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DESIGN OF SEPARATION PROCESSES: FROM THE EMPIRICAL METHODS TO THE COMPUTER-AIDED STRATEGIES

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Mexico



INTRODUCTION

Chemical/petrochemical industries…

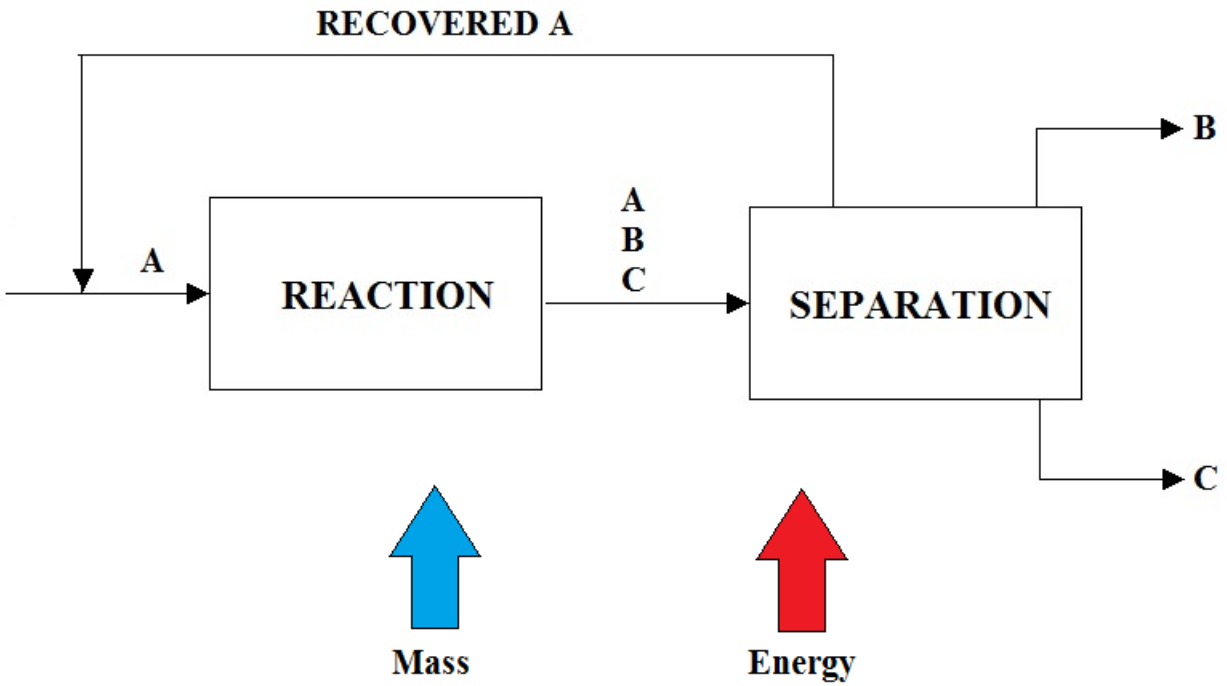


Figure 1. A general flowsheet for a process plant



Figure 2. An ExxonMobil facility for the production of ethylene and other chemical products.[1]

[1] ExxonMobil Singapore Chemical Plant Expansion in Operation (2013), at news.exxonmobil.com. Last consulted April 12, 2016.

SEPARATION PROCESSES

Based on mass transfer

Liquid-liquid extraction

Adsorption

Absorption

Based on mass and energy transfer

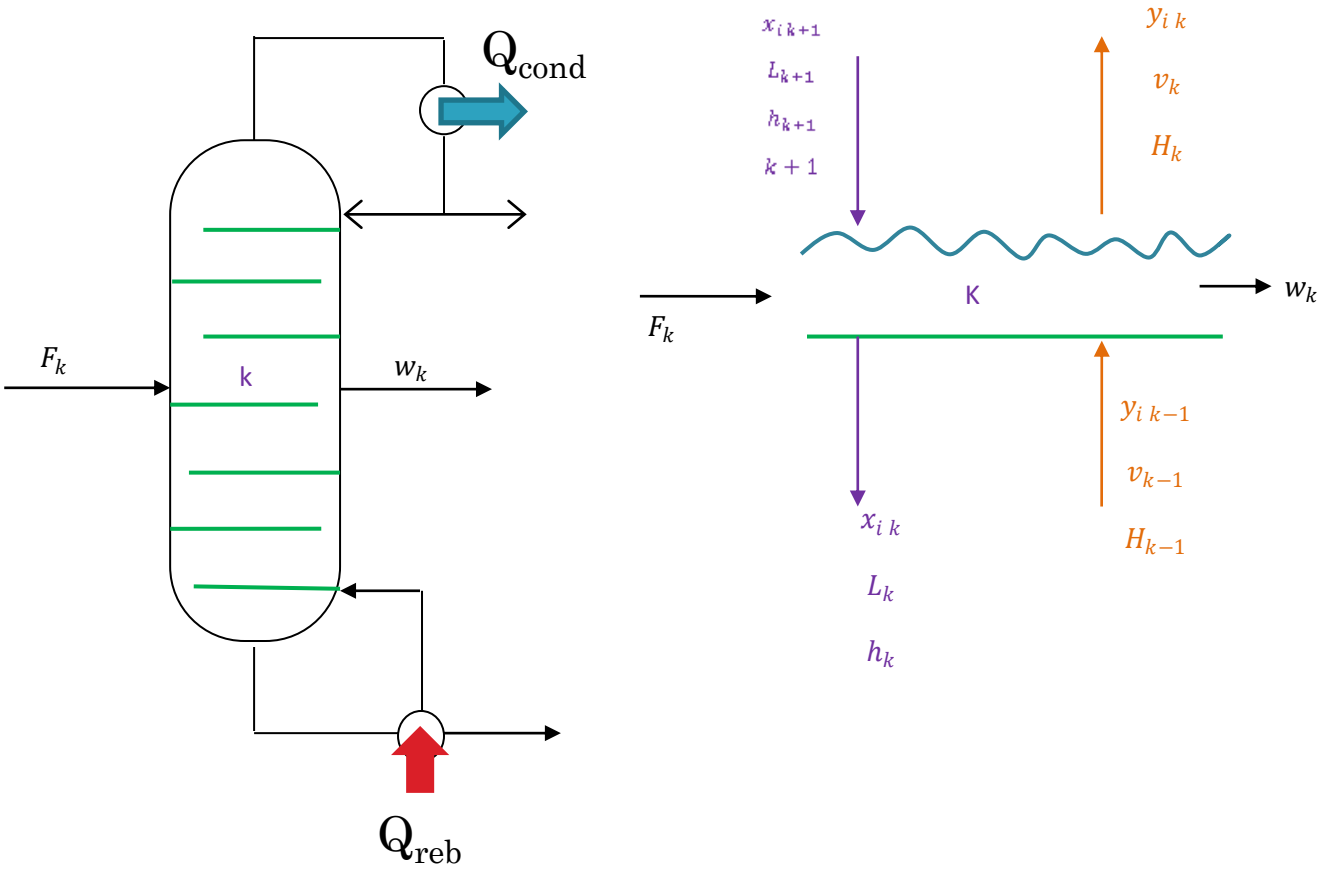
Distillation

Cristallyzation

Pervaporation

DISTILLATION

- ✓ Is one of the most used separation processes.
- ✓ Separates liquid mixtures
- ✓ Mature technology
- ☒ Low thermodynamic efficiency


Q_{cond}
F_k
k
w_k
Q_{reb}
$x_{i\,k+1}$
L_{k+1}
h_{k+1}
$k+1$
$y_{i\,k}$
v_k
H_k
K
F_k
w_k
$y_{i\,k-1}$
v_{k-1}
H_{k-1}
$x_{i\,k}$
L_k
h_k

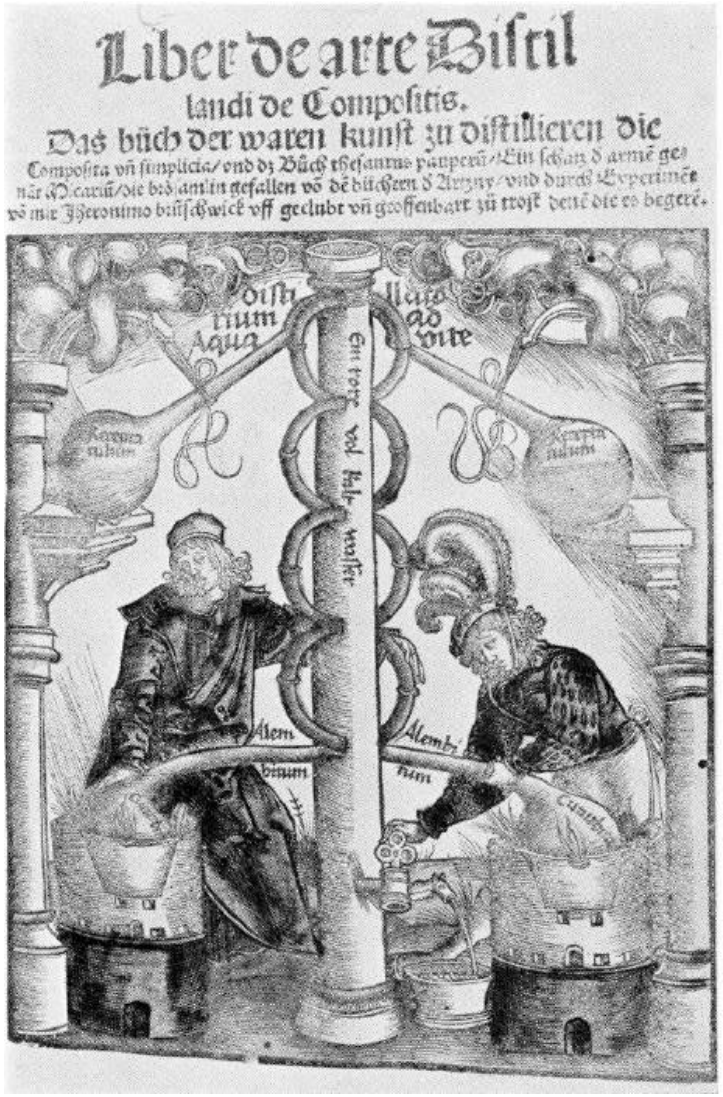




[2] Sulzer – Separation Technologies, at sulzer.com. Last consulted May 16, 2016.

[3] FLEXITRAY. Valve trays, at koch-glitsch.com. Last consulted May 16, 2016.

- Distillation is used since the ancient ages, but...



...it was more an art than a science

[4] A.J. Liebmann (1956) History of distillation, Journal of Chemical Education, 33(4), 166-173

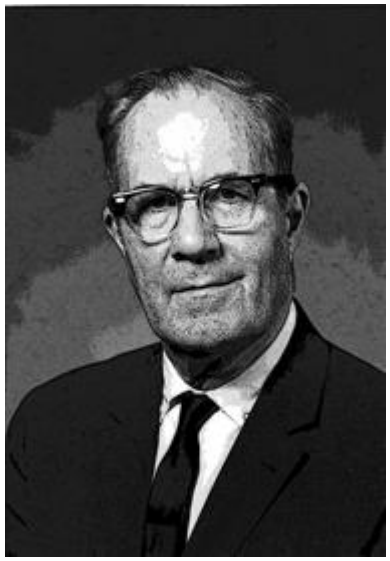
DESIGN OF DISTILLATION COLUMNS

Given a mixture with a known feed composition…

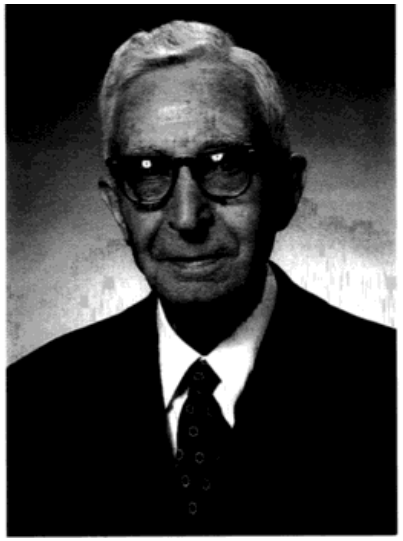


How can I obtain the pure components with the desired purity and recovery??

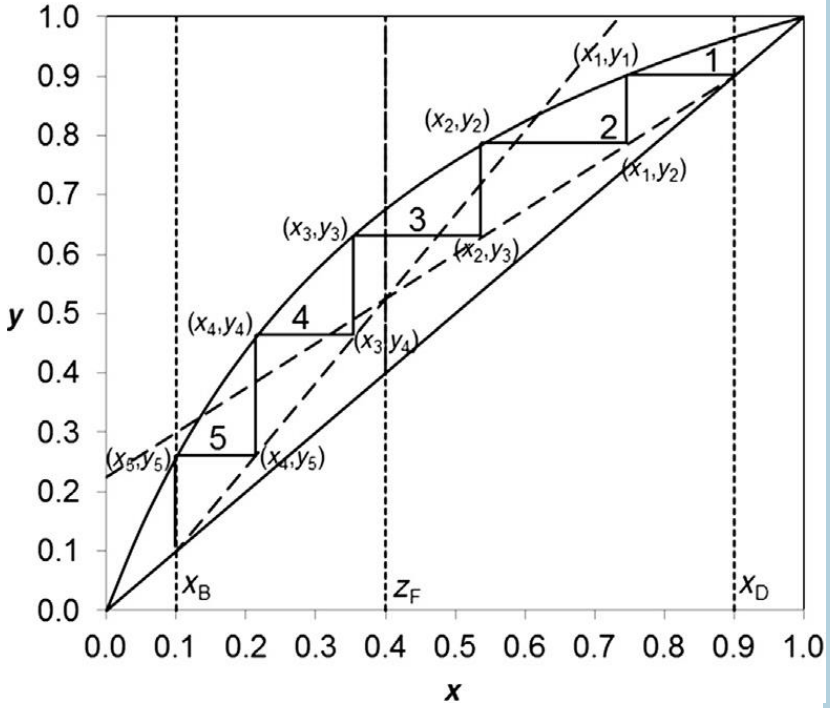
McCabe-Thiele method (1925)



W.L. McCabe[5]



E.W. Thiele[6]



[5] Department of Chemical & Biomolecular Engineering, NC State University, che.ncsu.edu. Last consulted May 16, 2016
[6] Memorial tributes: National Academy of Engineering, Volume 8, at nap.edu. Last consulted May 16, 2016
[7] E. Sorensen (2014) Principles of binary distillation, at Distillation: Fundamentals and Principles, A. Górak and E. Sorensen (Eds), Elsevier

Fenske-Underwood-Gilliland-Kirkbride method

Fenske equation (1932)[8]

$$N_{min} = \frac{ln\left[\left(\frac{x_D}{1-x_D}\right)\left(\frac{1-x_B}{x_B}\right)\right]}{ln(\alpha)}$$

Underwood equations (1946)[9]

$$\sum_{i=1}^{nc} \frac{\alpha_{i,r} x_{i,B}}{\alpha_{i,r} - \Phi} = 1 - q$$

$$R_{min} + 1 = \sum_{i=1}^{nc} \frac{\alpha_{i,r} x_{i,D}}{\alpha_{i,r} - \Phi}$$

Gilliland correlation (1940)[10]

$$Y = 1 - exp\left[\frac{(1+54.4X)(X-1)}{(11+117.2X)X^{1/2}}\right]$$

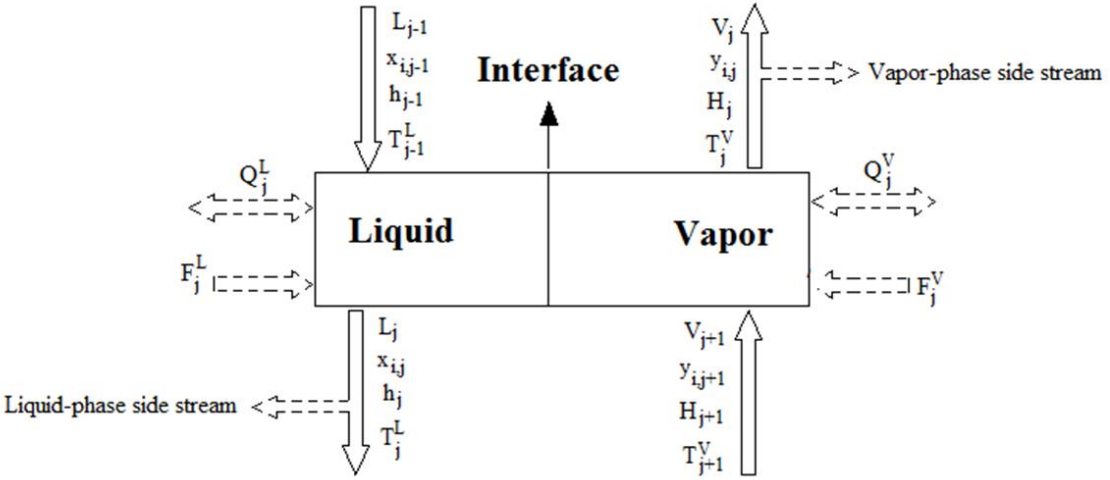
$$X = \frac{R - R_{min}}{R+1} \qquad Y = \frac{N - N_{min}}{N+1}$$

Kirkbride equation (1944)[11]

$$\frac{N_R}{N_S} = \left[\left(\frac{z_{HK}}{z_{LK}}\right)\left(\frac{x_{B,LK}}{x_{D,HK}}\right)^2 \frac{B}{D}\right]^{0.206}$$

[8] M.R..Fenske (1932) Fractionation of straight-run Pennsylvania gasoline, Ind. Eng. Chem., 42, 482.
[9] A.J.V.Underwood (1946) Fractionation distillation of multicomponent mixtures – Calculation of mínimum reflux ratio, J. Inst. Petrol., 32, 614.
[10] E.R.Gilliland (1940) Multicomponent rectification: estimation of number of theoretical plates as a function of reflux ratio, Ind. Eng. Chem., 32, 1220.
[11] G.G.Kirkbride (1944) Process design procedure for multicomponent fractionators, Pet. Refin., 23, 87.

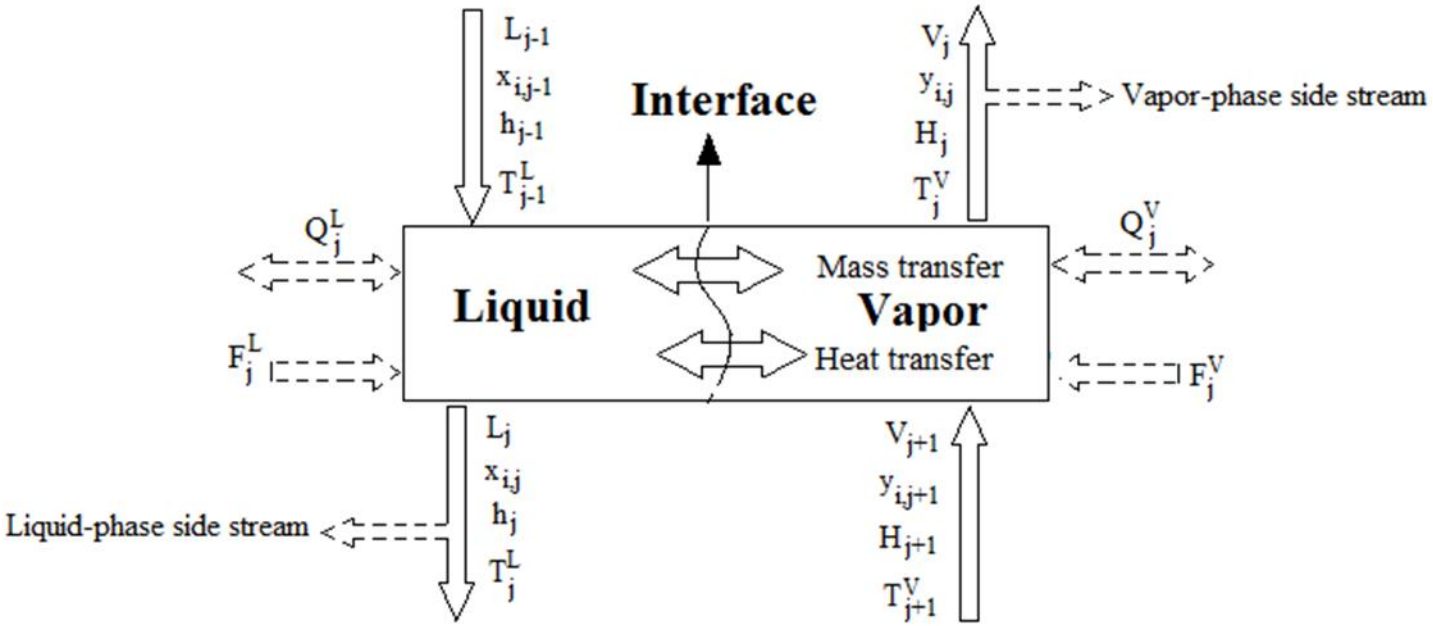
The equilibrium model: MESH equations



Mass balances (M)
Equilibrium equations (E)
Summation equations (S)
Energy balances (H)

[12] J.R. Friday, B.D. Smith (1964) An analysis of the equilibrium stage separations problem – formulation and convergence, AIChE J., 10(5), 698.
[13] R. Taylor, R. Krishna, H. Kooijman (2003) Real-world modeling of distillation, CEP Magazine, July 2003, 28.

The rate-based model: MERSQH equations



Mass balances (M)
Energy balances (E)
Rate equations (R)

Summation equations (S)
Hydraulic equations (H)
Equilibrium equations(Q)

[14] R. Taylor, R. Krishna, H. Kooijman (2003) Real-world modeling of distillation, CEP Magazine, July 2003, 28.
[15] R. Taylor, R. Krishna (1993) Multicomponent mass transfer, John Wiley and Sons, New York.

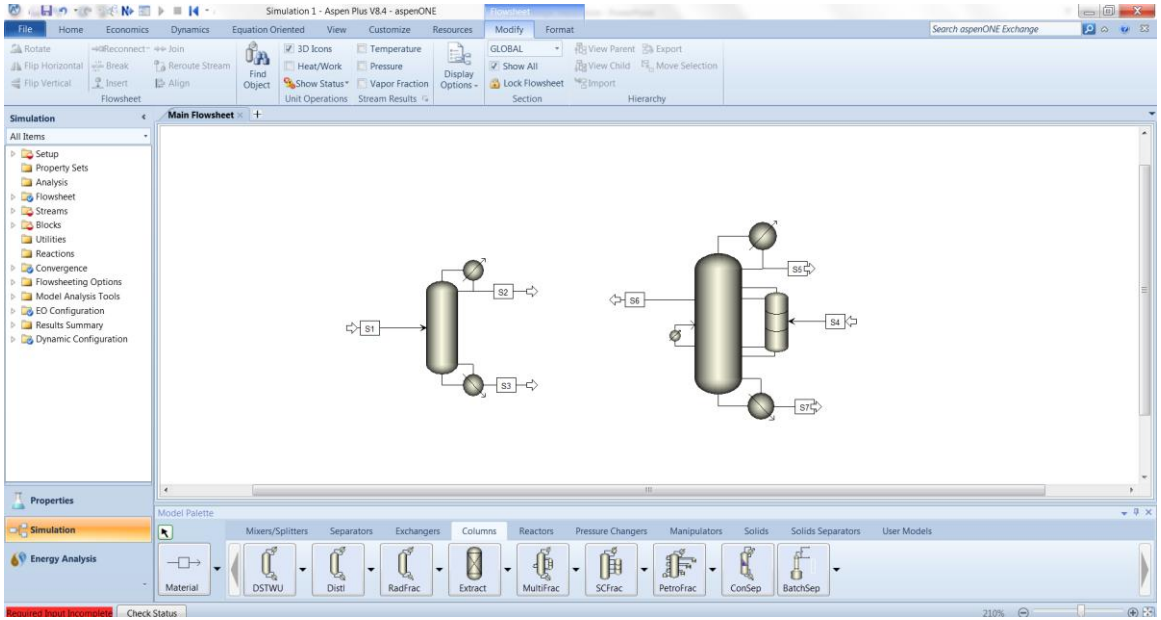
Modular process simulators

aspentech

CHEMCAD

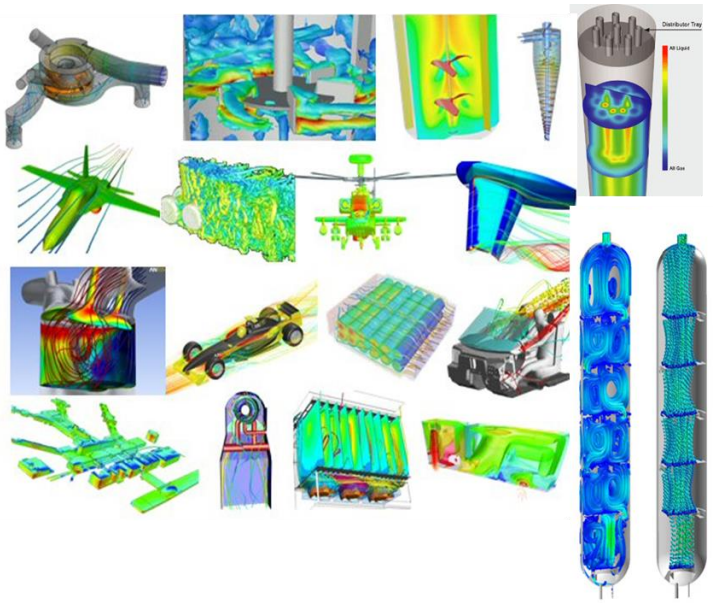
CC-STEADY STATE
CC-DYNAMICS
CC-BATCH
CC-THERM
CC-SAFETY NET
CC-FLASH

HYSYS®



Computational fluid dynamics (CFD)

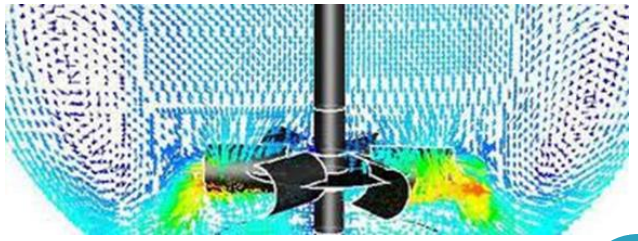
ANSYS® FLUENT®



$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q\right)+\nabla\cdot\left(\alpha_q \rho_q \vec{v}_q\right)=\sum_{p=1}^{n}\left(m_{pq}-m_{qp}\right)+S_q$$

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q \vec{v}_q\right)+\nabla\cdot\left(\alpha_q \rho_q \vec{v}_q \vec{v}_q\right)=-\alpha_q \nabla p+\nabla\cdot\bar{\bar{\tau}}_q+\alpha_q \rho_q \vec{g}+$$

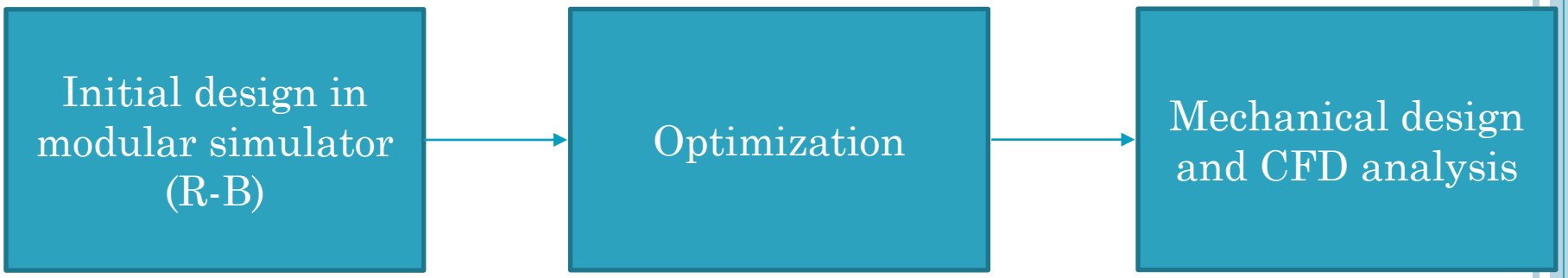
$$\sum_{p=1}^{n}\left(\vec{R}_{pq}+m_{pq}\vec{v}_q-m_{qp}\vec{v}_q\right)+\left(\vec{F}_q+\vec{F}_{lift,q}+\vec{F}_{vm,q}\right)$$



$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q h_q\right)+\nabla\cdot\left(\alpha_q \rho_q \vec{u}_q h_q\right)=-\alpha_q \frac{\partial p_q}{\partial t}+\bar{\bar{\tau}}_q:\nabla\vec{u}_q-\nabla\cdot\vec{q}_q$$

$$+S_q+\sum_{p=1}^{n}\left(\vec{Q}_{pq}+m_{pq}h_{pq}-m_{qp}h_{qp}\right)$$

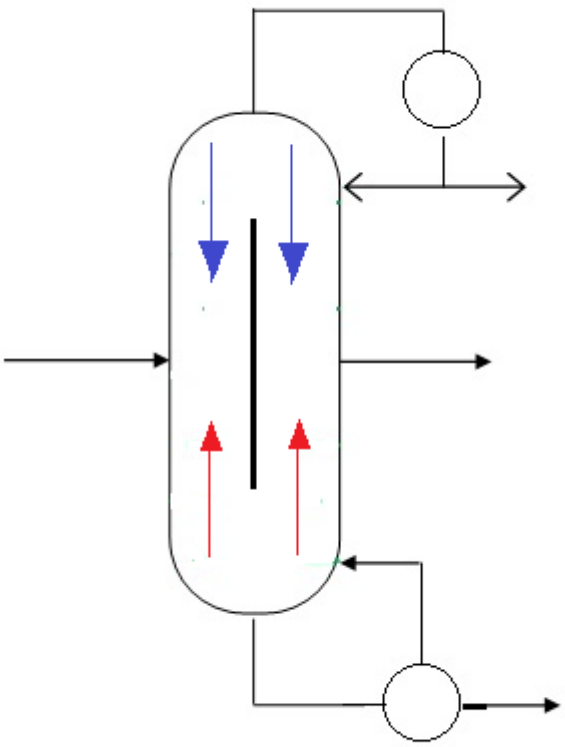
DESIGN PROCEDURE



EXAMPLES

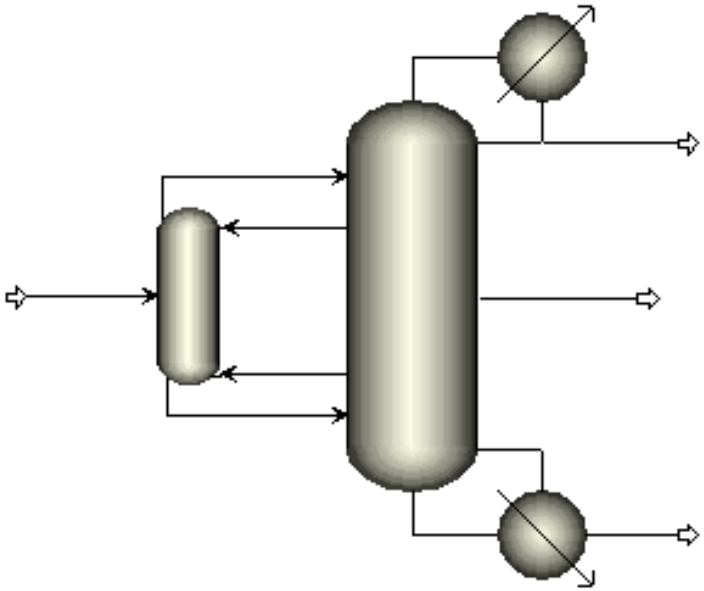


DIVIDING WALL COLUMN



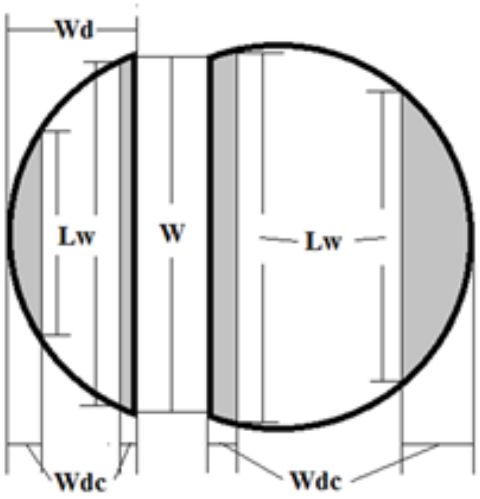
- Reduces energy consumption
- Reduces utilities costs
- Reduces number of equipment
- Reduces equipment cost
- Better controllability

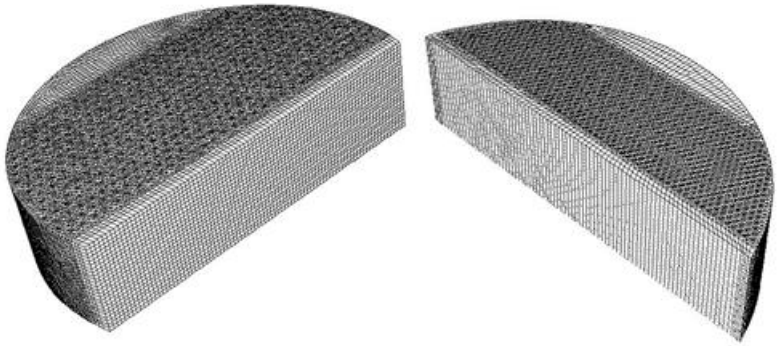
- Analysis in modular simulator…

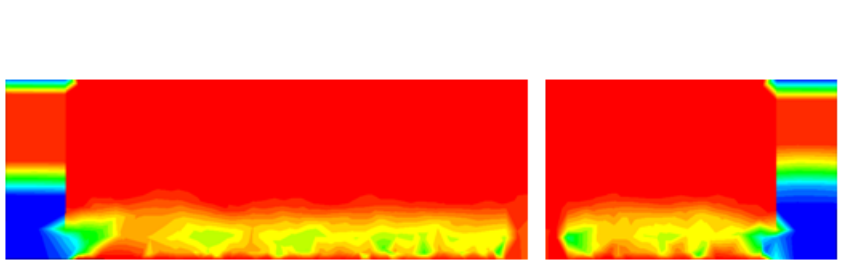


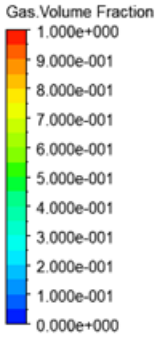
- Preliminary design
- Mass and energy balances
- Optimization
- Control (Open-loop, closed-loop)

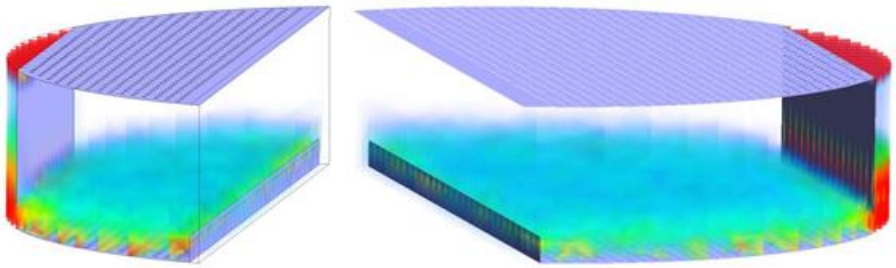
- Operation of the column? Design of the DWC trays? Hydrodynamics?





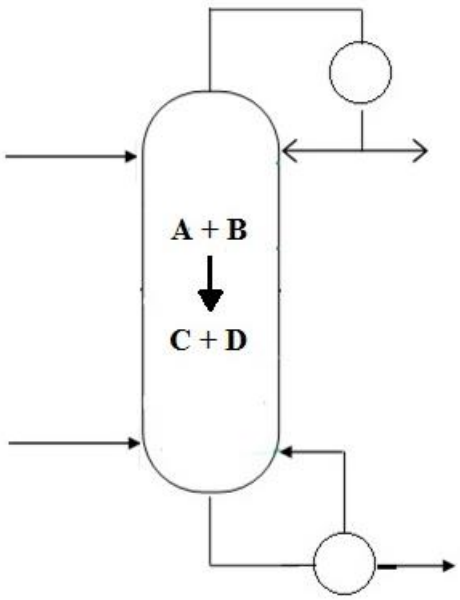






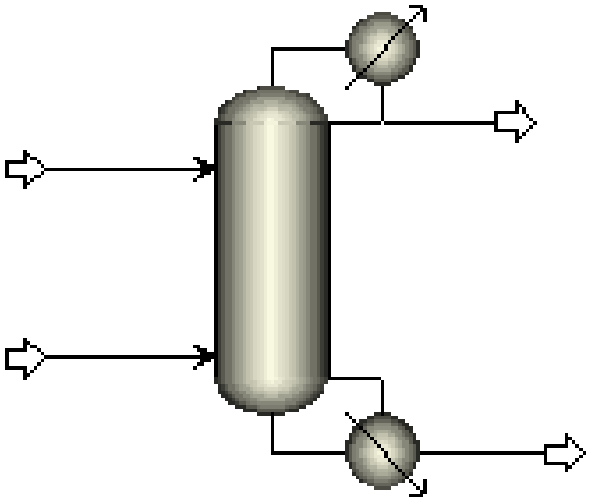
[16] M.A. Rodríguez-Ángeles, F.I. Gómez-Castro, J.G. Segovia-Hernández, A.R. Uribe-Ramírez (2015) Mechanical design and hydrodynamic analysis of sieve trays in a dividing wall column for a hydrocarbon mixture, Chem. Eng. Process., 97, 55.

HIGH-PRESSURE REACTIVE DISTILLATION COLUMN



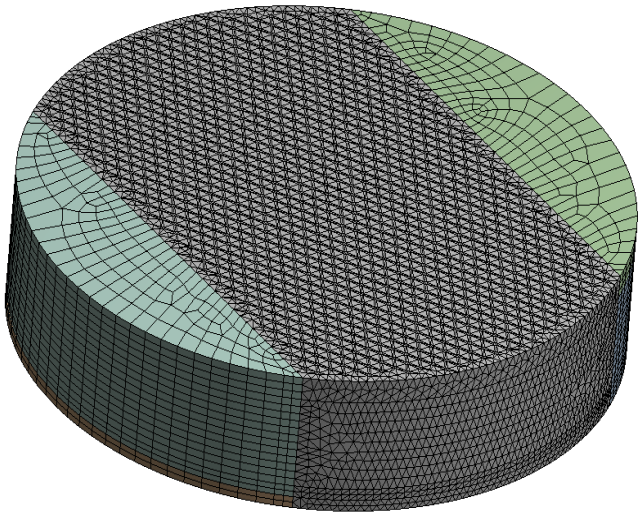
- May overcome equilibrium limitations
- Reduces energy consumption
- Reduces utilities costs
- Reduces number of equipment
- Reduces equipment cost

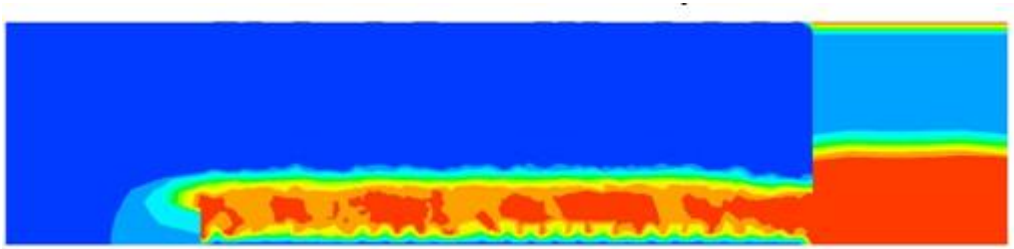
- Analysis in modular simulator…

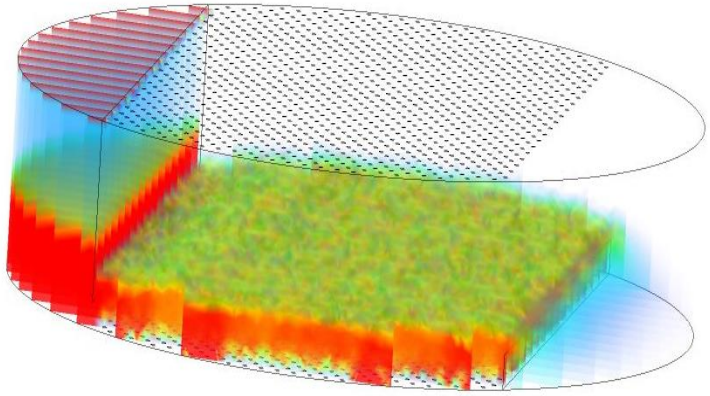


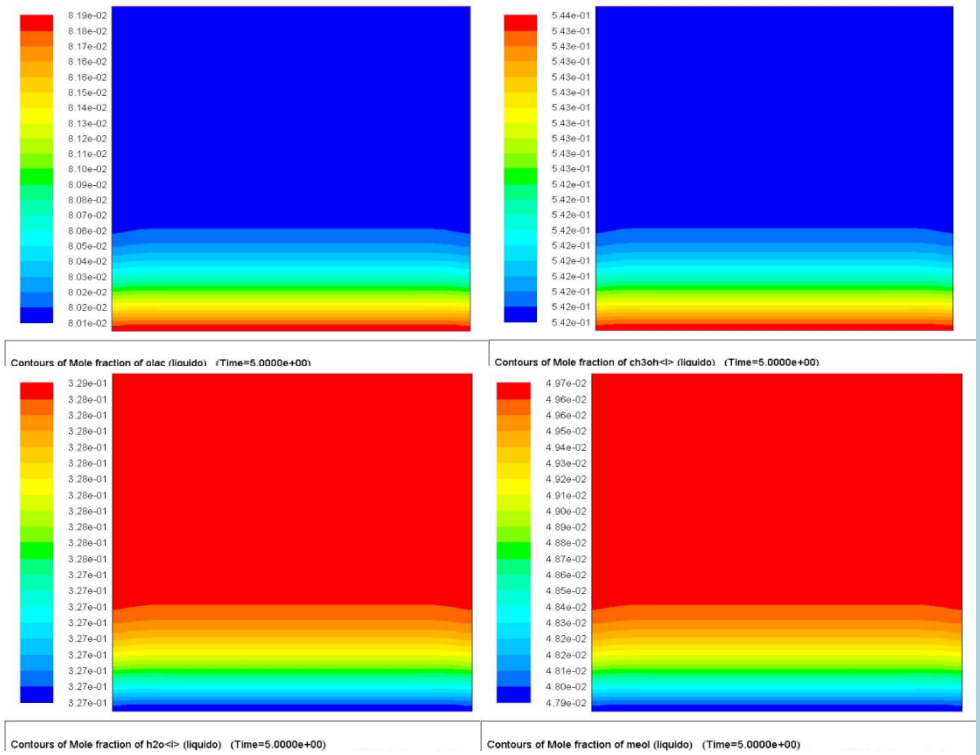
- Preliminary design
- Mass and energy balances
- Optimization

- Design of the RDC trays under the required pressure? Hydrodynamic performance?








8.19e-02
8.18e-02
8.17e-02
8.16e-02
8.16e-02
8.15e-02
8.14e-02
8.13e-02
8.12e-02
8.11e-02
8.10e-02
8.09e-02
8.08e-02
8.07e-02
8.06e-02
8.05e-02
8.04e-02
8.03e-02
8.02e-02
8.02e-02
8.01e-02
Contours of Mole fraction of glac (liquido) (Time=5.0000e+00)
5.44e-01
5.43e-01
5.43e-01
5.43e-01
5.43e-01
5.43e-01
5.43e-01
5.43e-01
5.43e-01
5.43e-01
5.43e-01
5.42e-01
5.42e-01
5.42e-01
5.42e-01
5.42e-01
5.42e-01
5.42e-01
5.42e-01
5.42e-01
5.42e-01
Contours of Mole fraction of ch3oh<l> (liquido) (Time=5.0000e+00)
3.29e-01
3.28e-01
3.28e-01
3.28e-01
3.28e-01
3.28e-01
3.28e-01
3.28e-01
3.28e-01
3.28e-01
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3.27e-01
3.27e-01
3.27e-01
3.27e-01
3.27e-01
3.27e-01
3.27e-01
3.27e-01
Contours of Mole fraction of h2o<l> (liquido) (Time=5.0000e+00)
4.97e-02
4.96e-02
4.96e-02
4.95e-02
4.94e-02
4.93e-02
4.92e-02
4.91e-02
4.90e-02
4.89e-02
4.88e-02
4.87e-02
4.86e-02
4.85e-02
4.84e-02
4.83e-02
4.82e-02
4.82e-02
4.81e-02
4.80e-02
4.79e-02
Contours of Mole fraction of meol (liquido) (Time=5.0000e+00)

CONCLUDING REMARKS

- Computer-aided methods are nowadays a helpful tool for the design of separation processes.
- A combined design strategy using modular simulators and CFD-based simulators has been proposed.
- Such approach is helpful specially when designing non-conventional separation processes.
- Experimental validation is still required, mainly for the mass transfer correlations.

ACKNOWLEDGMENTS

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- I.Q. Mayra Margarita May-Vázquez





THANK YOU

