Separation Science and Technology Education: Chemical Engineering Perspective

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Separation Science and Technology as a Convergence Platform for SusChEM
San Francisco, CA

Outline

1. Separations in Chemical Engineering: Multi-scale perspective
2. Challenges in Undergraduate Education
3. Graduate Education

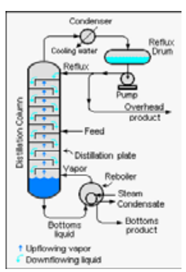
1. Separations in Chemical Engineering: Multi-scale Perspective

Separations in Chemical Engineering

Grams

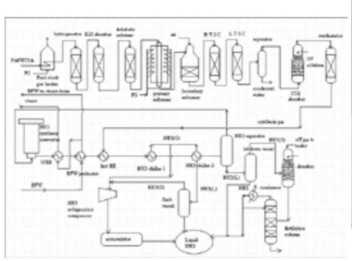
Separation science (molecular level)

Equilibrium	Kinetics



Unit operation (process level)

Mass balance	Heat balance

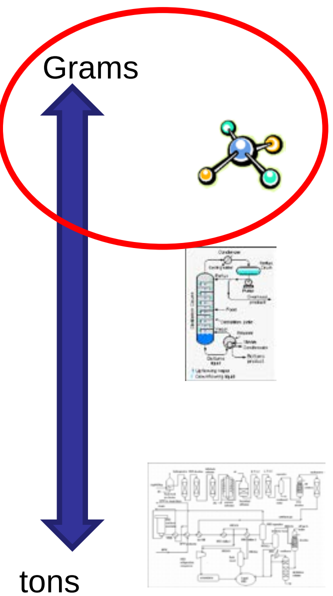


Separation process system (plant level)

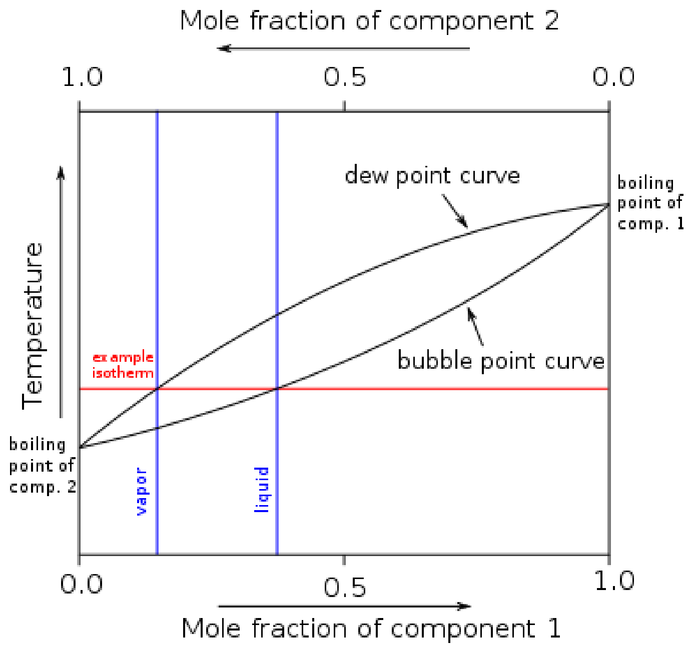
Integration with other operations	Control

tons

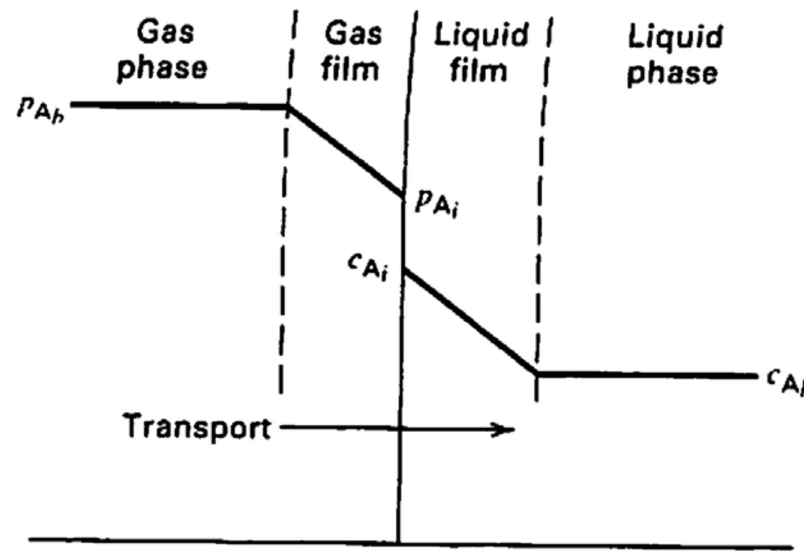
Separation science



Equilibria



Mass transfer

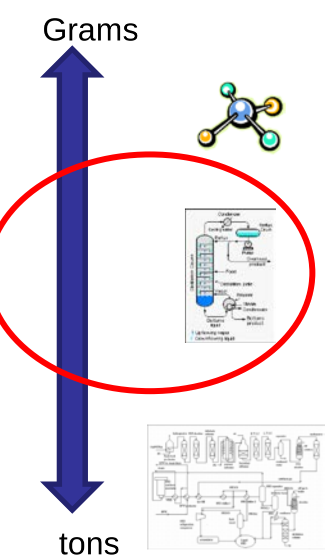


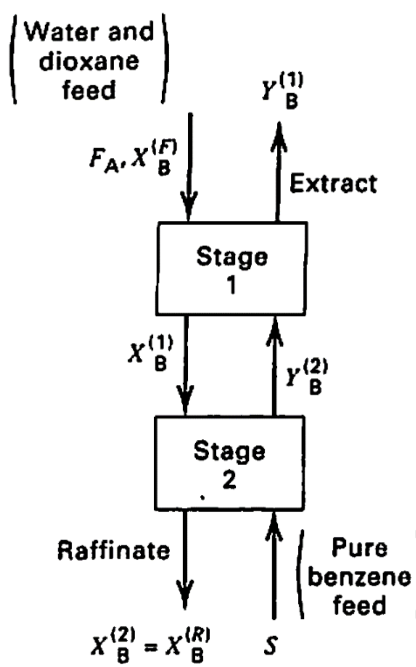
Materials

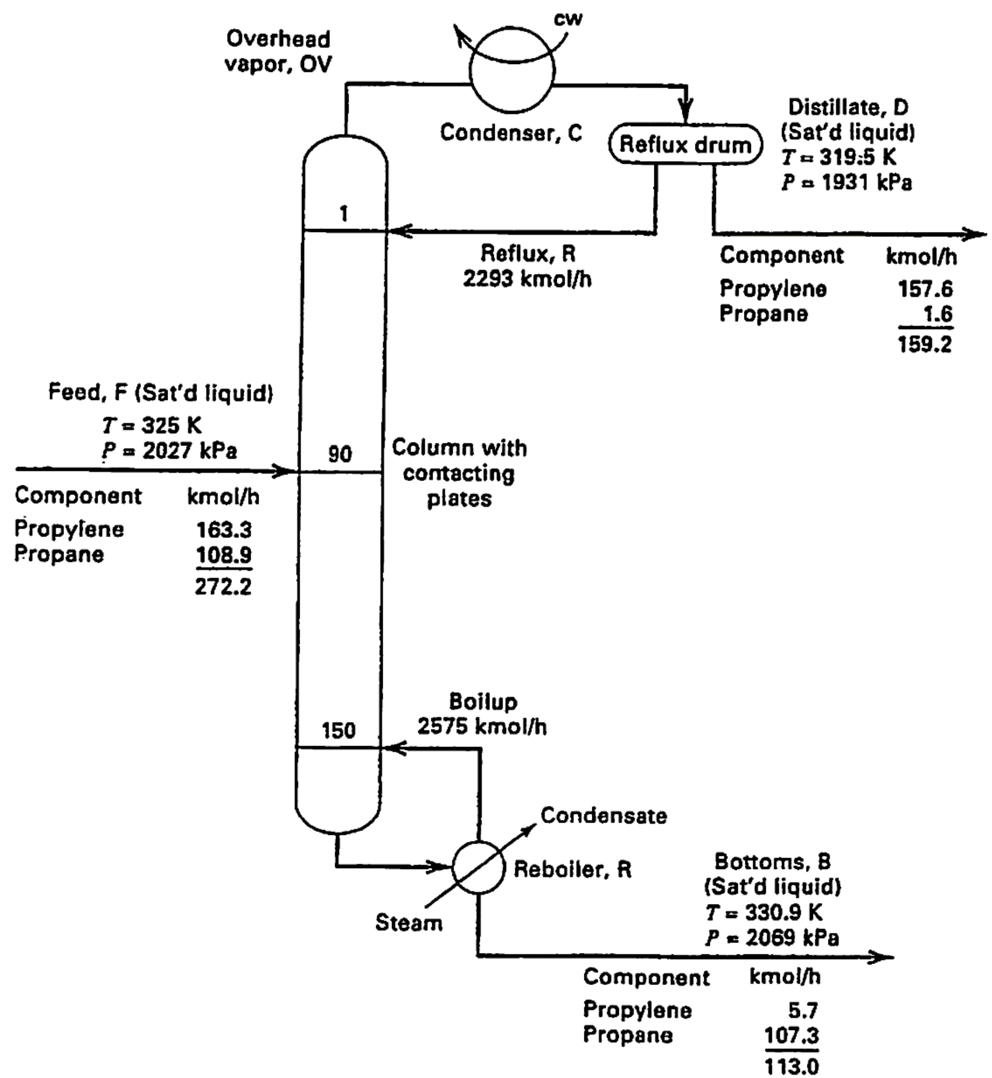
Seader and Henley, 2006

Separation processes

Unit design:
Determine unit size (capital cost) and utility requirements







Seader and Henley, 2006

Separation process system synthesis

Example 1: Separation process sequence

Distillation column sequence to separate multiple components

Membrane cascade to increase recovery

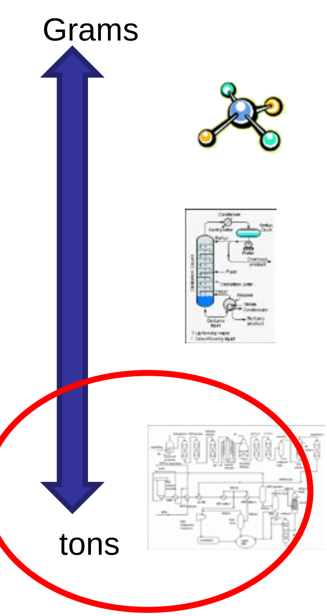
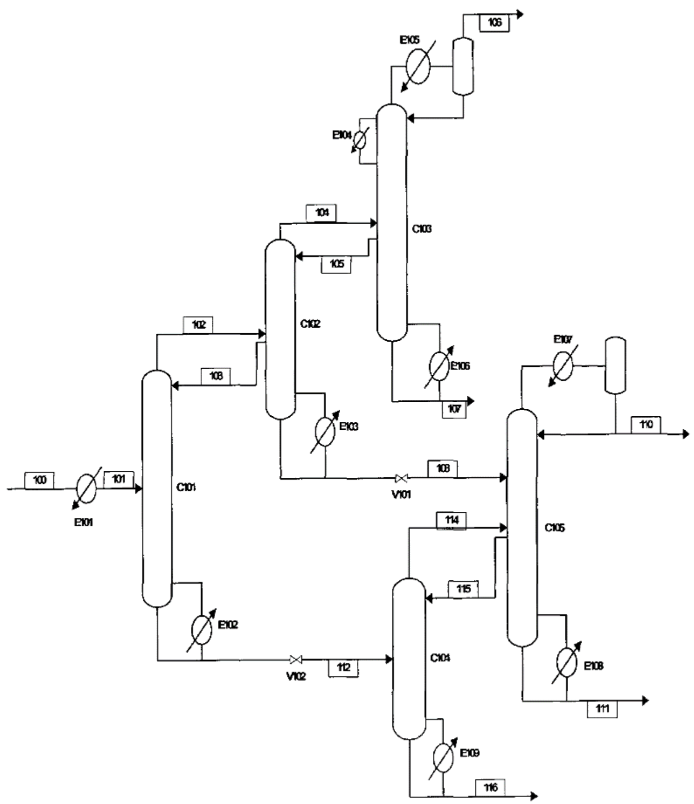
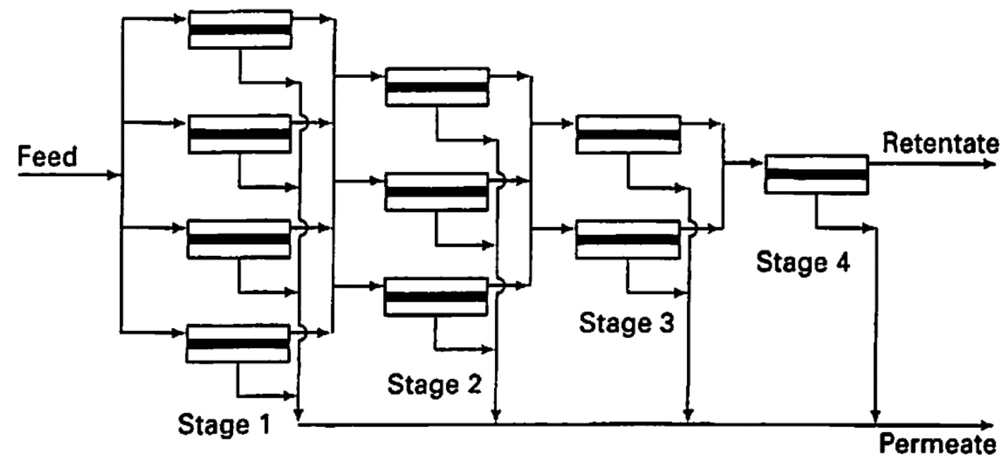


FIGURE 1



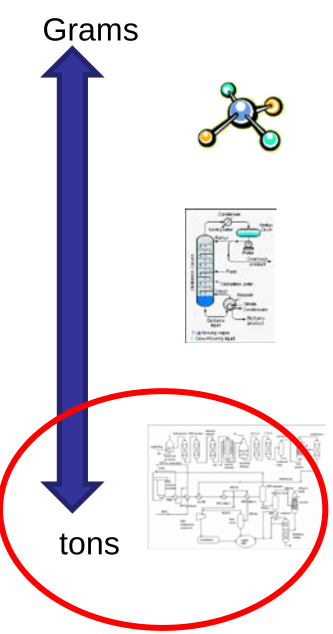


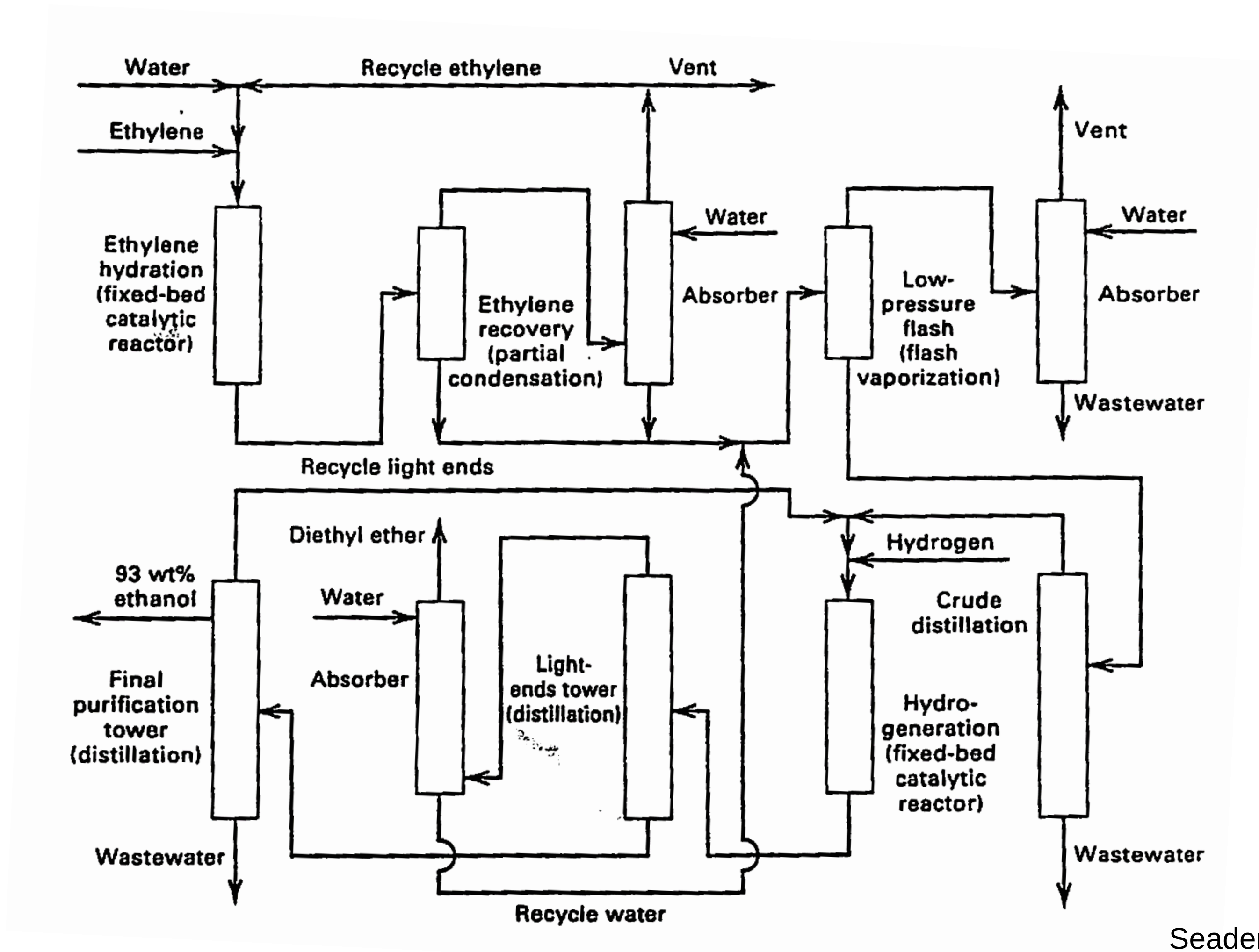
Reyneke et al. US 7311813 B2

Separation process system synthesis (continued)

Example 2: Ethylene hydration to produce ethanol

- 2 reactors
- 7 separation units (3 absorbers, 3 distillation columns, 1 flash)

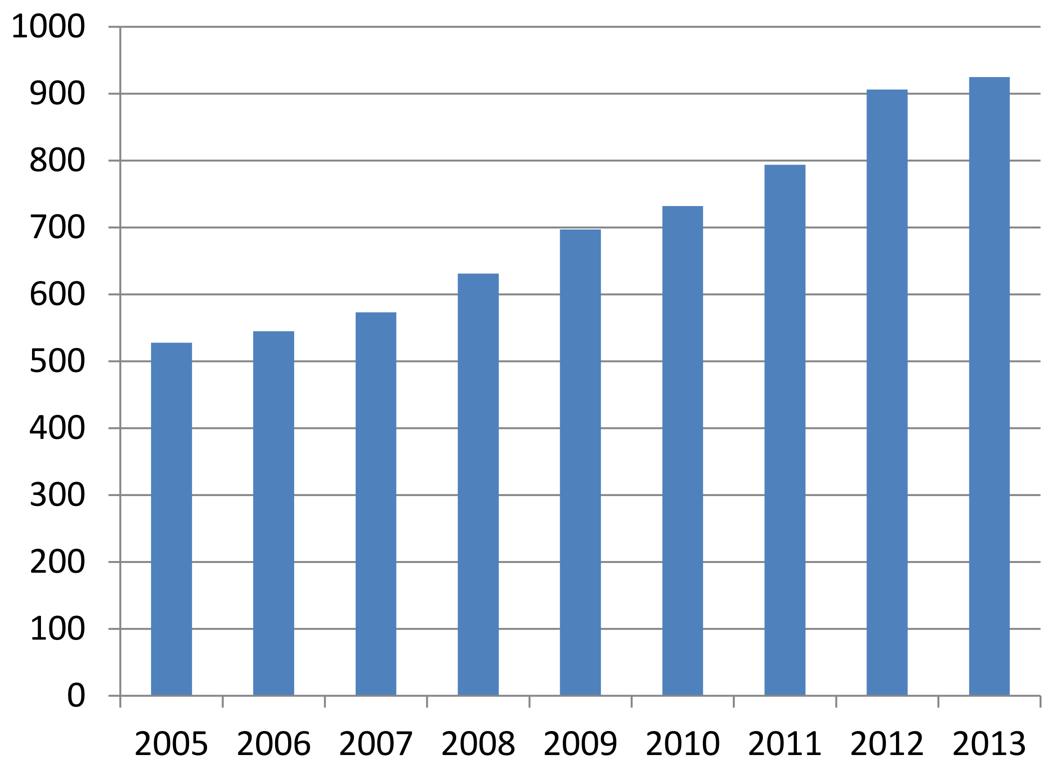




Seader and Henley, 2006

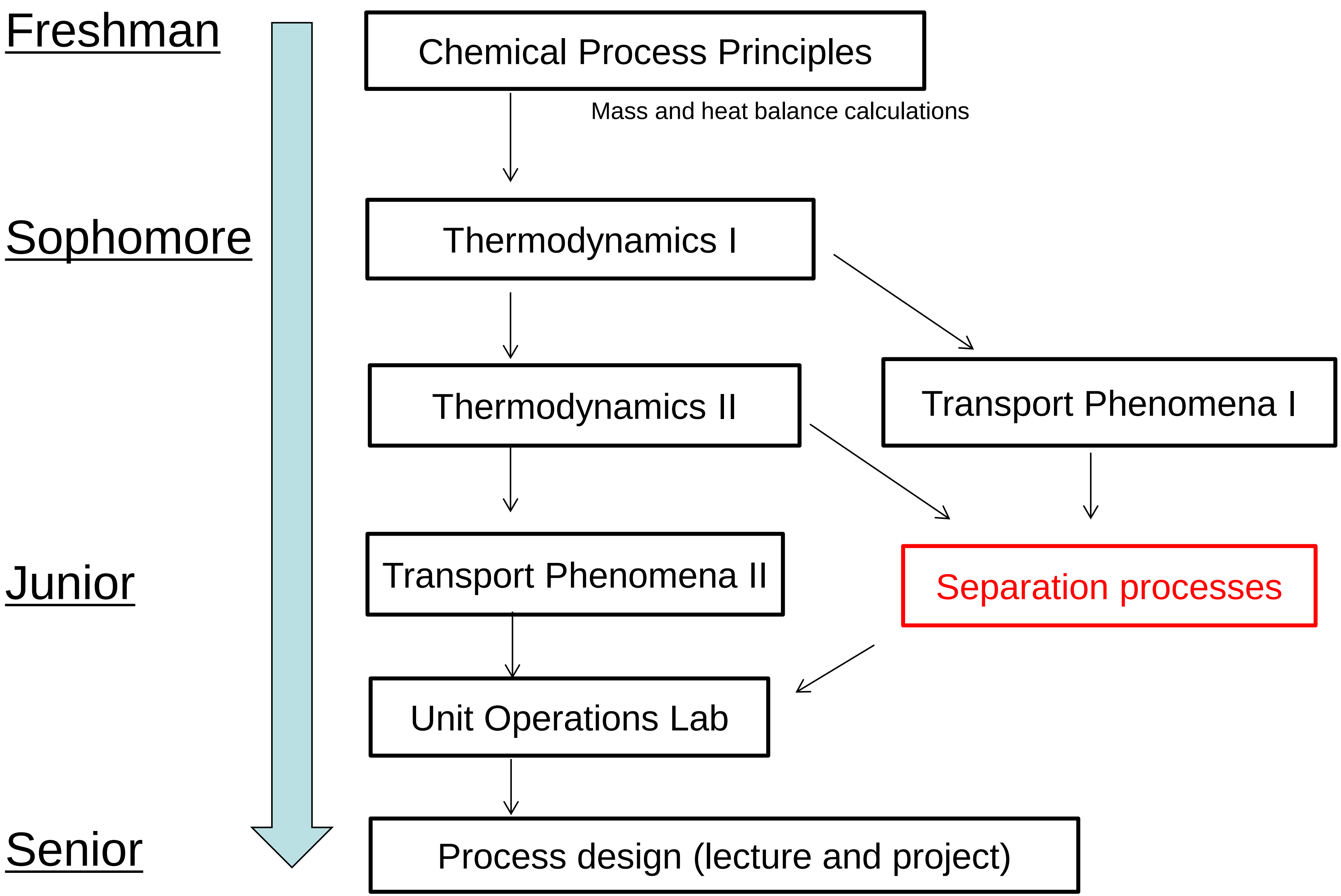
2. Undergraduate education

Enrollment in Chemical & Biomolecular Engineering at Georgia Tech

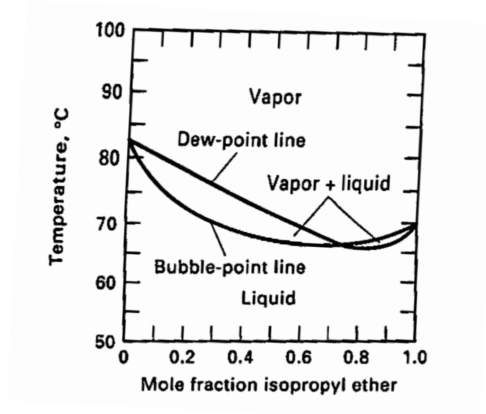


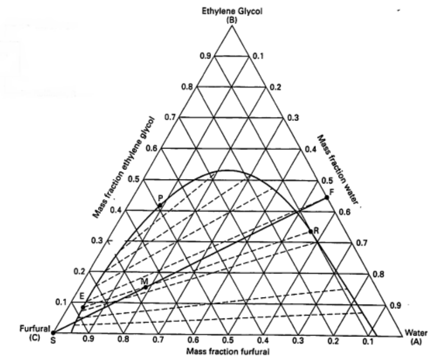
Popularity for energy and sustainability: Class size increasing

Curriculum at Georgia Tech: Courses related directly to separations



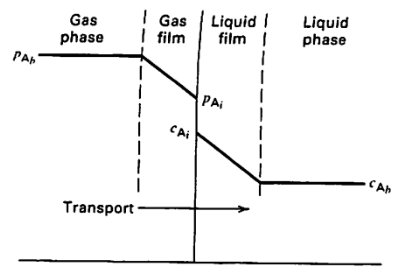
Topics in undergraduate separation course





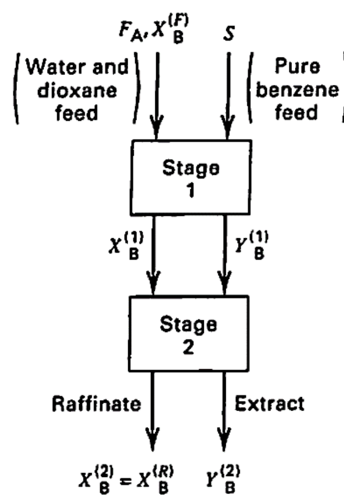
Equilibrium

- Vapor-liquid
- Liquid-liquid



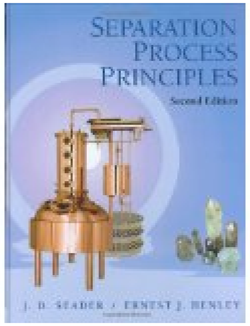
Kinetics

- Mass transfer
- Diffusion



Unit design and operation

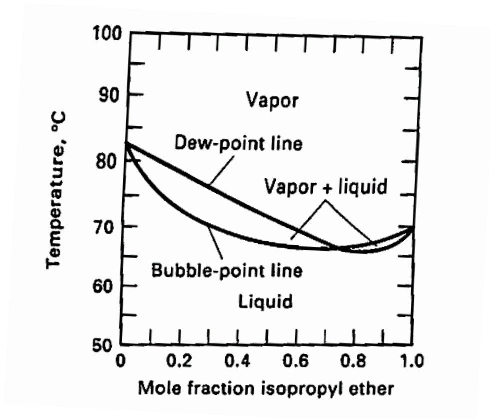
- Single stage vs. multi-stage
- Co-current vs. counter-current
- Continuous vs. batch



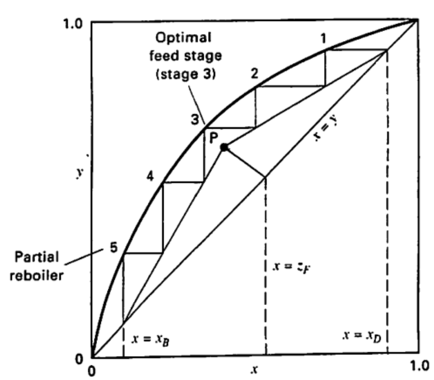
Seader and Henley, 2006

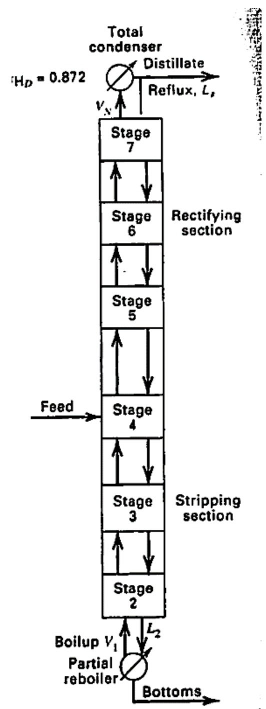
From physical properties to separation process design
Example: distillation column

Vapor-liquid equilibrium

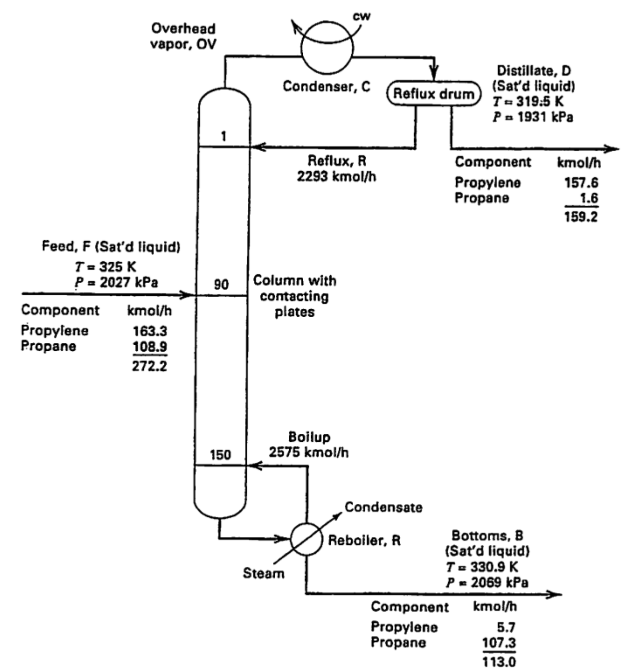


Stage calculations





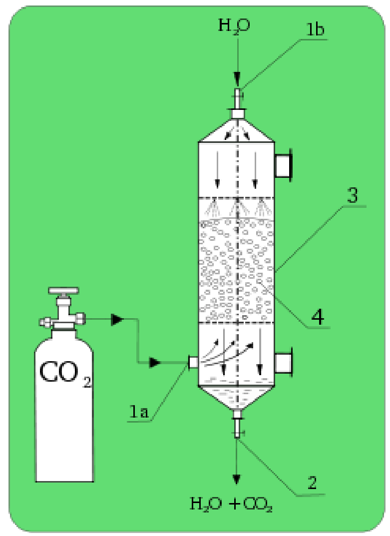
Mass balance and unit design



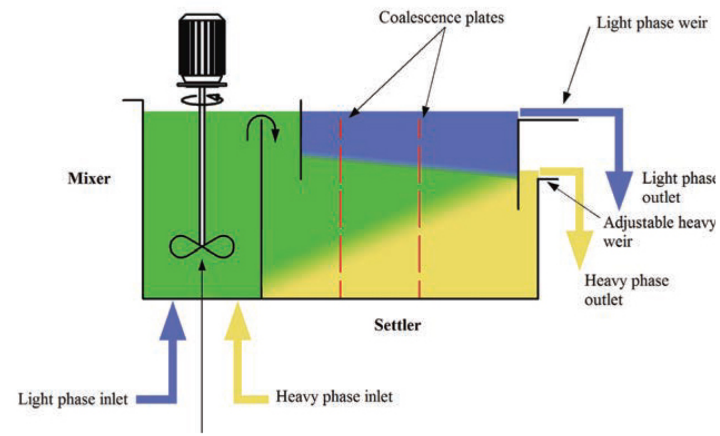
Separation techniques covered in undergraduate course

Distillation

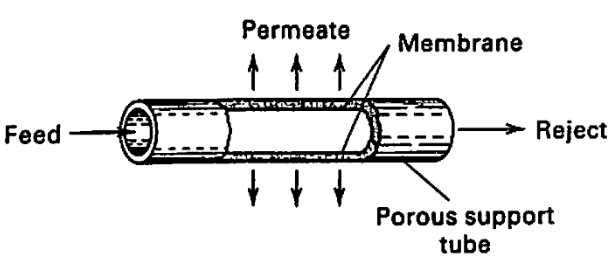
Absorption



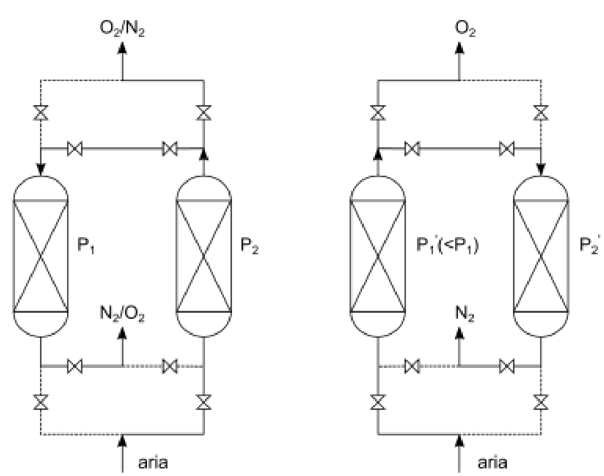
Extraction



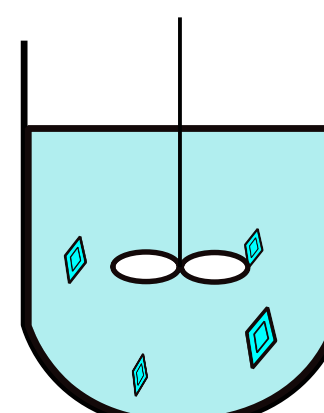
Membrane (liquid and gas)



Adsorption and ion exchange



Crystallization

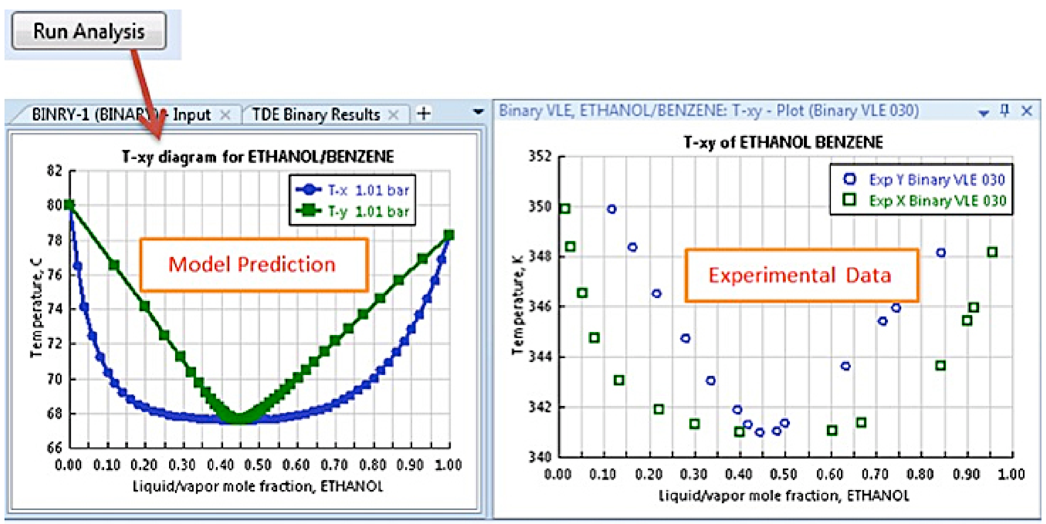


www.wikipedia.com

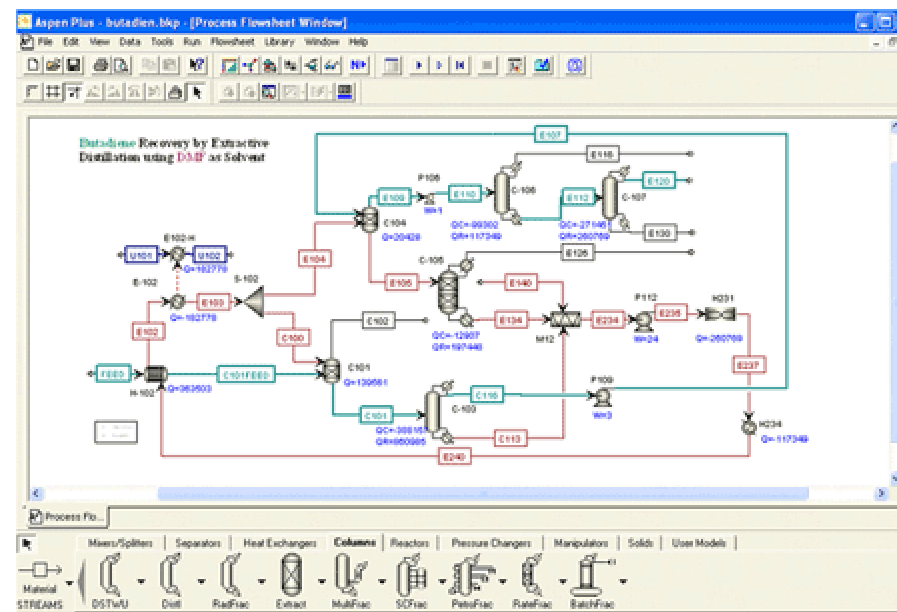
Computer-aided engineering in separations

Students use Aspen Plus® from sophomore until senior in multiple courses

Physical property database



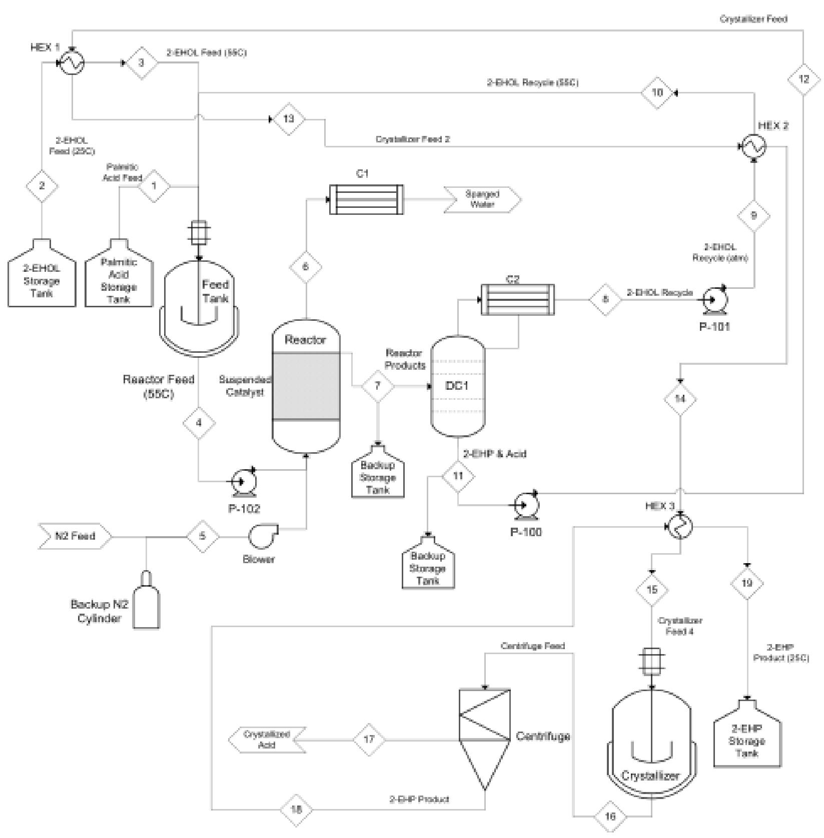
Process flowsheet



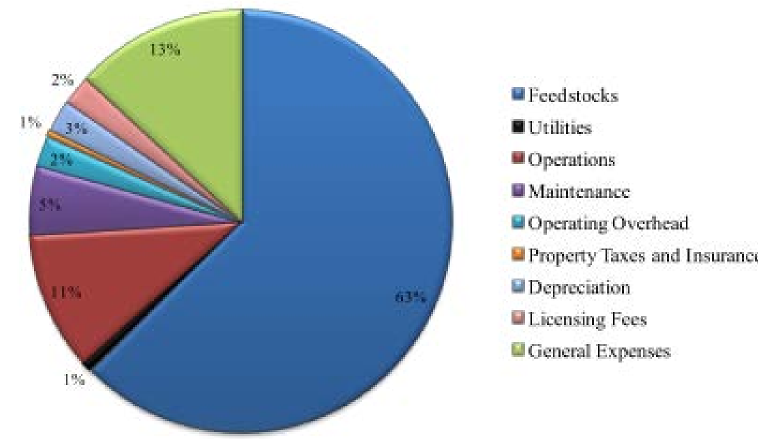
Covers most traditional chemicals (commodity chemicals)

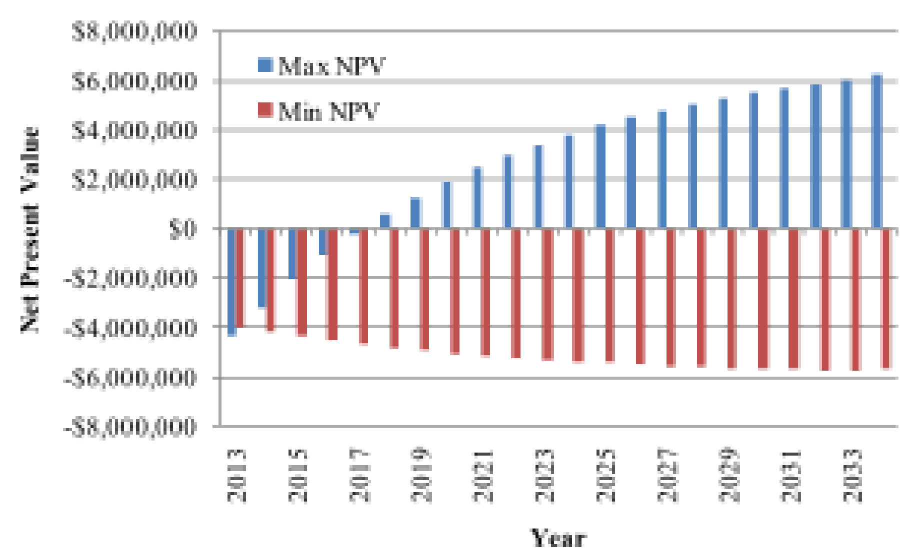
Capstone senior process design project

Process flow diagram
(from raw material to final product)



Process economics: cost and profitability





Industry involvement in capstone design course

Past sponsors include:

Sponsors are involved in this course through:

- Project problem development
- Guest lectures
- Evaluation of oral presentations
- Recruiting

We are currently looking for sponsor for 2015!

Introducing energy and sustainability in process design project

Algal biofuel processes

Sponsors

ALGENOL BIOFUELS
Cleaner - Greener - Cheaper

Chevron Human Energy

Life-cycle assessment for production of cosmetic esters

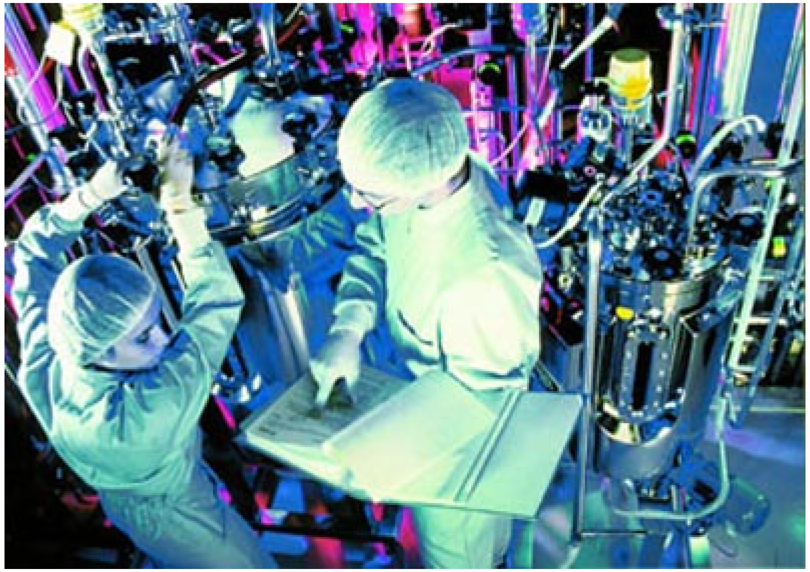
Sponsor

EASTMAN

http://www.solidworks.com/

Separations for biological and biochemical products

Same separation techniques as in traditional chemicals:
Chromatography (adsorption), membrane, centrifugation, etc.



Lack of

- Product information
- Property database
- Public information of process flow

www.novasep.com

www.pharmaceuticaltechnology.com

3. Graduate education

Graduate courses related separations

Chemical Engineering Core Courses (mandatory for 1st year graduate students)

- Chemical Process Safety
- Chemical Engineering Thermodynamics
- Transport Phenomena
- Mass Transfer
- Kinetics and Reactor Design
- Mathematical Modeling of Chemical Processes
- Chemical Engineering Elective

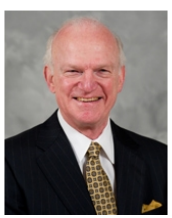
No “Separation” course!
Courses related closely to separations are in red

Separation faculty in Chemical Engineering at Georgia Tech

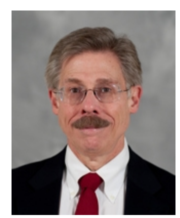
Sankar Nair
Nanoporous materials for adsorption and membrane

Christopher Jones:
Carbon capture adsorption materials

Krista Walton
Metal organic framework, adsoption



Ronald Rousseau
Crystallization



William Koros
Membranes

Charles Eckert:
Supercritical separations

Yoshiaki Kawajiri
Chromatography, adsorption

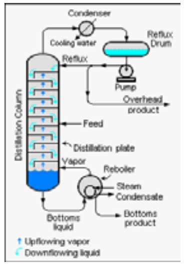
Amyn Teja
Thermodynamics

Ryan Lively
Membrane
hollow fiber adsorbent

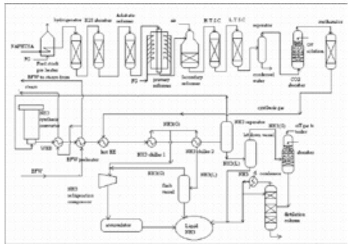
Graduate research programs in US

Grams

Current focus in most research programs in the US, heavily on materials



Smaller number of research programs in US



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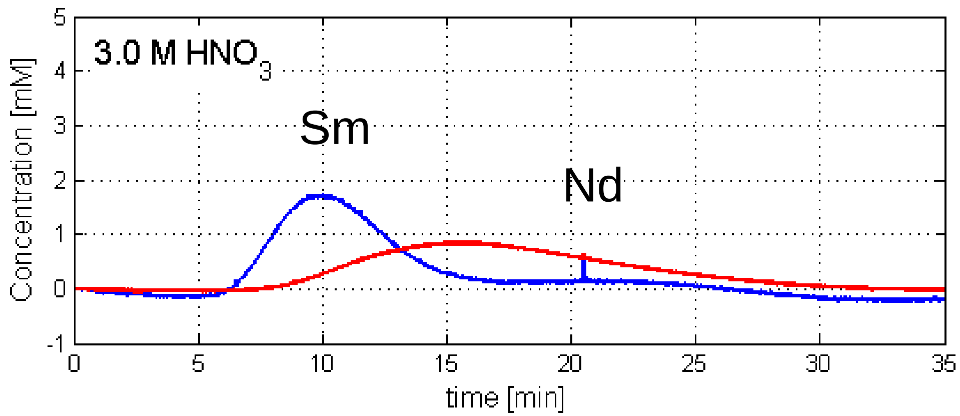
Process-level research example: Multi-column chromatography

Collaborators: David Hobbs (Savannah River National Laboratory)
Tatsuya Suzuki (Nagaoka University of Technology, Japan)

Chromatogram of lanthanides



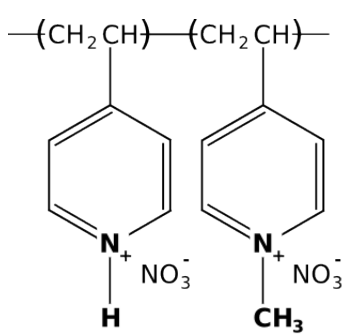
Mathematical model

$$(1-\varepsilon_b)\frac{\partial q_i}{\partial t} = k_{a,i}(C_i - C_i^{eq})$$

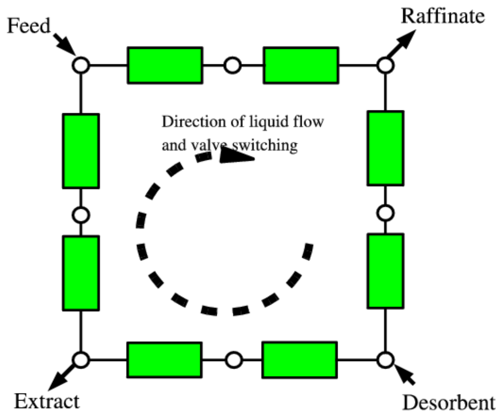
$$\varepsilon_b \frac{\partial C_i}{\partial t} + (1-\varepsilon_b)\frac{\partial q_i}{\partial t} + u\frac{\partial C_i}{\partial x} = 0$$

$$q_i = k_{D,i} C_i^{eq}$$

Tertiary pyridine resin



Simulated moving bed chromatography

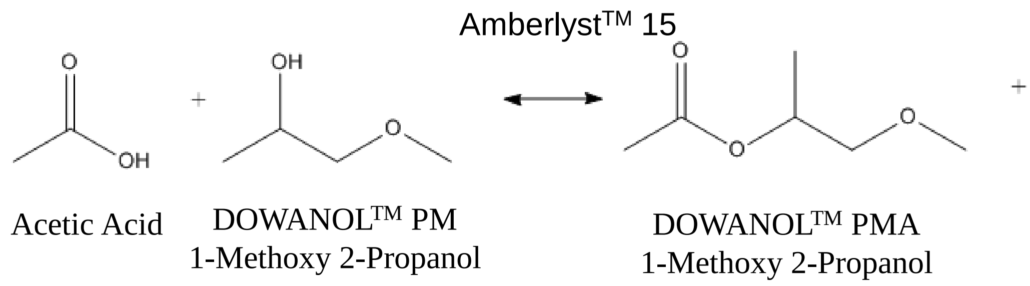


Sreedhar, Hobbs, Kawajiri, Separation and Purification Technology, in press
Sreedhar, Suzuki, Hobbs, Kawajiri, Journal of Separation Science, in press

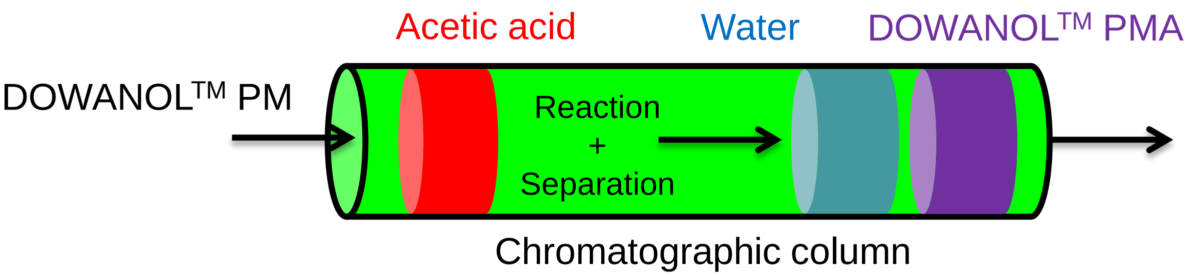
Industrial collaboration for process engineering

Dow University Partnership Program

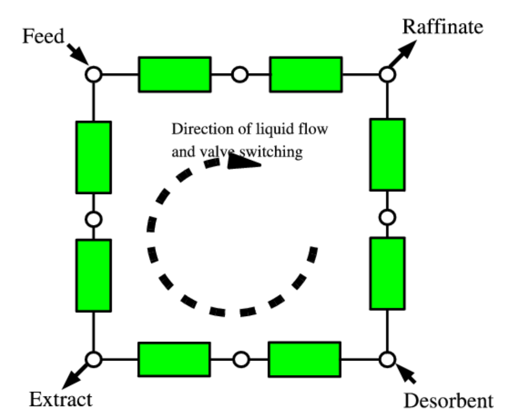
Production of Dowanol™ PMA



Reaction in a chromatographic column



Multi-column continuous reactive chromatographic separation



Agrawal, Oh, Sreedhar, Donaldson, Frank, Shultz, Bommarius, Kawajiri, Journal of chromatography A (in press).
Oh, Agrawal, Sreedhar, Donaldson, Shultz, Frank, Bommarius, Kawajiri, Chemical Engineering Journal (in press).

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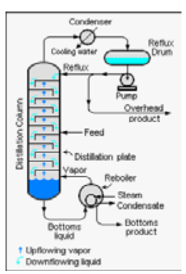

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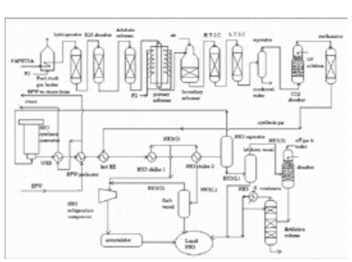

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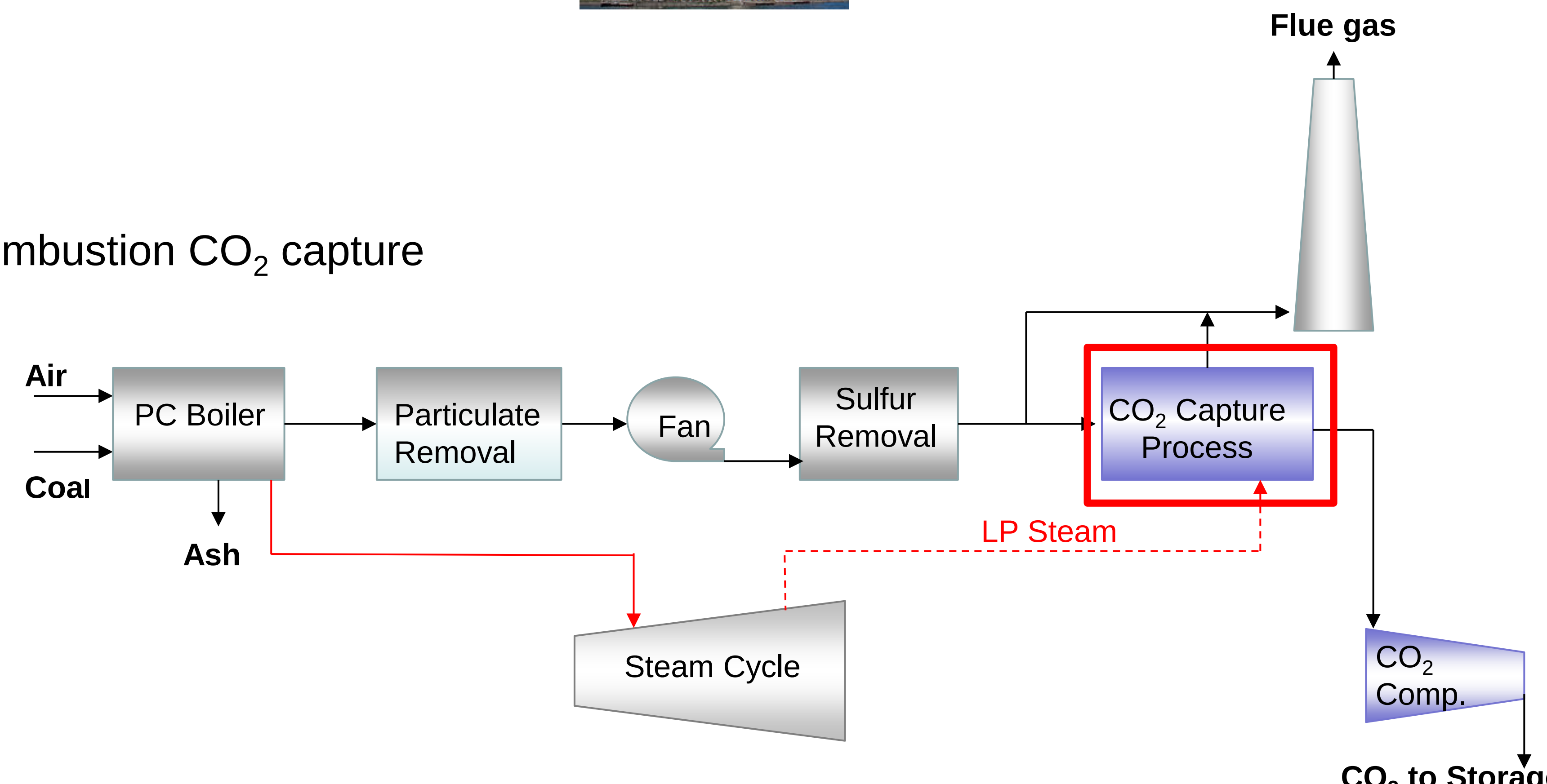
Graduate research project example
CO_2 capture from flue gas in coal-fired power plant

Post-combustion CO_2 capture

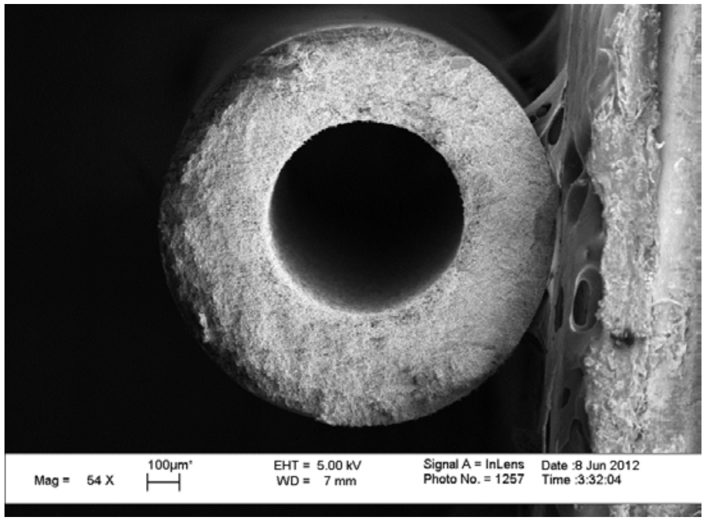


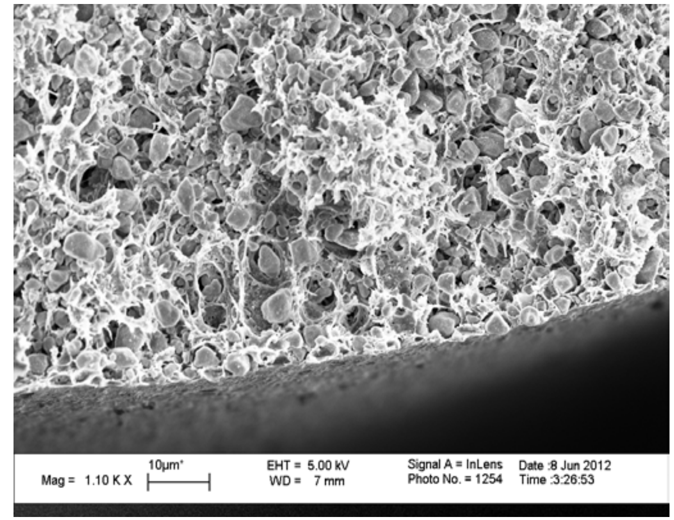
Target by NETL:

CO_2 recovery ≥ 90%

Increase in cost of electricity ≤ 35%

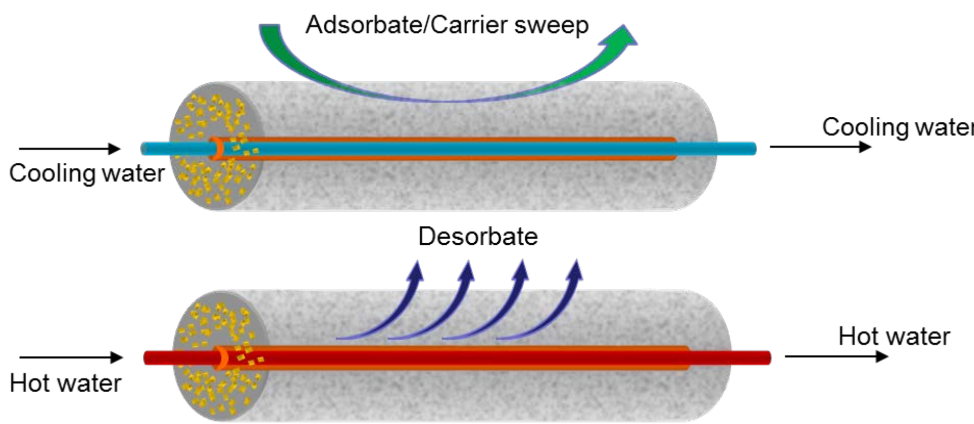
Collaborative research: CO_2 capture by hollow fiber adsorbent material



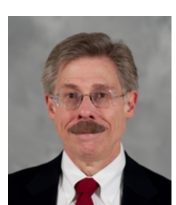


CO_2 adsorption

CO_2 desorption



Christopher Jones



William Koros

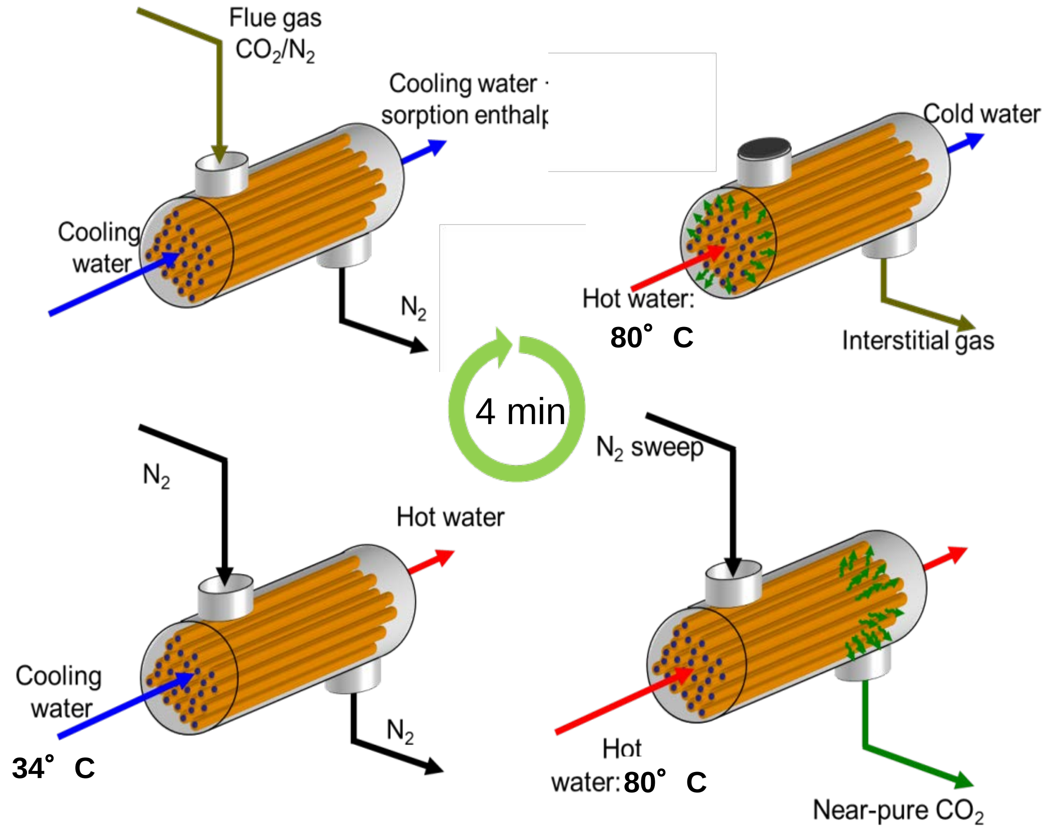
Ryan Lively

Matthew Realff

Yoshiaki Kawajiri

Development of separation process

Rapid temperature swing adsorption process



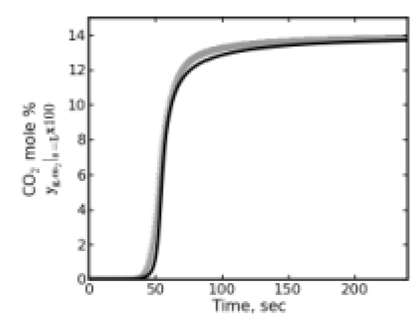
Mathematical models to design process and operation

$$\rho_f C_{pf}\frac{\partial T_f}{\partial t} - \frac{\lambda_f}{(1-\varepsilon_f)}\left(\frac{\partial^2 T_f}{\partial r^2}+\frac{1}{r}\frac{\partial T_f}{\partial r}+\frac{\partial^2 T_f}{\partial z^2}\right) = \rho_f \Delta H_{ads}\frac{\partial q_i}{\partial t}$$

$$\rho_w C_{pw}\frac{\partial T_w}{\partial t} + \rho_w C_{pw} u_w \frac{\partial T_w}{\partial z} = A_I h_w \left(T_w - T_f|_{r=r_{ID}}\right)$$

$$\rho_g C_{pg}\frac{\partial T_g}{\partial t} + \rho_g C_{pg} u_g \frac{\partial T_g}{\partial z} = A_O h_g \left(T_f|_{r=r_{OD}} - T_g\right)$$

Model validation with experiments

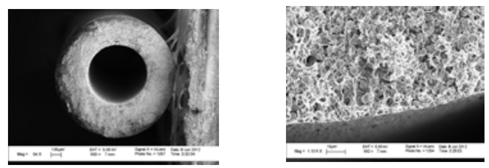


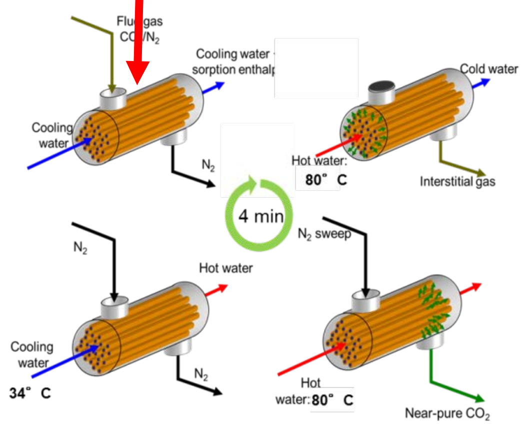
Rezaei, Swernath, Kalyanaraman, Lively, Kawajiri, Realff: Chemical Engineering Science 2014, 113, 62-76
Kalyanaraman, Fan, Lively, Koros, Jones, Realff, Kawajiri, Chemical Engineering Journal, in press

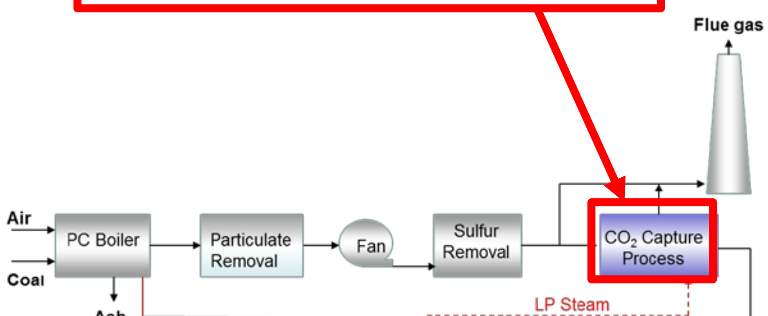
From molecular level to plant level

Grams

tons







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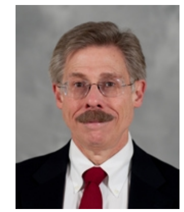
Jones


Koros


Lively


Kawajiri


Realff

Development of separation material

Separation process modeling and design

Process integration, technoeconomic evaluation

Summary

1. Separations in chemical engineering covers multiple scales

2. Challenges in undergraduate education includes:
    - Enrollment keeps incrasing
    - Integration with sustainability and energy topics
    - Computer aided design
    - Biological and biochemical processes

3. Challenges in graduate education includes
    - Few process-level and plant-level research projects
    - Collaborations with industry
    - Multi-scale collaborative research

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