Intensification Concepts for Gas-to-Liquids Processes

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The University of Texas at Austin

NSF Workshop on Process Intensification

Washington, DC,

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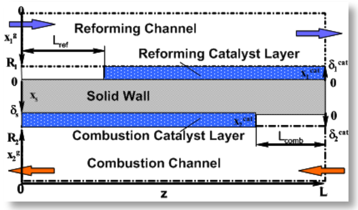
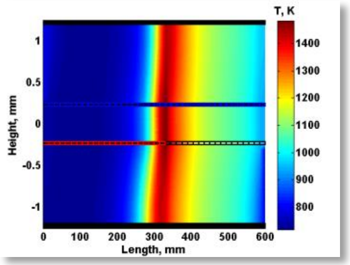
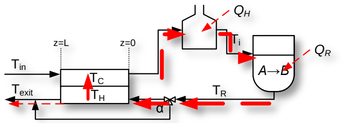






Distributed Natural Resources

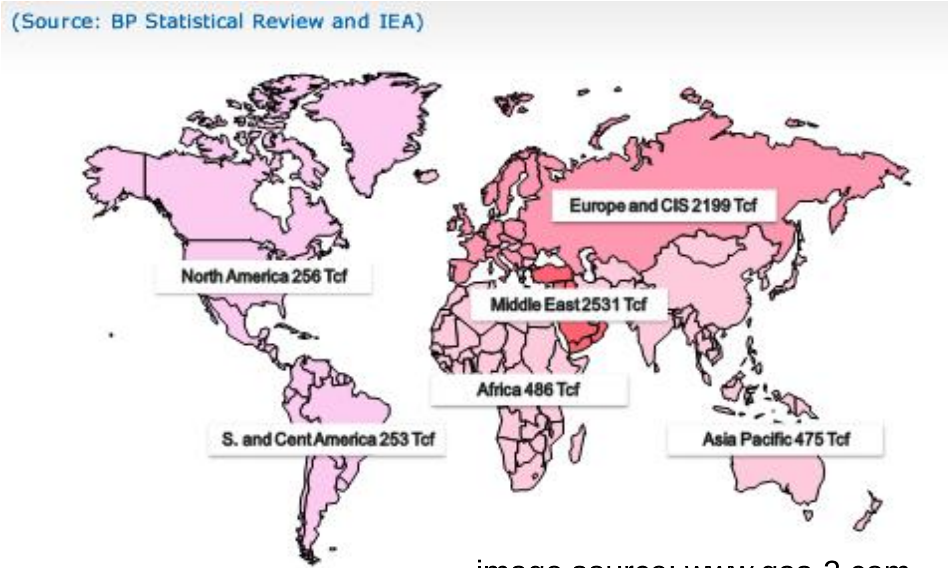


image source: www.gas-2.com

image source: www.gereports.com

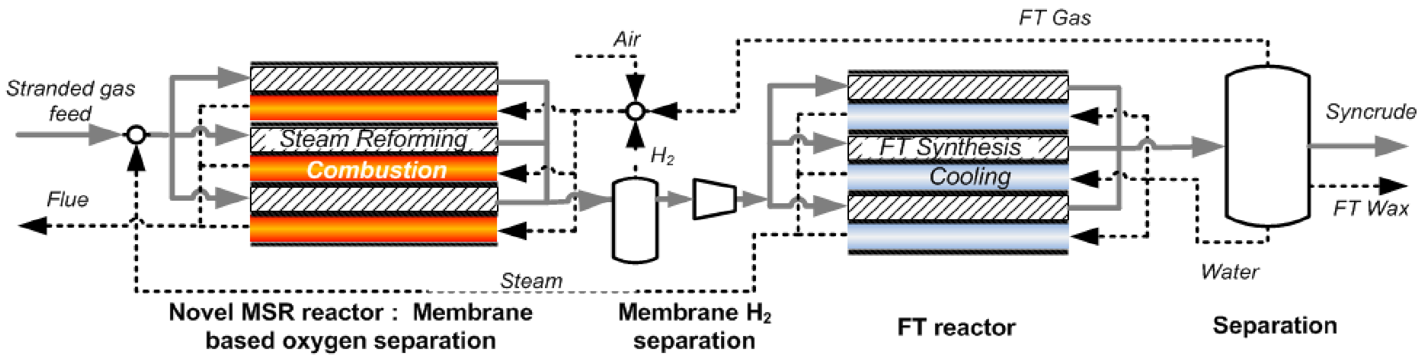
- **Stranded gas**: Small remote deposits that are too difficult and/or expensive to extract
- 7000 tcf worldwide

- **Associated gas:** flared or reinjected
- 4.5 trillion megajoules wasted in 2011

Monetization: conversion to liquids, GTL technologies (Fischer-Tropsch, liquefaction): poor scale-down

Develop new flexible processing capacity at small scales

Application: Small, Modular GTL Systems

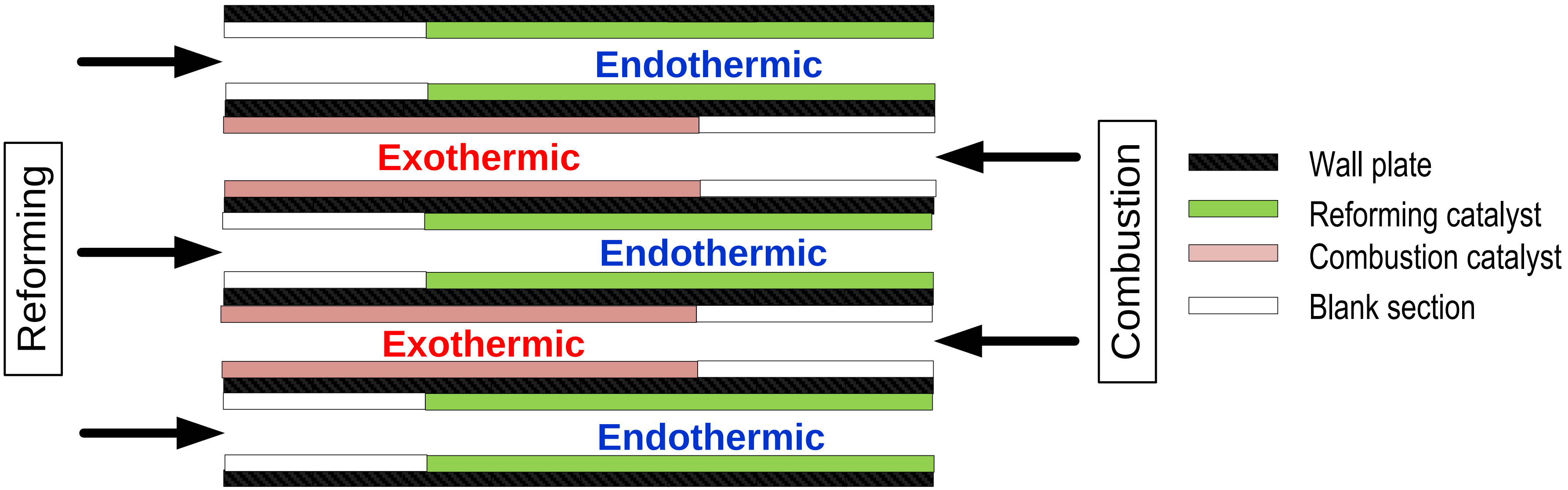


Specific challenges

- **water management:** scarce, location-dependent resource; steam needed/generated at multiple pressures
- **hydrogen management:** reforming product H_2:CO ratio is not optimal for FT synthesis: separation or high recycling?
- **process control**

Not a "chemical integrated circuit"

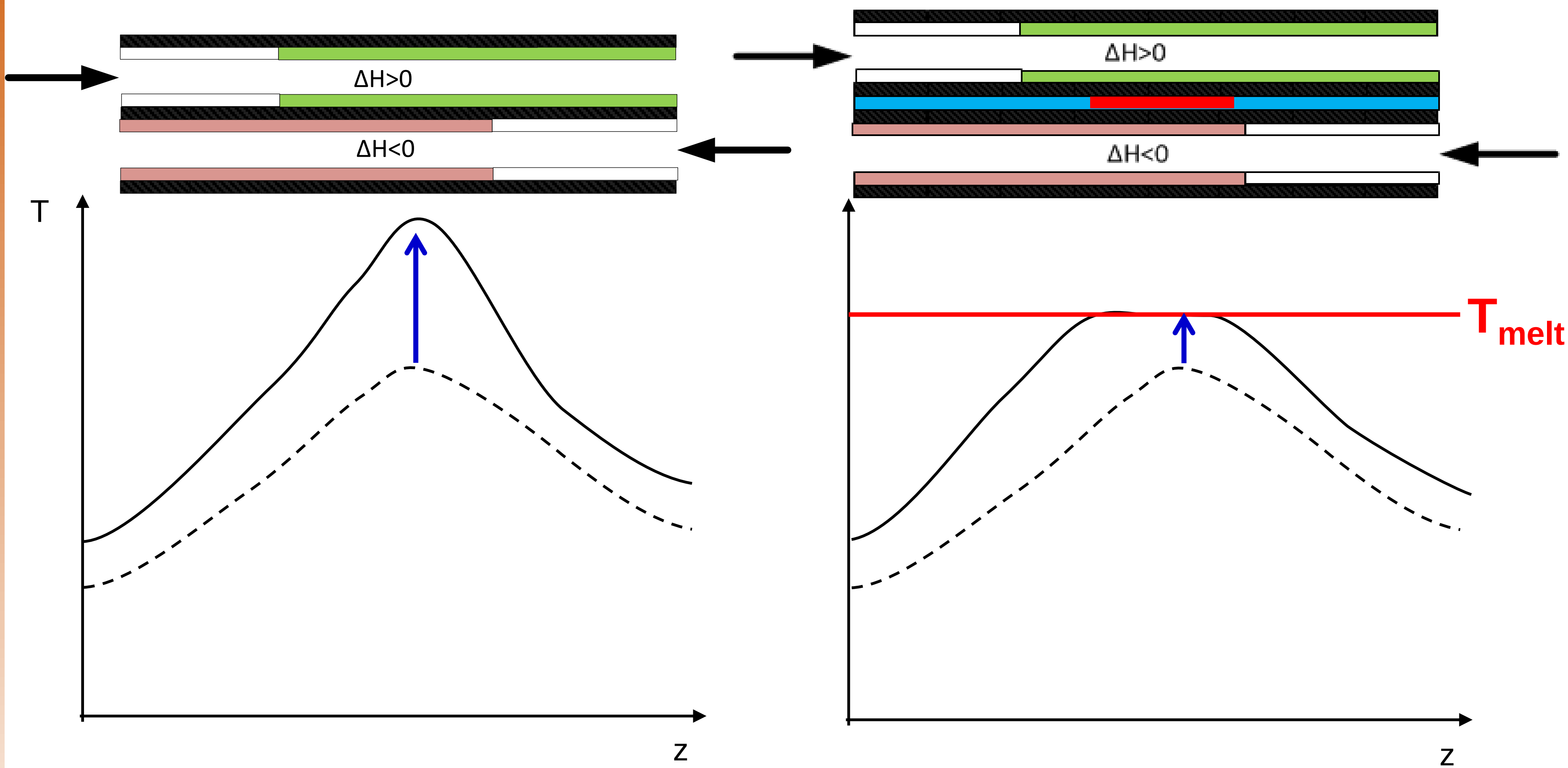
Robust Autothermal Microchannel Reactors



- Single integrated physical device has fewer “control handles”
- Millimeter thick channels make measurement and actuation difficult
- Match heat generation and consumption: offset catalyst layers

Process intensification: difficult control

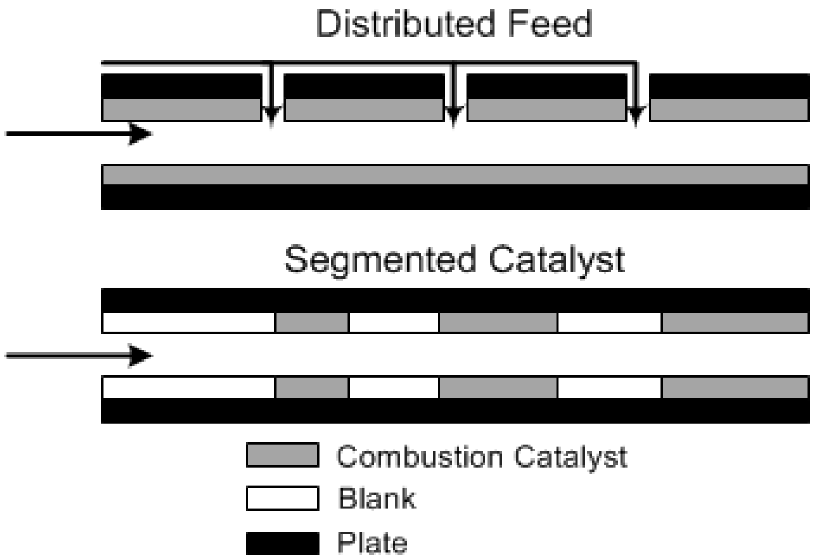
Temperature Control with Phase Change Material

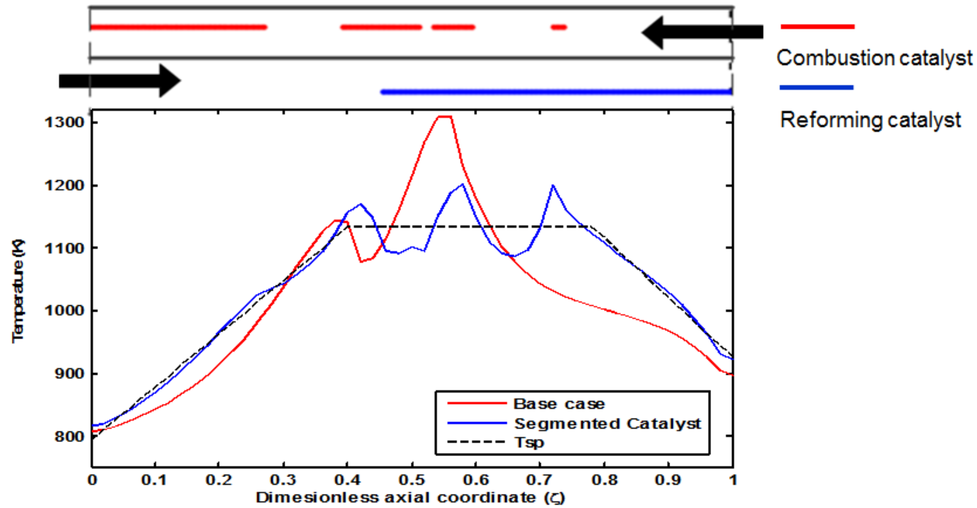


- Phase change layer absorbs heat at constant temperature when melting: Prevents temperature extremes caused by disturbances

Pattison and Baldea, *AIChE J., 2013*

Segmented Combustion Catalyst Configuration

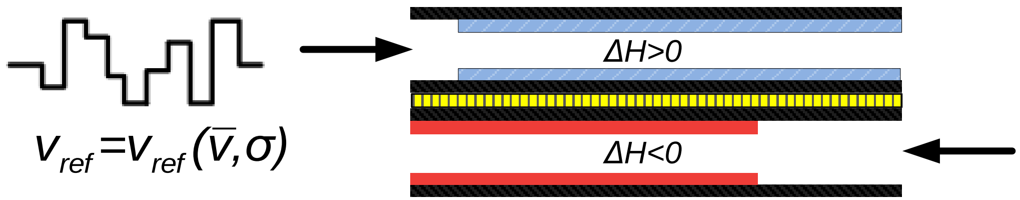




- Alternating catalytically active and inactive segments can emulate a distributed feed and modulate the rate of heat generation axially
- Formulate optimization to select:
  - the optimal parametric temperature trajectory and
  - the optimal catalyst segmentation to track the trajectory

Pattison, Estep and Baldea, *Ind. Eng. Chem. Res., 2013*

Optimal Design Under Uncertainty



- Geometry is fixed and must be determined at design stage
- **Online adjustments are not possible**

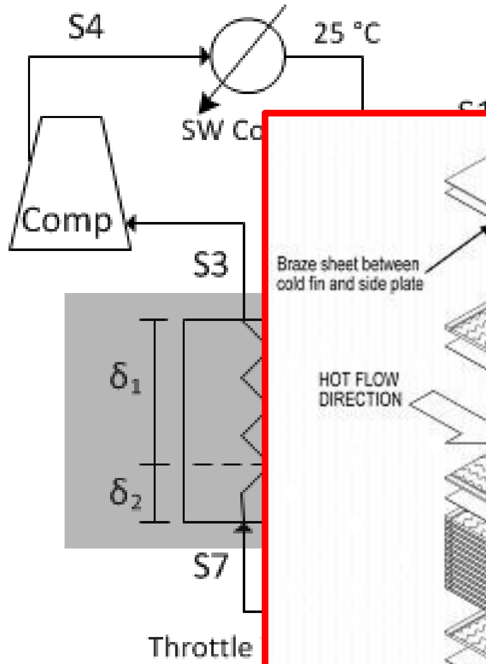
Model-based optimal design under uncertainty

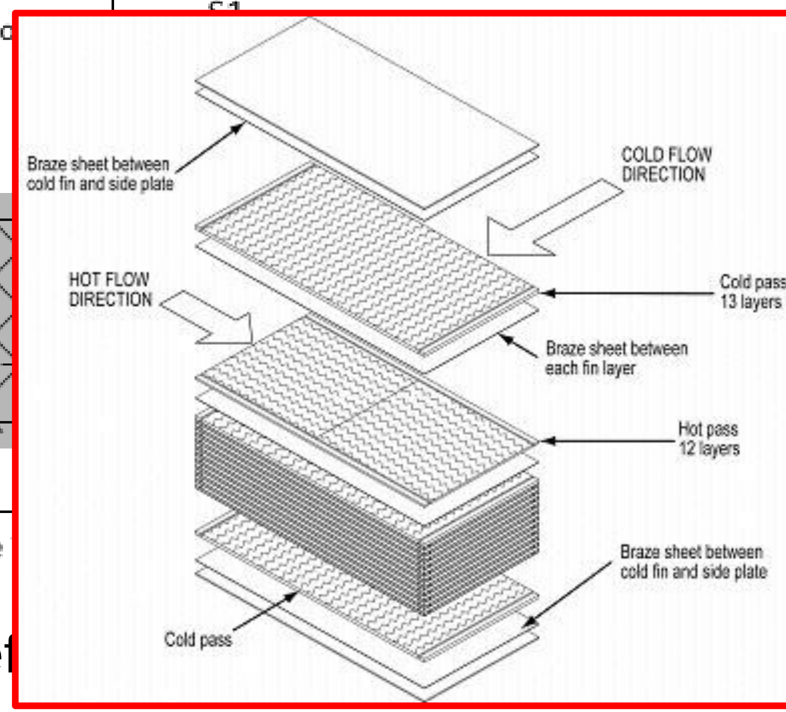
- Shape dynamic behavior via stochastic optimization of PCM thickness, catalyst geometry
- Usual approach: study a large number of scenarios
- **<u>Identification-based optimization (IBO):</u>** represent disturbances as multi-level random signals, impose on system model during dynamic optimization iterations

  10 reduction in computation time

Wang and Baldea, *Comput. Chem. Eng.*, 2014

Cryogenic Liquefaction Process



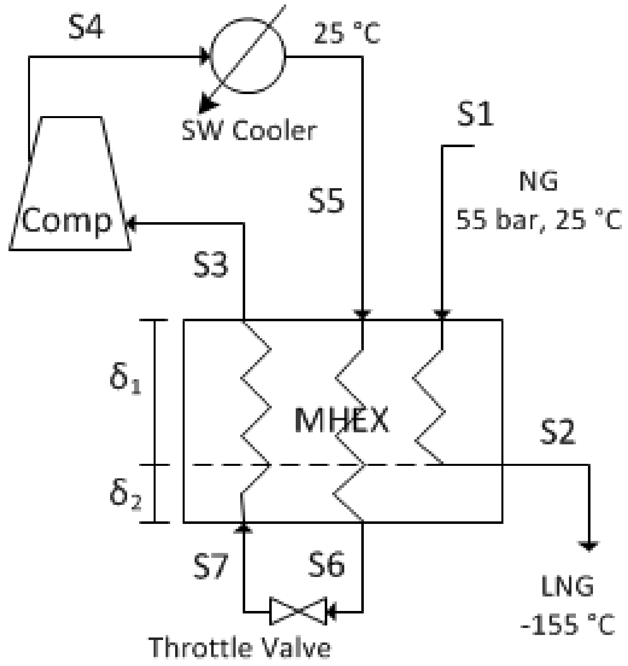


lack & Veatch
APE 24, 2014

http://www.lytron.com/

- PRICO Process (mixed-ref
- Design challenges:
  - Integration: refrigeration generated and trapped in the process
  - Intensification: multi-stream heat exchanger (MHEX)

Simultaneous Flowsheet and Unit Optimization

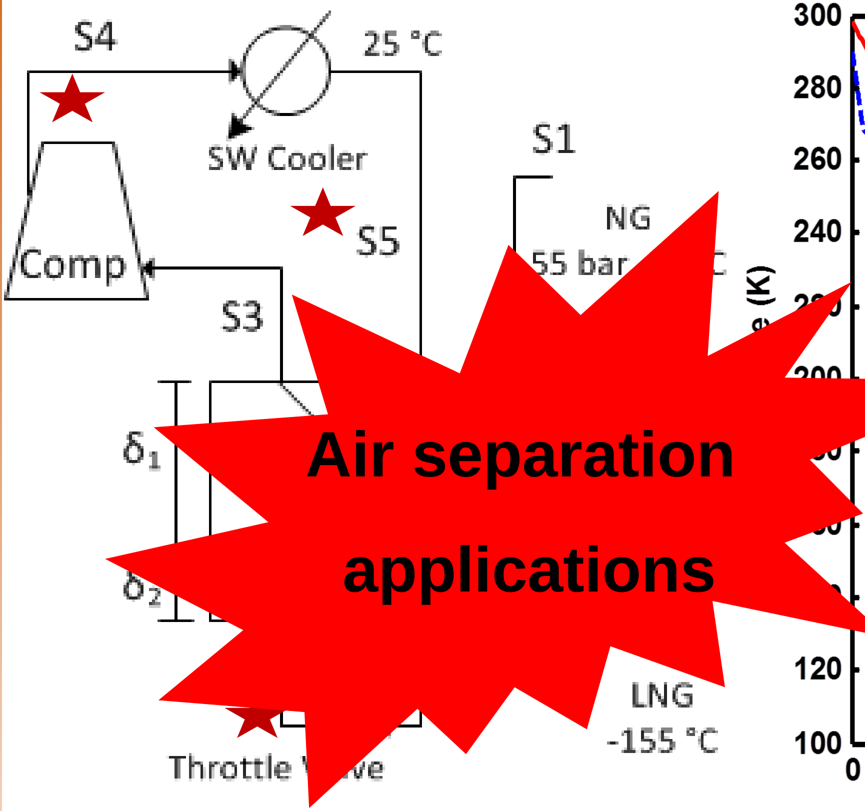


PRICO is a trademark of Black & Veatch
Pattison and Baldea, *ESCAPE 24,* 2014

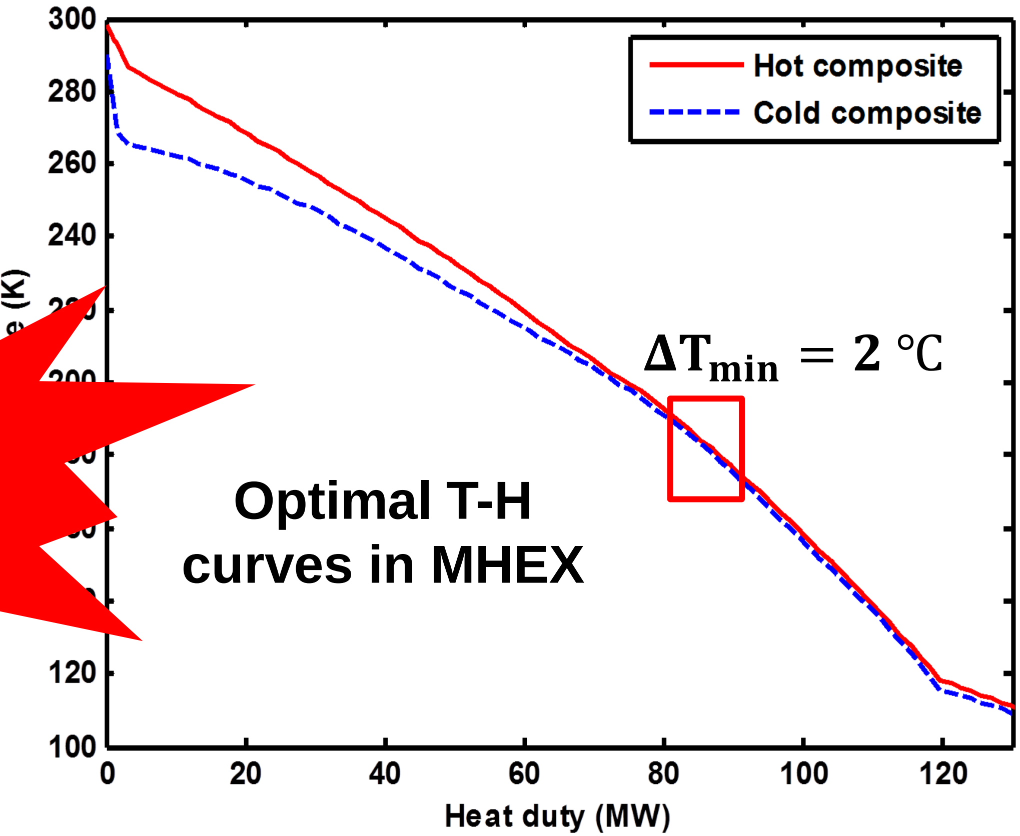
- Optimization includes composition of refrigerant (N2 + C1-C4)
- Phase transitions in MHEX: highly nonlinear, discontinuous model
- Equation-oriented pseudo-transient model: improve basin of convergence of model equations
- Time-relaxation-based optimization

Pattison and Baldea, *AIChE J.,* 2014

PRICO Liquefaction Process



Air separation applications



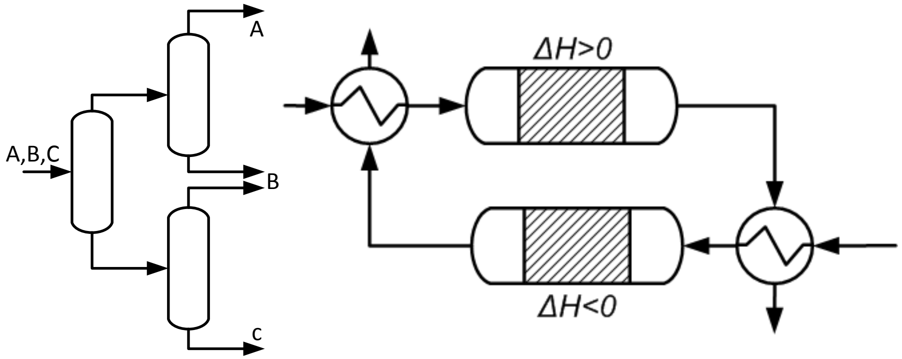
Optimal T-H curves in MHEX

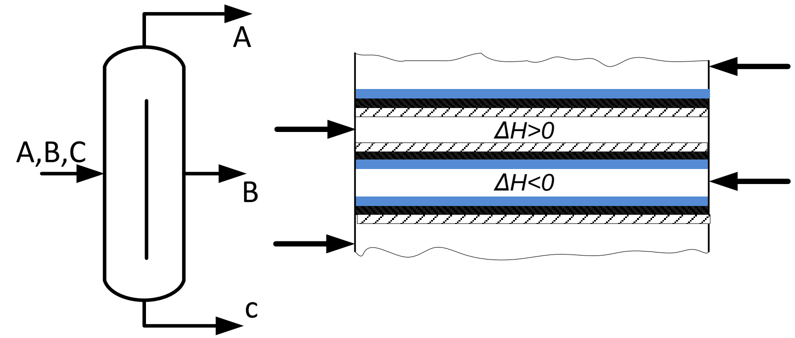
Pattison and Baldea, *ESCAPE 24,* 2014

- Tight heat integration (2°C approach)
- Optimal process uses 5.7% less power than previous designs.

Kamath et al., *AIChE J.,* 2012

PI: Future Challenges





Models readily available in process simulator “parts bin”

?

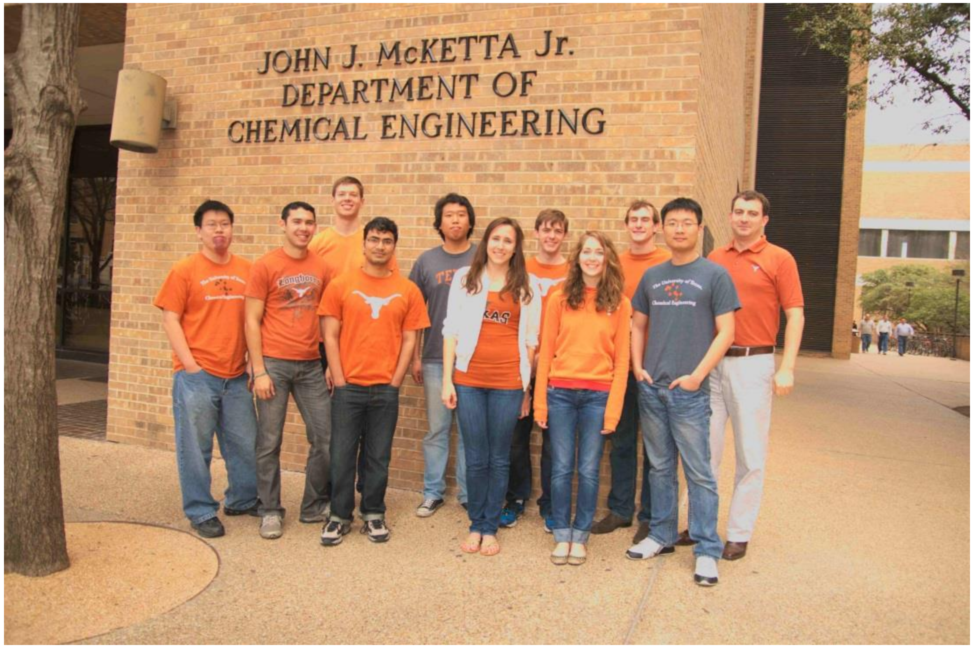
Theory: break unit ops paradigm

Synthesis of intensified processes: Phenomena-based Superstructure? (presentation by Dr. Mario Eden)

Flowsheet “co-simulation” / optimization (Lang et al., 2009)

Smart manufacturing: embed control capability

Acknowledgements



- ACS-PRF
- Ventech Engineering, Ltd., Velocys, Ltd
- Texas Wisconsin California Control Consortium

Context

Process intensification (PI):

> *"Any chemical engineering development that leads to substantially* ***smaller****, cleaner, safer and more energy efficient technology" (Reay et al., 2013) or "that combine[s]* ***multiple operations into fewer devices****." (Tsouris and Joseph, 2003)*

Multum in parvo (Lat.) : much in little

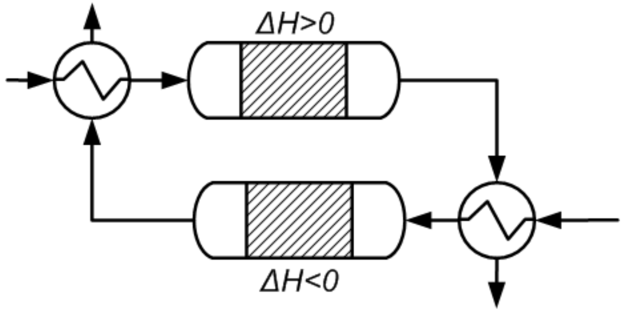
Paradigm

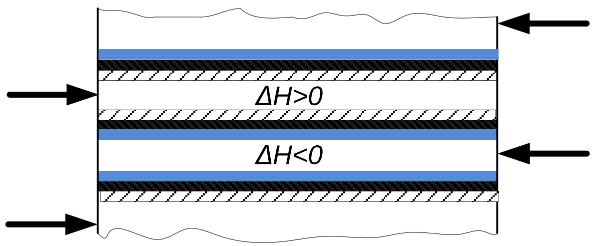
- Process should be governed by intrinsic rates
- Identify limiting factor(s) in a process (transport, transfer)
- Address them via changes in system operation (batch $\rightarrow$ continuous), device geometry, external energy fields
- Scale-up by "numbering-up"

PI: Multiple Phenomena, Scale-Independent

Integrated | *Intensified*

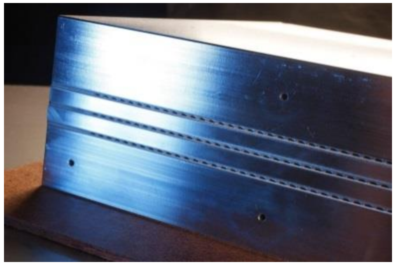
Reaction





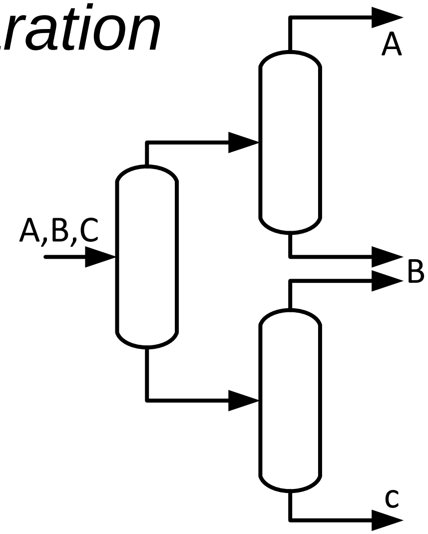
mm channels

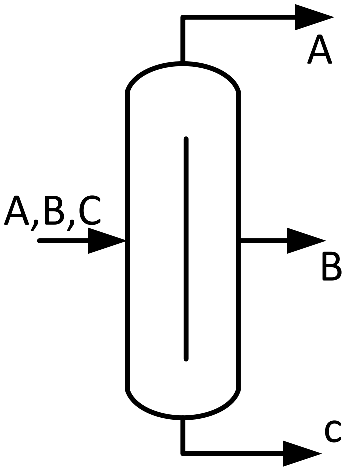
<1m length



www.velocys.com

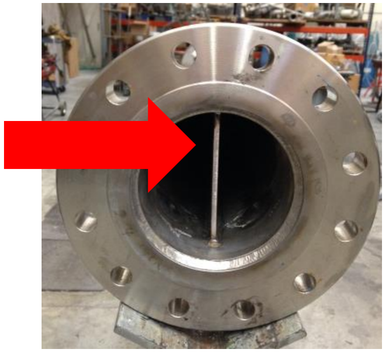
Separation





cm diameter

Several meters tall



Courtesy of Bailee Roach

PI: Multiple Phenomena, Scale-Independent

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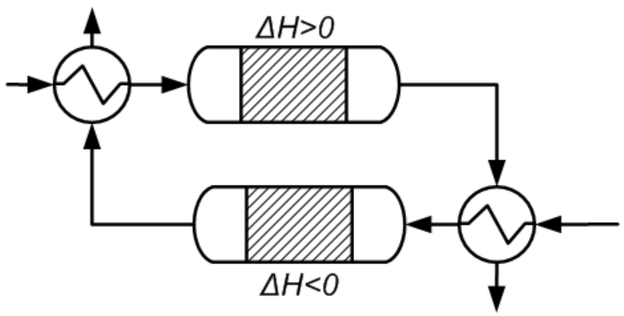
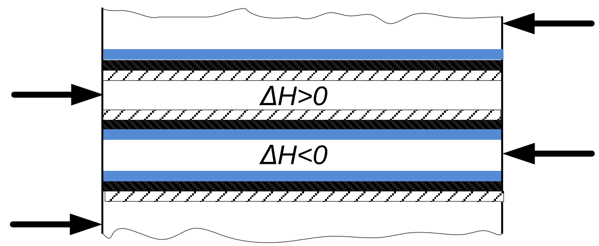




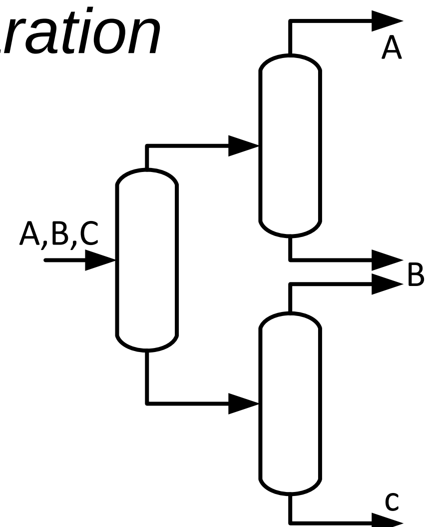
mm channels

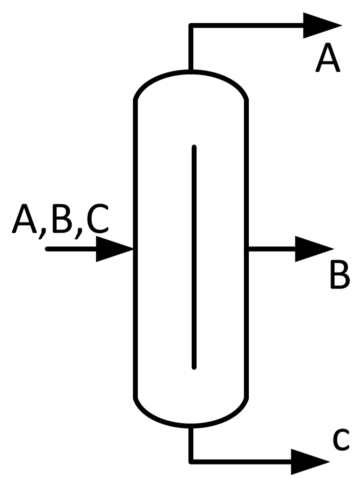
<1m length

10x smaller size

Zanfir and Gavriilidis, CES, 2003

Separation





cm diameter

30% capital savings, use up to 40% less energy

Schultz et al., CEP, 2002, Kiss and Bildea, CEPPI, 2011

PI practice ahead of theory

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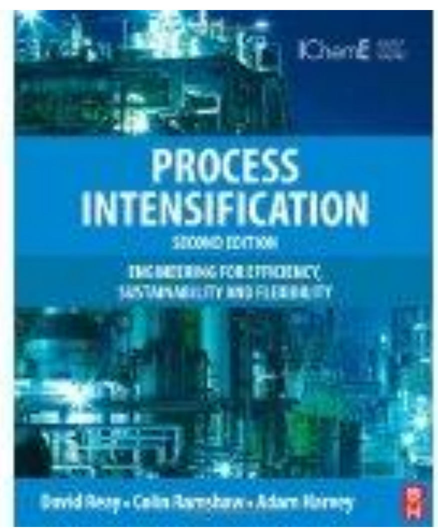
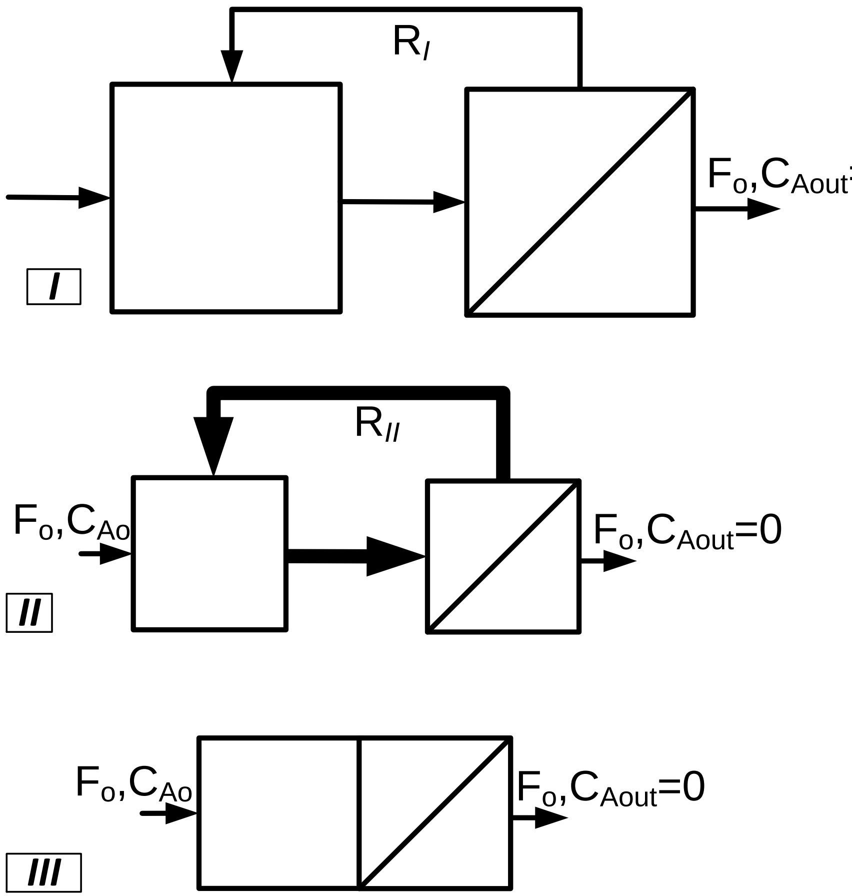
Multum in parvo (Lat.) : much in little

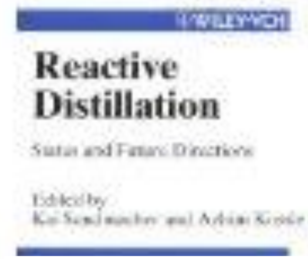
Stankiewicz and Moulijn, 2003



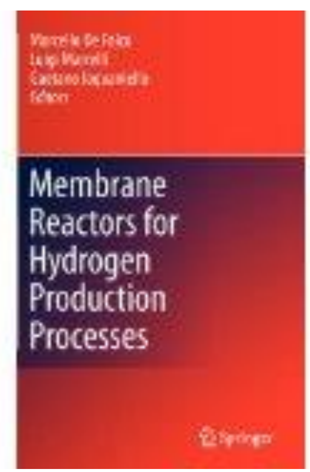
Reay et al., 2013

Integration vs. Intensification



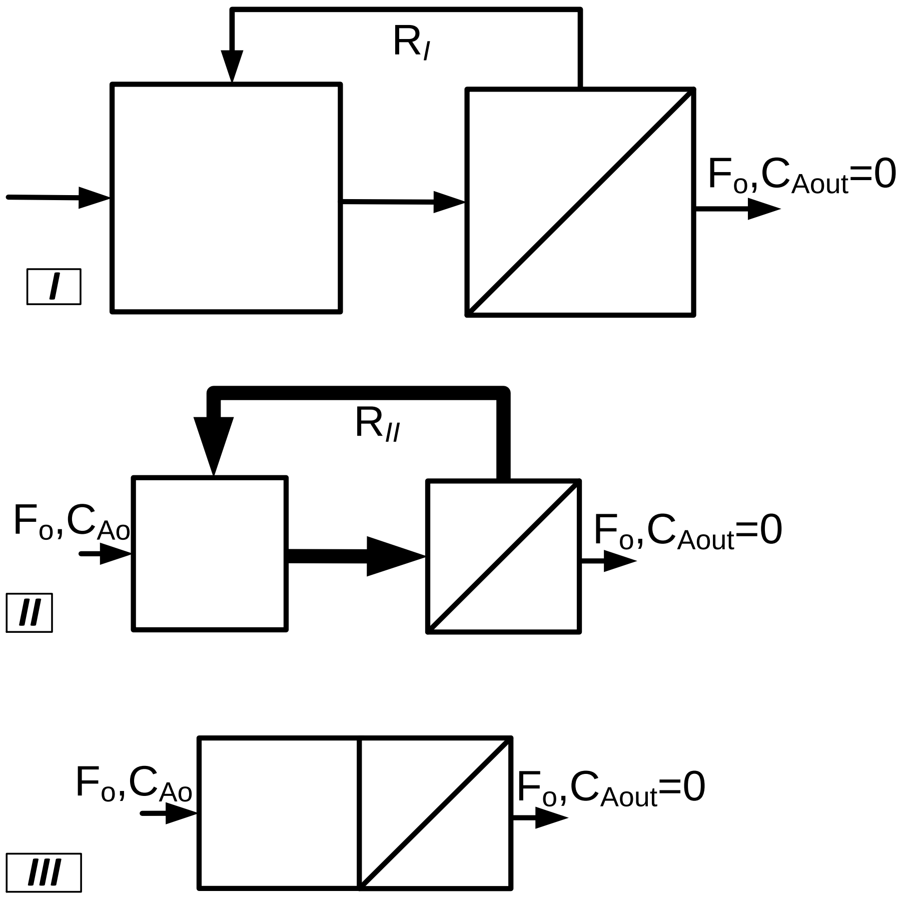


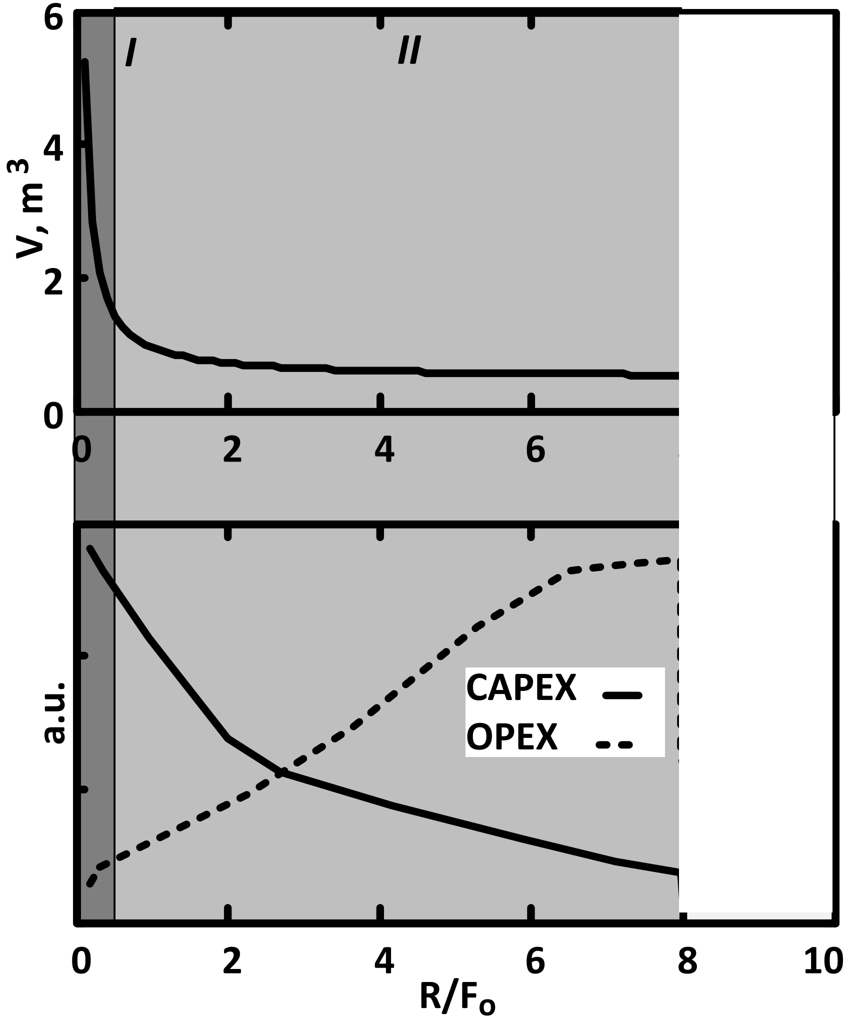
- "The front-runner of industrial process intensification" (Harmsen, 2007)



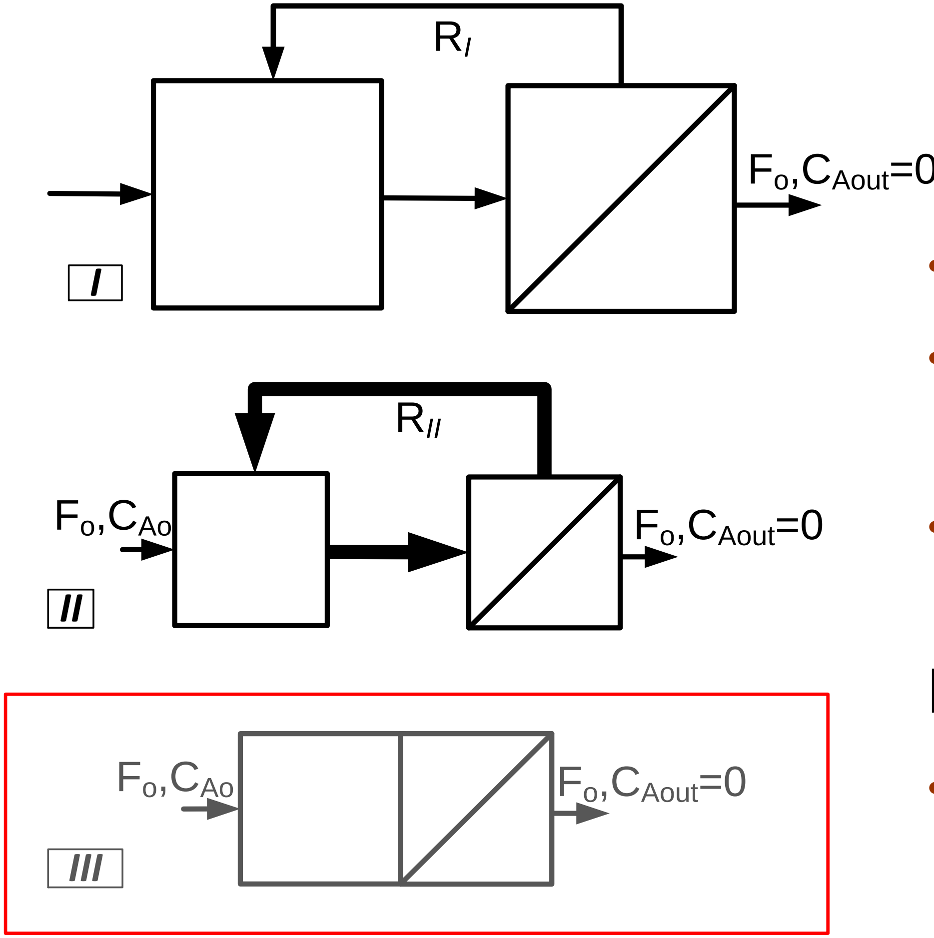
- Fundamental changes in design, operation

Integration vs. Intensification





Integration vs. Intensification



- Reduced number of units
- Reduced unit size and holdup
- Reduced OPEX (no recycling)

BUT

- Reduced number of degress of freedom

Schembecker and Tlatlik, 2003; Nikacevic et al., 2012

Conclusions

- Intensification fosters dynamic complexity
  - Better economics/improved efficiency: more difficult control
  - Scale independent
- Accomplishments
  - “cool” applications and commercial success
- Future
  - Theory: new process synthesis, simulation, optimization framework; will likely lead to new applications
  - Embed control considerations at the control stage
  - Applications: smarter manufacturing, interaction with power system

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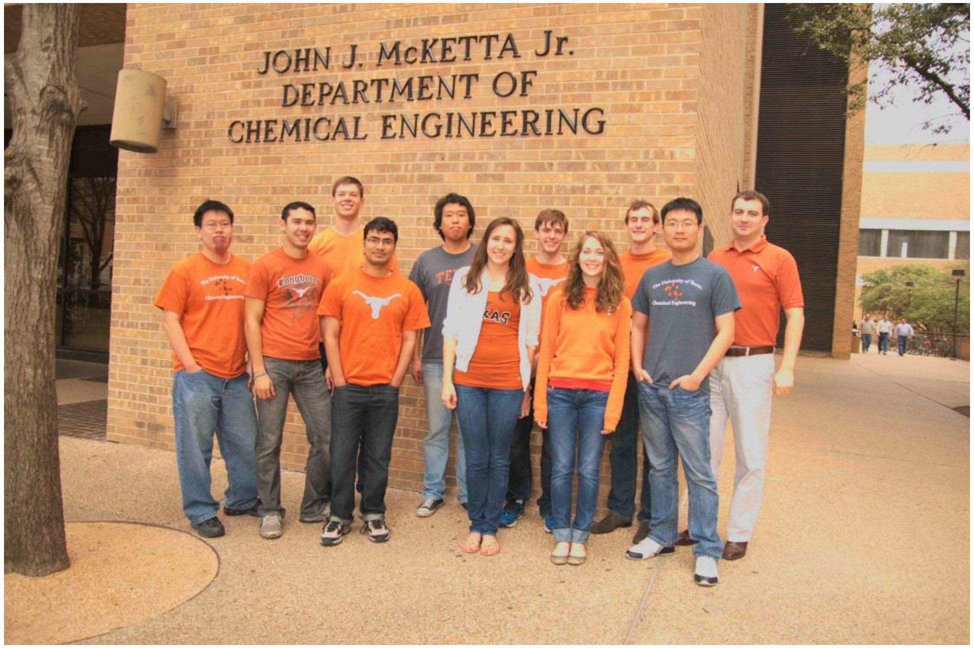

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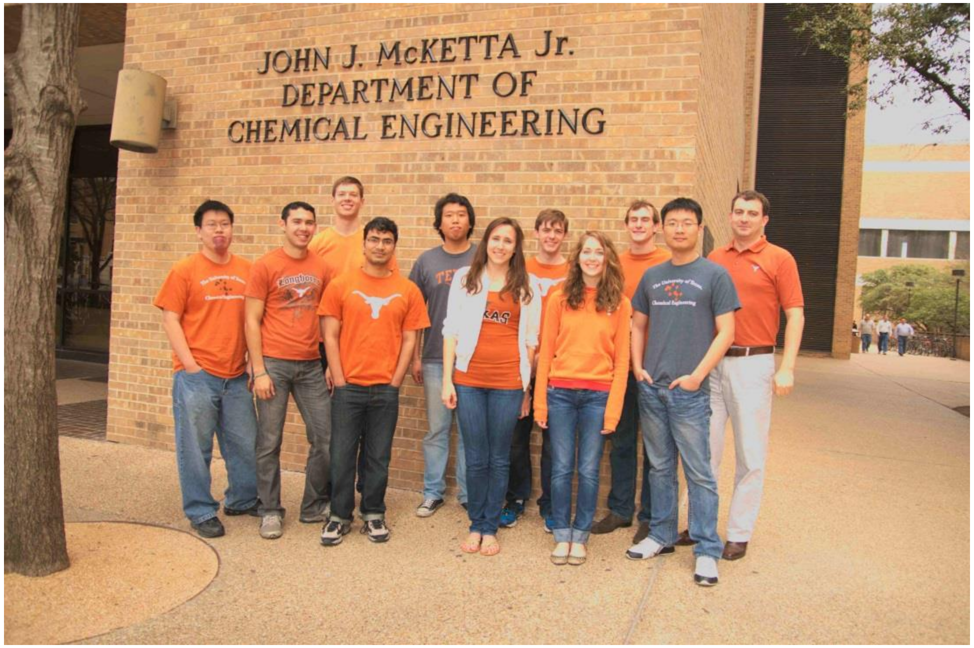

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