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

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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.\textsuperscript{[1]}

\textsuperscript{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
- Crystallization
- Pervaporation
DISTILLATION

✓ Is one of the most used separation processes.

✓ Separates liquid mixtures

✓ Mature technology

✗ Low thermodynamic efficiency
Distillation is used since the ancient ages, but...

...it was more an art than a science

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

E.W. Thiele

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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
Fenske-Underwood-Gilliland-Kirkbride method

Fenske equation (1932)\(^8\)

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

Underwood equations (1946)\(^9\)

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

Gilliland correlation (1940)\(^10\)

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

\[
X = \frac{R - R_{\text{min}}}{R + 1}
\]

\[
F = \frac{N - N_{\text{min}}}{N + 1}
\]

Kirkbride equation (1944)\(^11\)

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

The equilibrium model: MESH equations

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

\[ \text{Mass balances (M)} \]
\[ \text{Equilibrium equations (E)} \]
\[ \text{Summation equations (S)} \]
\[ \text{Energy balances (H)} \]

\[ \text{J.R. Friday, B.D. Smith (1964) An analysis of the equilibrium stage separations problem – formulation and convergence, AIChE J., 10(5), 698.} \]
The rate-based model: MERSQH equations

Mass balances (M)  Summation equations (S)
Energy balances (E)  Hydraulic equations (H)
Rate equations (R)  Equilibrium equations (Q)

Modular process simulators
Computational fluid dynamics (CFD)

\[ \frac{\partial}{\partial t} (\alpha_q \rho_q v_q) + \nabla \cdot (\alpha_q \rho_q \tilde{v}_q) = \sum_{p=1}^{n} (m_{pq} - m_{qp}) + S_q \]

\[ \frac{\partial}{\partial t} (\alpha_q \rho_q \tilde{v}_q) + \nabla \cdot (\alpha_q \rho_q \tilde{v}_q \tilde{v}_q) = -\alpha_q \nabla p + \nabla \cdot \tau_q + \alpha_q \rho_q g + \sum_{p=1}^{n} (\bar{R}_{pq} + m_{pq} \tilde{v}_q - m_{qp} \tilde{v}_q) + (\bar{F}_q + \bar{F}_{lift,q} + \bar{F}_{vm,q}) \]

\[ \frac{\partial}{\partial t} (\alpha_q \rho_q h_q) + \nabla \cdot (\alpha_q \rho_q \tilde{u}_q h_q) = -\alpha_q \frac{\partial p_q}{\partial t} + \tau_q : \nabla \tilde{u}_q - \nabla \cdot \tilde{q}_q + S_q + \sum_{p=1}^{n} (\bar{Q}_{pq} + m_{pq} h_q - m_{qp} h_q) \]
DESIGN PROCEDURE

Initial design in modular simulator (R-B) → Optimization → Mechanical design and CFD analysis
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?
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?
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.
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