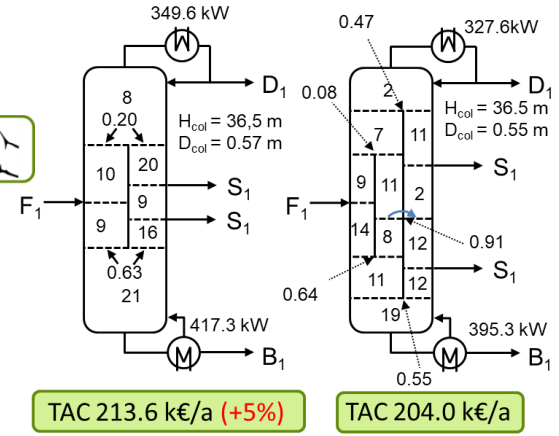
Skiborowski, M, 2020, Comput. Aided Chem. Eng. (48), 991-996.

Evaluation of complex processes

- 4-product separation with
  - Kaibel column (*13 DDoF*) (dividing wall + 2 side streams)
  - Multi-DWC (*21 DDoF*) (2 dividing walls + 2 side streams)

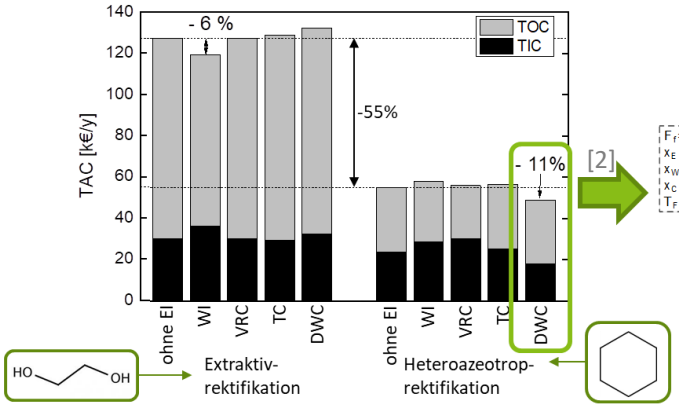


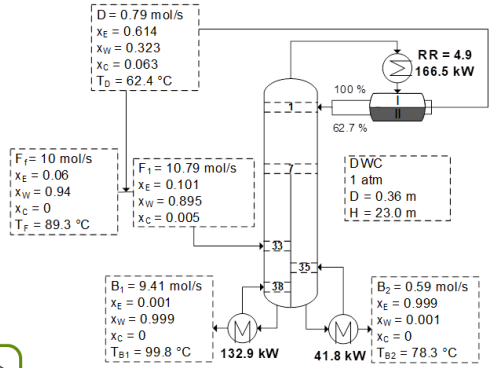
Waltermann, Sibbing & Skiborowski, Chem. Eng. Process., 2019, 146, 107688



TAC 213.6 k€/a (+5%)

TAC 204.0 k€/a





- MSA-based distillation
  - Extractive distillation
  - Heteroazeotropic distillation

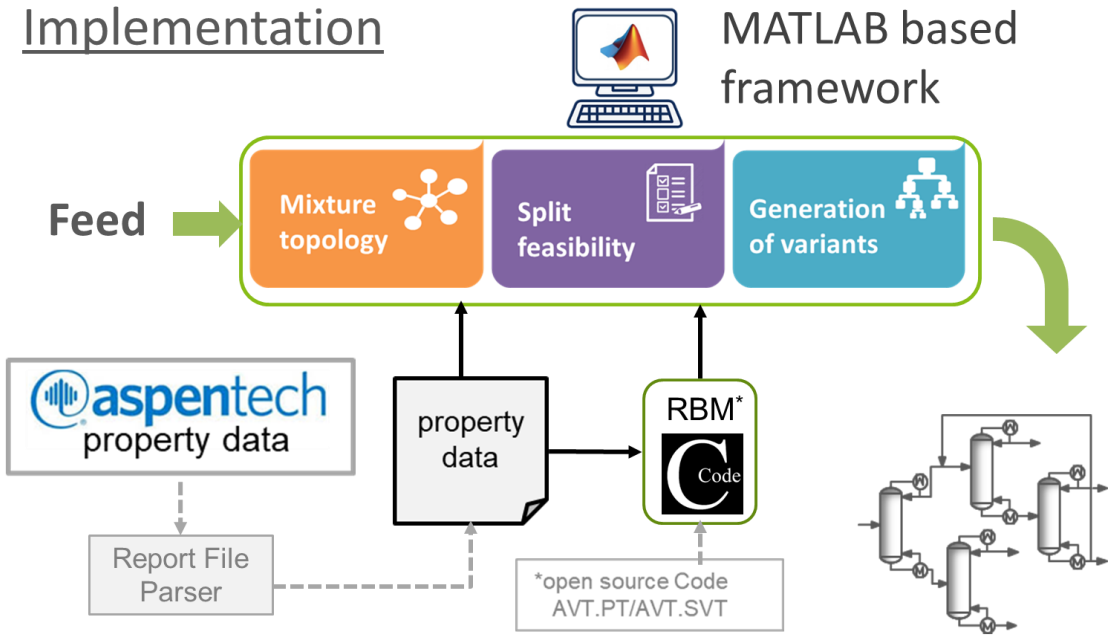
Waltermann & Skiborowski, Comp. Chem. Eng., 2020, 133, 106676

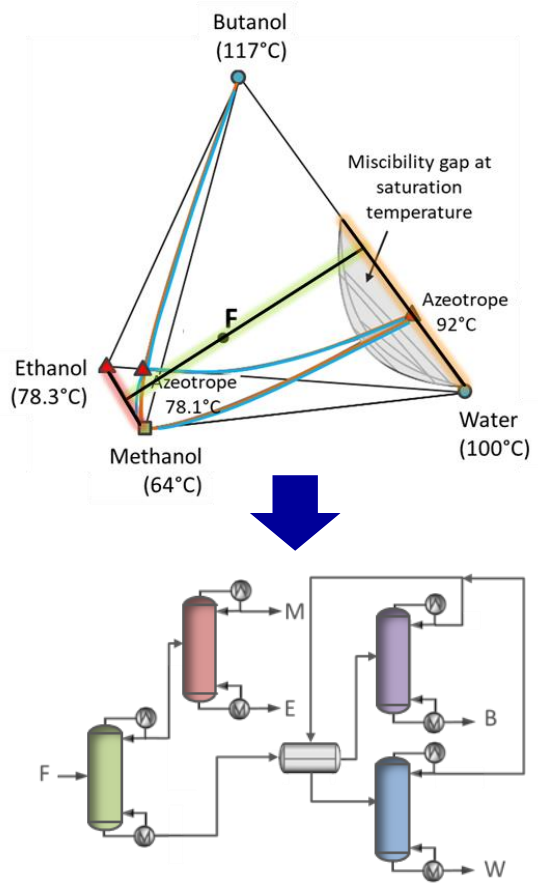
Objectives for further development

- Continuous extension of the design space
  - further options for energy integration
  - hybrid (membrane-assisted) process concepts
- Integration of MSA selection
  - computer-aided molecular design
  - solvent-based process synthesis
- Experimental validation and dynamic control
  - lab-scale experiments with extended Petlyuk configuration

Machine-based creativity

- Thermodynamic-based process synthesis

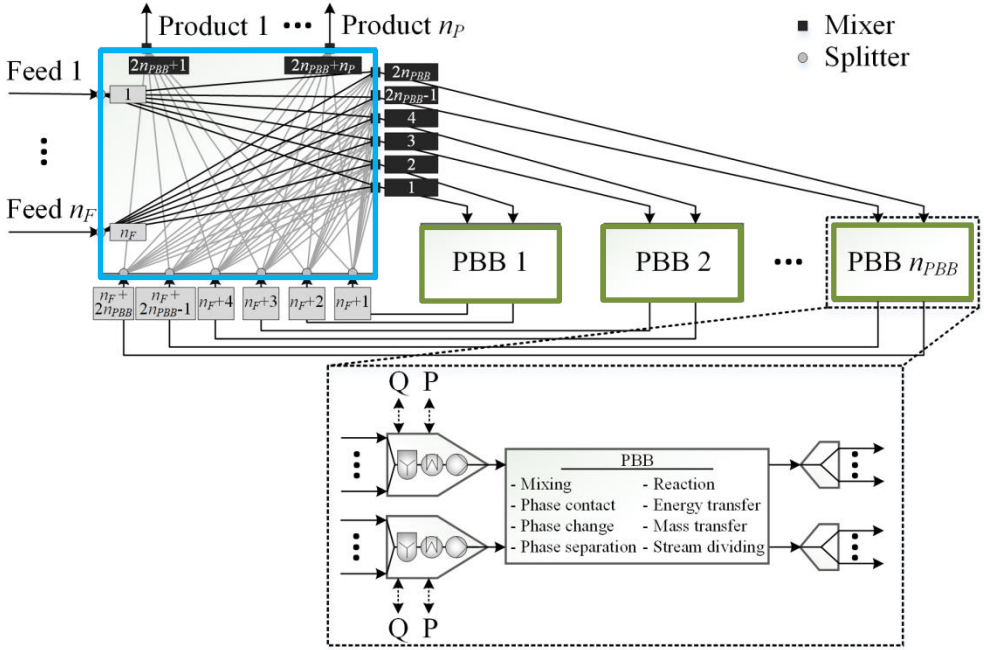




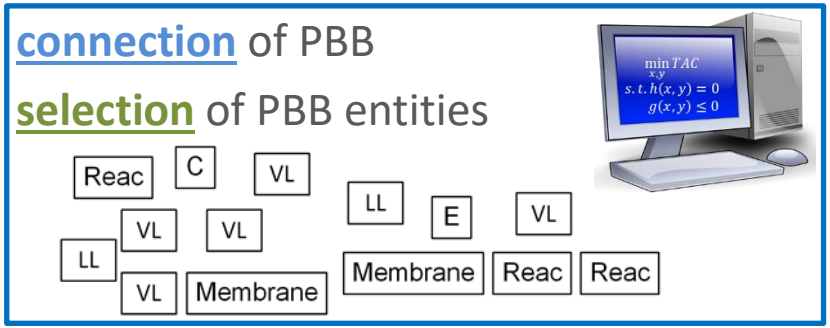
Sasi, T., Wesselmann, J., Kuhlmann, H., Skiborowski, M., 2019, Comput. Aided Chem. Eng. (46) 49–54.
Sasi, T., Kruber, K., Ascani, M. and Skiborowski, M, 2020, Comput. Aided Chem. Eng. (48), 1009-1014.

Phenomena-based process synthesis

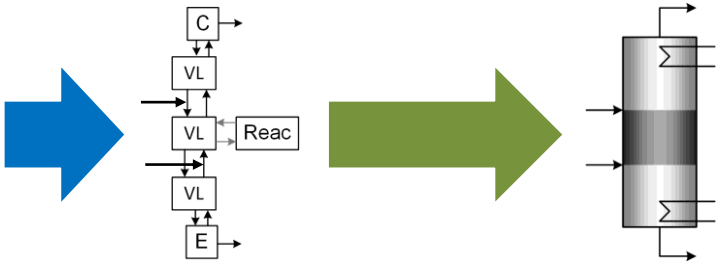
- Designing processes from abstract building blocks



- Generation of innovative processes
  - connection of PBB
  - selection of PBB entities



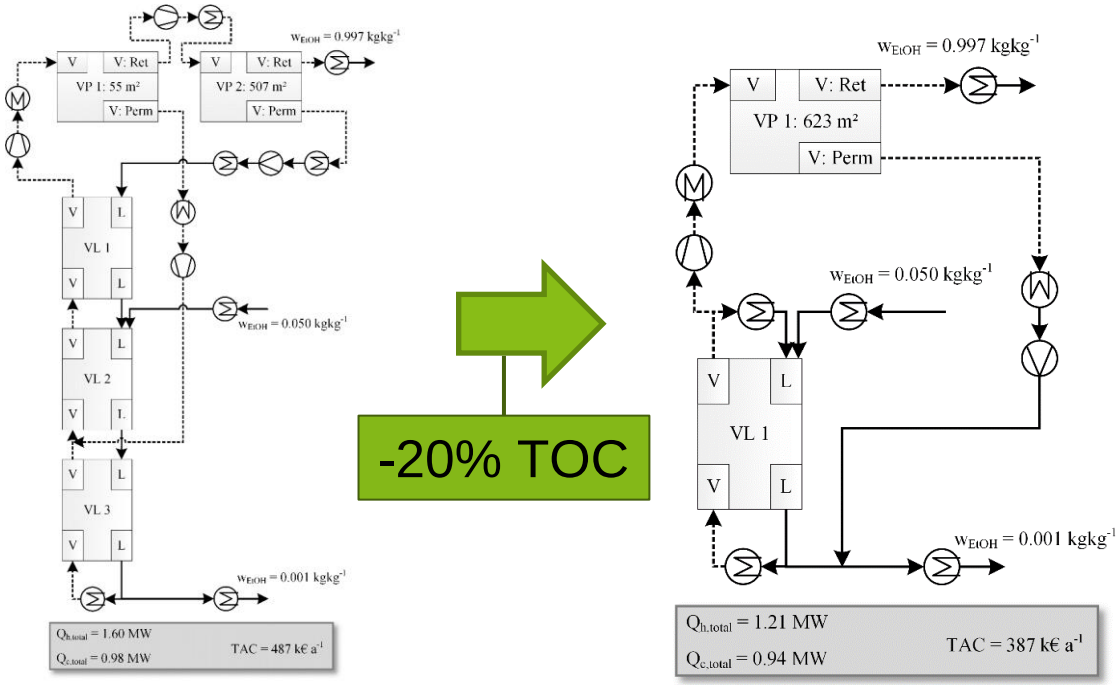
  - translation into real equipment

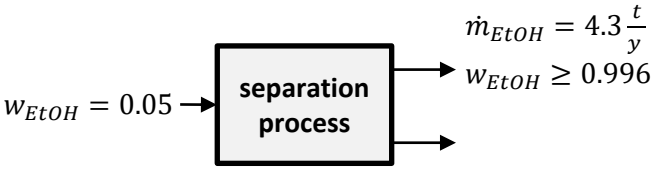


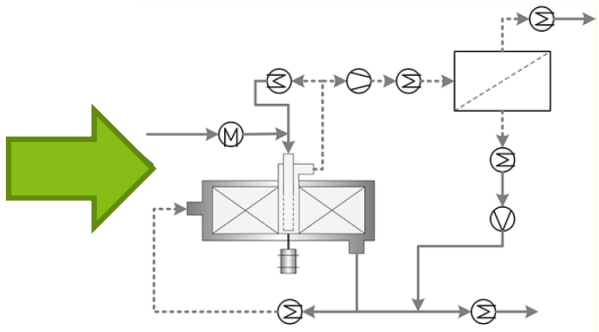
Kuhlmann and Skiborowski, 2017, Ind. Eng. Chem. Res., 56 (45), pp 13461–13481
Kuhlmann, Veith, Möller, Nguyen, Górak and Skiborowski, 2018, Ind. Eng. Chem. Res. 2018, 57, 3639–3655

Phenomena-based process synthesis

- Simple example – Ethanol dehydration







≈ **Hi**Gee **S**tripper **M**embrane process**

** Gudena, Rangaiah and Lakshminarayanan, Ind. Eng. Chem. Res. 2013, 52, 4572−4585

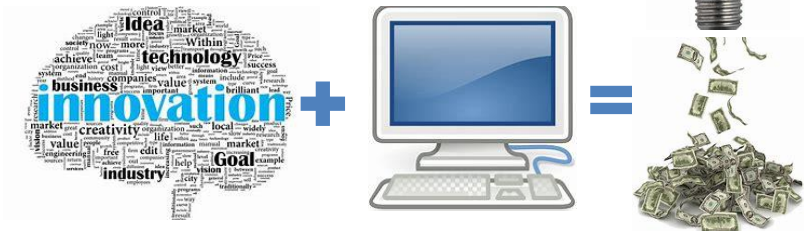
≈ **M**embrane **A**ssisted **V**apor **S**tripping*

* Vane, Alvarez, Huang and Baker, J Chem Technol Biotechnol, 2008, 831275–1287

Kuhlmann and Skiborowski, 2017, Ind. Eng. Chem. Res., 56 (45), pp 13461–13481
Kuhlmann, Veith, Möller, Nguyen, Górak and Skiborowski, 2018, Ind. Eng. Chem. Res. 2018, 57, 3639−3655

Summary

- There is a need for systematic methods for Process Intensification
  - in order to extend the search space and
  - in order to evaluate process concepts.



- There is "**no free lunch**"

  - no single technology will provide the best process for all applications and
  - no single design method will identify the best process variant.

- Biggest impact from **symbiosis of PSE and PI** and **integration across disciplines**.

Thank you for your attention!

I am happy to answer any questions.