



Outline

# A Hybrid Simulation-Optimization Approach for the Design of Internally Heat-integrated Distillation Column

- Motivation
- Concepts and general configuration of HIDiC with single heat exchangers
- Examples and conclusions
- Future work (inclusion of LCA and environmental impact evaluation in the optimization problem)



**Motivations** 

# A Hybrid Simulation-optimization Approach For The Design Of Internally Heat-integrated Distillation Column

#### ✓ Motivation (I)

#### ✓ Environmental aspects (THERE IS NOT PLANET "B")

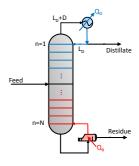
- Increasing energy efficiency in chemical processes not only provides economic benefits but also reduces emissions resulting for process operations => more efficient and sustainable chemical processes







- Distillation columns are one of the major energy consumers in chemical processes and therefore represent a key point in terms of energy efficiency

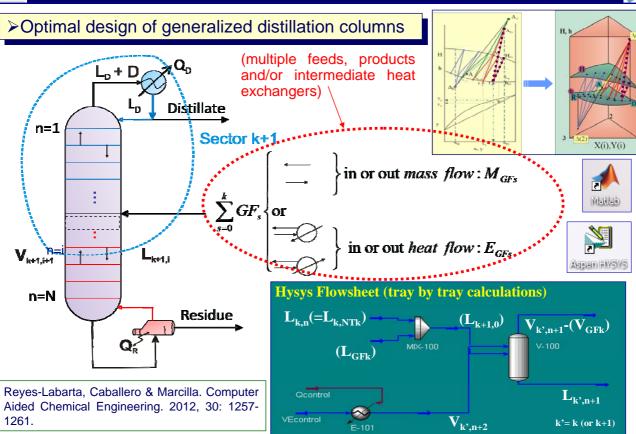


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Motivation (TT): Simula:

# Motivation (II): Simulation-Optimization approaches





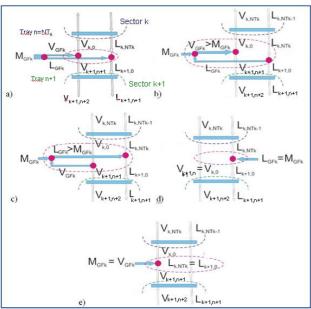


#### Optimal design of generalized distillation columns



#### > Optimal location of all the side streams:

#### (two phases) Side feed stream



Schematic representations of the internal existing streams at the zone connecting consecutive sectors in the case of a generalized feed side stream (GFk).

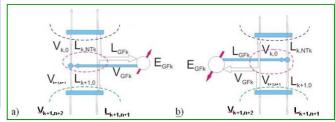
 $\frac{x_{k,n,L} / x_{k,n,H}}{z_{opt,k,L} / z_{opt,k,H}} \le 1$ 

where  $z_{opt}$  refers to the phase composition at the optimal change point of sector k. L and H are the indexes for light and heavy key components, respectively.

#### Side product stream (liquid or vapor)



#### •Intermediate Heat exchanger



Marcilla, Reyes-Labarta & Serrano. "Review and extension of the McCabe-Thiele method covering multiple feeds, products and heat transfer stages" (2012). <a href="https://hdl.handle.net/10045/23195">http://hdl.handle.net/10045/23195</a>

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Optimal design of absorption systems (MINLP)

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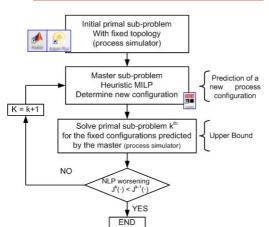
## Motivation (II): Simulation-Optimization approaches

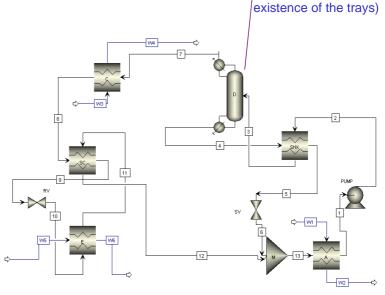


**Distillation Column** 

(binary variables associated with the





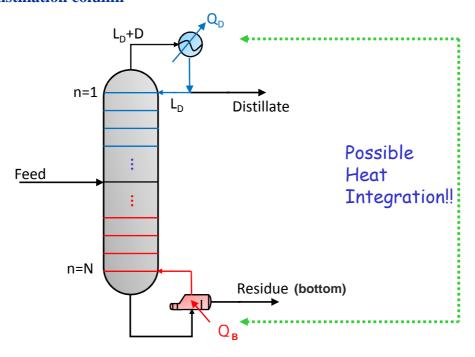


Reyes-Labarta et al. Computer Aided Chemical Engineering. 2011, 29: 301-305.





#### **≻**Conventional distillation column



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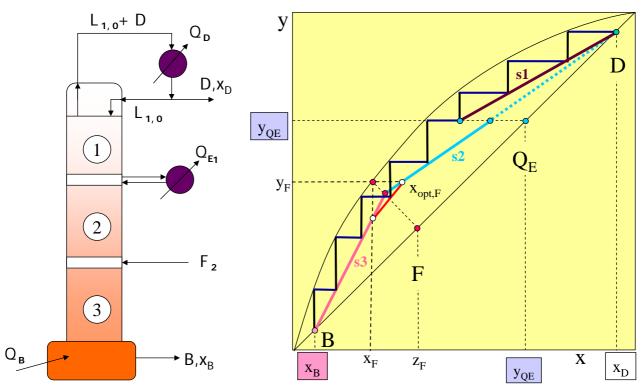
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# Design of Internally Heat-Integrated Distillation Columns (HIDiC)



## Inter-Condenser and inter-reboiler benefits (McCabe-Thiele Method)

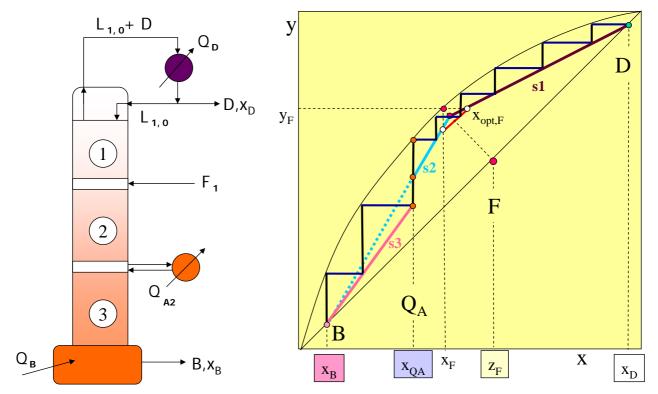


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## Inter-Condenser and inter-reboiler benefits (McCabe-Thiele Method)



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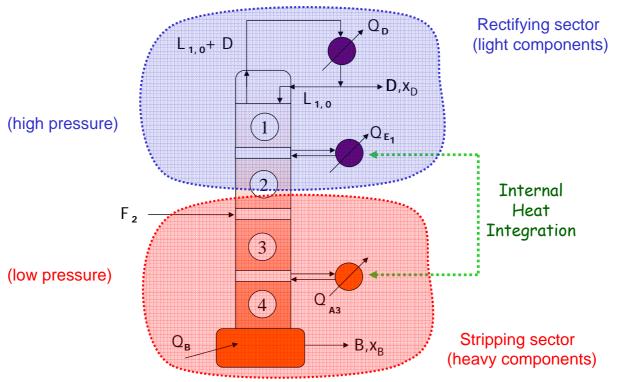
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# Design of Internally Heat-Integrated Distillation Columns (HIDiC)



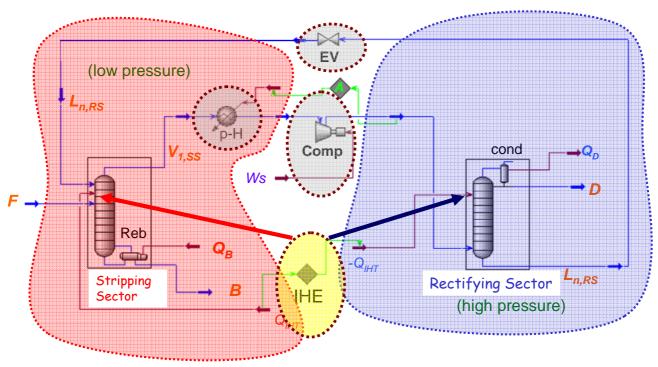
# ➤ General representation of an internally heat-integrated distillation column







## ➤ General configuration of an internally heat-integrated distillation column



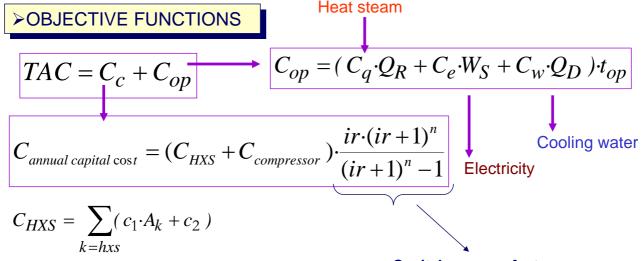
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# Design of Internally Heat-Integrated Distillation Columns (HIDiC)





$$C_{compressor} = 5.8 \cdot 10^{\left[k1 + k2 \cdot \log(W_S) + k3 \cdot \log^2(W_S)\right]}$$

Capital recovery factor:

ir = interest rate

n = life time of the equipment (years)

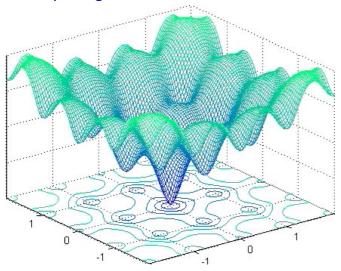
$$A_k = \frac{Q_k}{U_k \, \Delta T_k^{lm}}$$





#### SIMULATION-OPTIMIZATION APPROACH

We propose an approach that combines the advantages of commercial process simulator (Aspen-Hysys) to converge distillation columns, with the advantages of using a metaheuristic algorithm (PSO: particle swarm optimization) which initially has the ability to escape from local optima and not require gradient information



The original particle swarm optimization algorithm (Kennedy Eberhart, 1995)

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## Design of Internally Heat-Integrated Distillation Columns (HIDiC)



#### >NUMERICAL EXAMPLES

## Systems studied:

- benzene + toluene
- propylene + propane
- methanol + water
- benzene + cyclohexane + toluene
- methanol + acetone + water
- methanol + ethyl-acetate + water
- propylene + i-butane + propane

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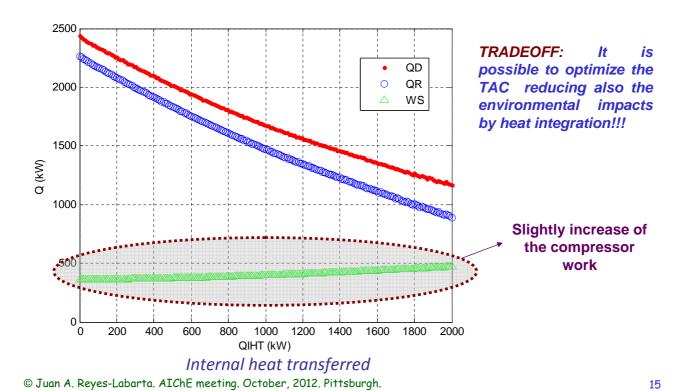
- benzene + toluene + ethyl-benzene + styrene





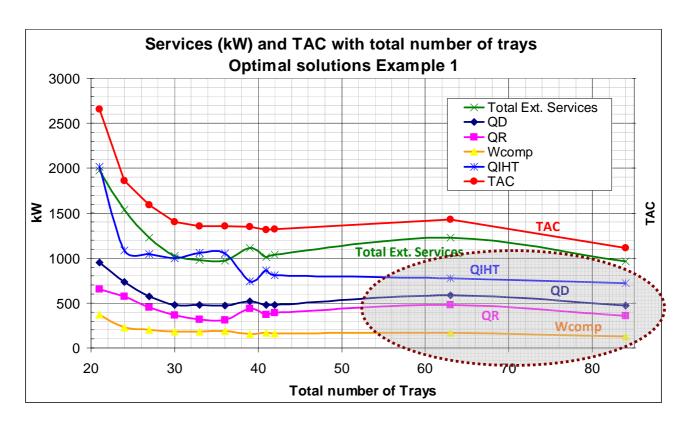


Condenser and reboiler duties, and compressor shaft work vs overall internal heat transferred (QIHT)



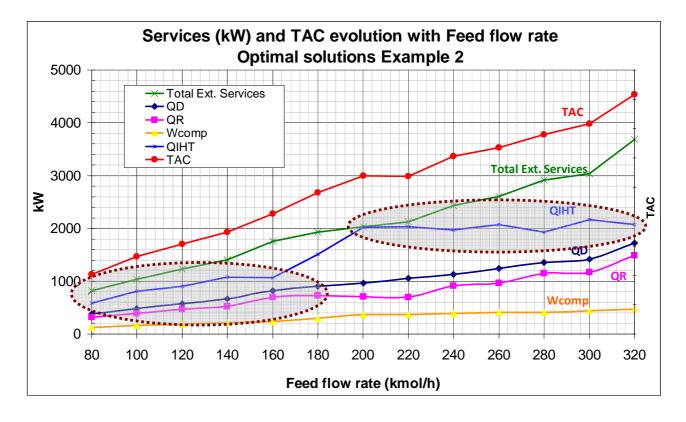
# Design of Internally Heat-Integrated Distillation Columns (HIDiC)











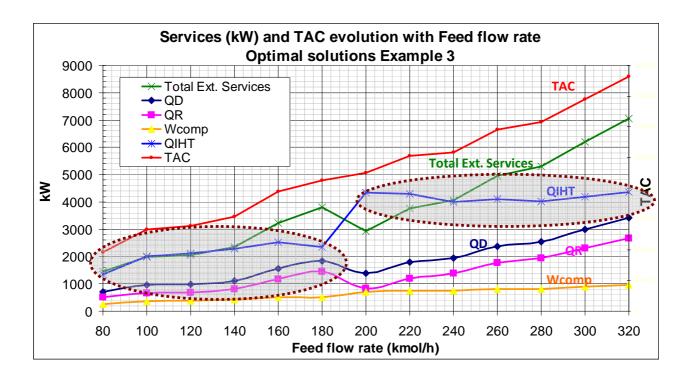
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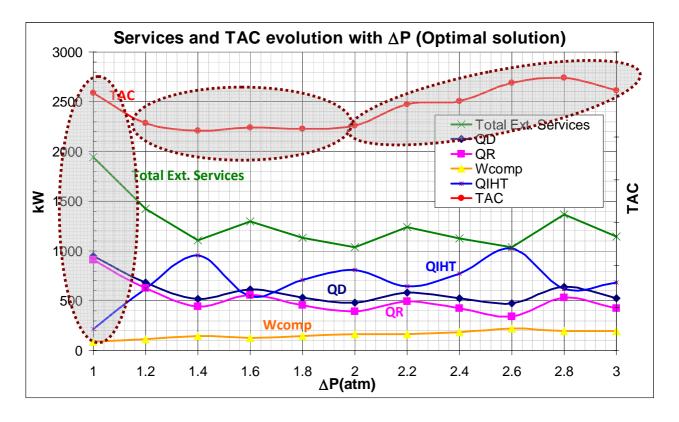
# Design of Internally Heat-Integrated Distillation Columns (HIDiC)











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## Design of Internally Heat-Integrated Distillation Columns (HIDiC)



## ➤ General Conclusions (I)

- The economic interest of HIDiC depends on the ratio between the cost of the electricity and the cost of the heating steam. However, environmentally friendly and more energy efficient technologies should be introduced to provide more sustainable processes that minimize the environmental impacts.
- HIDiC with a small number of intermediate heat exchangers can present interesting benefits, providing savings around 20-40% comparing with conventional distillation columns, depending on the components of the system, the flow rate and composition of the feed stream, and the product purities desired.
- The possibility of heat exchange between stages that are not at the same high in both sectors can also improve the efficiency of the configuration, together with the optimal location of the feed stream that is generally at the first stages of the stripping sector (but not always!!).
- The pressure difference between both sectors is also a key point of the process. The
  pressure of the rectifying sector should be high enough to allow the heat transfer
  between both sectors, but it should be as low as possible to minimize the compressor
  costs.





## ➤ General Conclusions (II)

 Traditional HIDiC (with heat transfer along the total length of each sector) are less efficient when we have flat temperature profiles inside the column (i.e. with small variation in the equilibrium composition of the different trays) and high products purity.

However, HIDiC with a small number of intermediate heat exchangers can improve the feasibility and efficiency of the configuration in this kind of separations.

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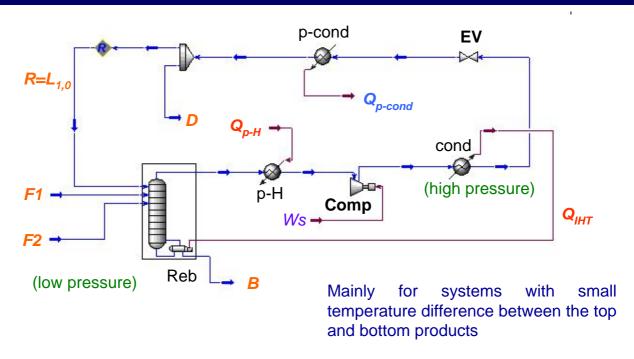
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## Design of sustainable processes



➤ General configuration of a classical vapour recompression distillation column (VRC)

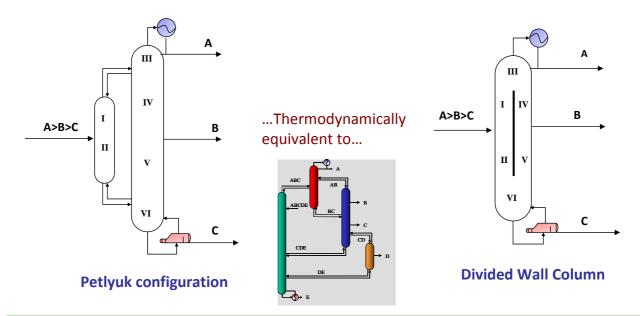




#### Energy efficiency: heat integration configurations



 Thermally coupled columns/sequences or its thermodynamically equivalent Divided Wall Column (DWC) configurations



Caballero, Reyes-Labarta & Grossmann. Computer Aided Chemical Engineering. 2003, 14(C): 59-64 and 2004, 18(C): 361-366.

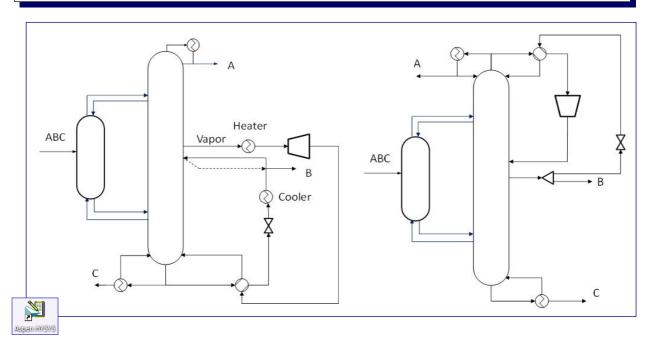
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## Motivation (II): Simulation-Optimization approaches



➤ New Vapor Compression Alternatives in Thermally Coupled Distillation Columns



Caballero, Navarro & Reyes-Labarta. Paper 399b. AIChE Meeting 2012. <a href="https://aiche.confex.com/aiche/2012/webprogram/Paper267695.html">https://aiche.confex.com/aiche/2012/webprogram/Paper267695.html</a>



#### Bibliography



-Reyes-Labarta, J.A. "Diseño de Columnas de Rectificación Y Extracción Multicomponentes". Biblioteca Virtual Miguel de Cervantes (Universidad de Alicante), 1998.

http://www.cervantesvirtual.com/FichaObra.html?Ref=4845&ext=pdf

http://hdl.handle.net/10045/10023

- -A. Marcilla, A. Gómez, J.A. Reyes, M.M. Olaya.; New Method for Quaternary Systems Liquid-liquid Extraction Tray to Tray Design. Industrial & Engineering Chemistry Research, 38, 3083-3095 (1999). http://dx.doi.org/10.1021/ie9900723
- -A. Marcilla, A. Gómez, J.A. Reyes; New Methods for Designing Distillation Columns of Multicomponent Mixtures. Latin American Applied Research and International Journal of Chemical Engineering, 27, 51-60 (1997). http://hdl.handle.net/10045/24679
- -Reyes, J.A.; Gomez, A.; Marcilla, A. Graphical concepts to orient the minimum reflux ratio calculation on ternary mixtures distillation. Industrial & Engineering Chemistry Research 39(10),3912-3919 (2000). <a href="https://dx.doi.org/10.1021/ie9907021">https://dx.doi.org/10.1021/ie9907021</a>
- -J.A. Reyes-Labarta, I.E. Grossmann; Disjunctive Programming Models for the Optimal Design Of Liquid-liquid Multistage Extractors and Separation Sequences. AIChE Journal. 2001, 47 (10), 2243-2252. http://dx.doi.org/10.1002/aic.690471011
- J.A. Reyes-Labarta y I.E. Grossmann. Optimal Synthesis of Liquid-liquid Multistage Extractors. Escape-11 (European Symposium of Computer Aided Process Engineering), Capec (Computer Aided Process Engineering Center). ISBN: 0-444-50709-4 (Dinamarca, 2001). http://dx.doi.org/10.1016/S1570-7946(01)80076-6

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#### Bibliography



- -Reyes-Labarta, J.A.; Caballero, J.A.; Marcilla, A. A Novel Hybrid Simulation-Optimization Approach for the Optimal Design of Multicomponent Distillation Columns. Computer Aided Chemical Engineering. 2012, 30, 1257-1261. http://dx.doi.org/10.1016/B978-0-444-59520-1.50110-X
- -Reyes-Labarta, J.A.; Brunet, R.; Caballero, J.A.; Boer, D.; Jiménez, L. Integrating process simulation and MINLP methods for the optimal design of absorption cooling systems. Computer Aided Chemical Engineering. 2011, 29, 301-305. <a href="http://dx.doi.org/10.1016/B978-0-444-53711-9.50061-4">http://dx.doi.org/10.1016/B978-0-444-53711-9.50061-4</a>
- -Brunet, R.; Reyes-Labarta, J.A.; Guillén-Gosálbez, G.; Jiménez, L.; Boer, D. Combined Simulation-Optimization Methodology for the Design of Environmental Conscious Absorption Systems. Computers and Chemical Engineering, 2012, 46, 205-216 http://hdl.handle.net/10045/24678
- -Marcilla et al. "Review and extension of the McCabe-Thiele method covering multiple feeds, products and heat transfer stages" (2012). http://hdl.handle.net/10045/23195
- -Reyes-Labarta, J.A.; Navarro M.A.; Caballero, J.A. A Hybrid Simulation-Optimization Approach for the Design of Internally Heat-Integrated Distillation Columns. Paper 488e. AIChE 2012 Annual Meeting (Energy Efficiency by Process Intensification). https://aiche.com/ex.com/aiche/2012/webprogram/Paper267732.html
- -Caballero, Reyes-Labarta & Grossmann. Synthesis of Integrated Distillation Systems. Computer Aided Chemical Engineering. 2003, 14(C): 59-64.
- -Caballero, Reyes-Labarta & Grossmann. Simultaneous Design of Heat Integrated and Thermally Coupled Distillation Systems. Computer Aided Chemical Engineering. 2004, 18(C): 361-366.
- -Caballero, Navarro & Reyes-Labarta. New Vapor Compression Alternatives In Thermally Coupled Distillation. Paper 399b. AIChE Meeting 2012 (Advances in process intensification) <a href="https://aiche.com/aiche/2012/webprogram/Paper267695.html">https://aiche.com/aiche/2012/webprogram/Paper267695.html</a>