Integrarea si Intensificarea Proceselor Chimice

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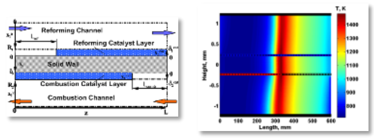
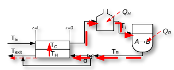
The University of Texas at Austin



Facultatea de Chimie si Inginerie Chimica

Universitatatea "Babes-Bolyai"

Cluj, 18 martie, 2015



Context

Process Integration (IP):

A holistic approach to process design, based on maximizing recovery and utilization of energy and materials from within the process, reducing the use of utilities and minimizing environmental impact (cf. Hallale, 2001, Cussler and Moggridge, 2001, El-Halwagi, 2006)

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 Porcelli, 2003)*

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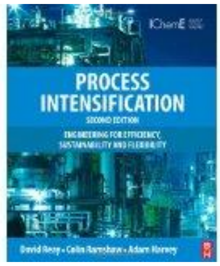
Multum in parvo (Lat.) : much in little

Stankiewicz and Moulijn, 2003



Reay et al., 2013

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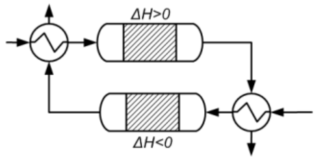
Paradigm

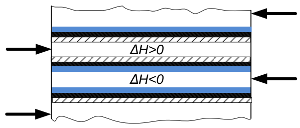
- Process should be governed by intrinsic rates
- Identify limiting factor(s) in a process (transport, transfer)
- Address them via changes in system operation (batch → continuous), device geometry, external energy fields
- Scale-up by "numbering-up"

PI: Multiple Phenomena, Scale-Independent

Integrated *Intensified*

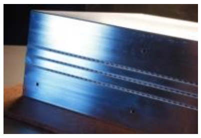
Reaction





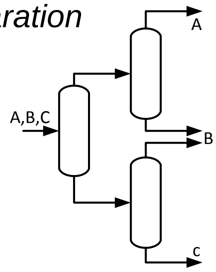
mm channels

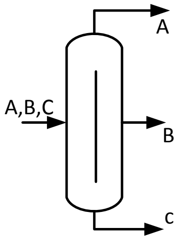
<1m length



www.velocys.com

Separation





cm diameter

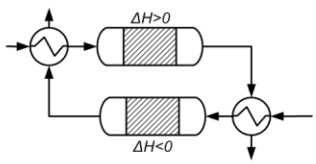
Several meters tall

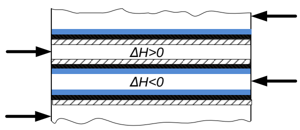
Courtesy of Bailee Roach

PI: Multiple Phenomena, Scale-Independent

Integrated *Intensified*

Reaction





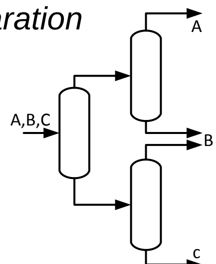
mm channels

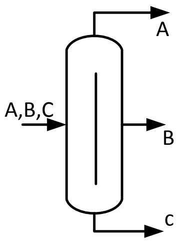
<1m length

10x smaller size

Zanfir and Gavriilidis, CES, 2003

Separation





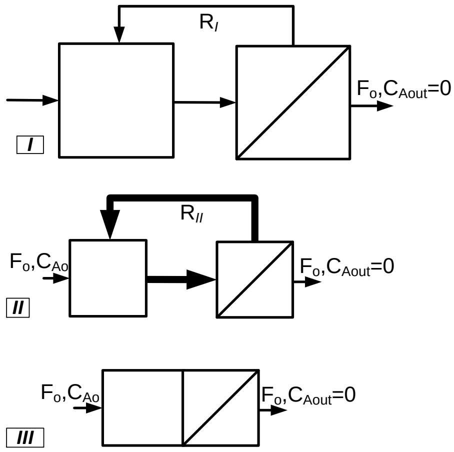
cm diameter

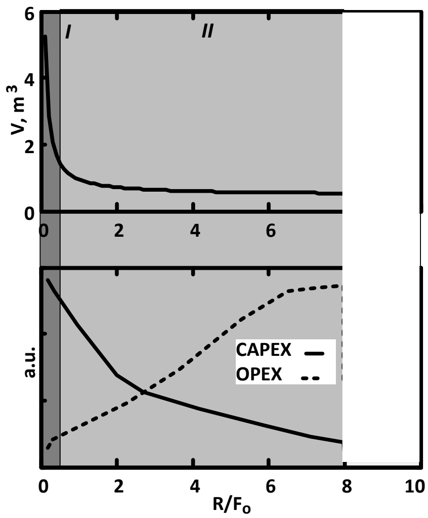
30% capital savings, use up to 40% less energy

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

PI practice ahead of theory

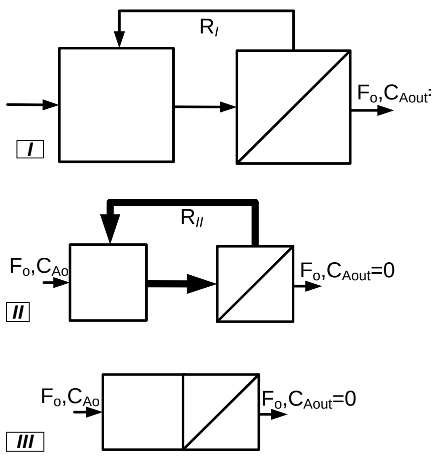
Integration vs. Intensification



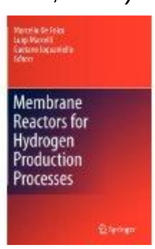


Baldea, FOCAPD, 2014

Integration vs. Intensification

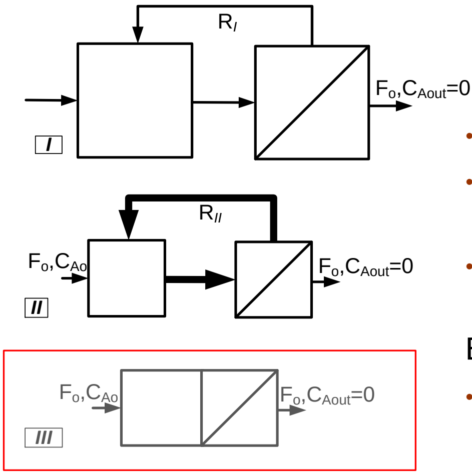


- "The front-runner of industrial process intensification" (Harmsen, 2007)



- Fundamental changes in design, operation

Integration vs. Intensification: Empirical



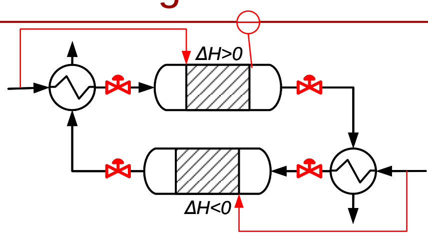
- Reduced number of units
- Reduced unit size and holdup
- Reduced OPEX (no recycling)

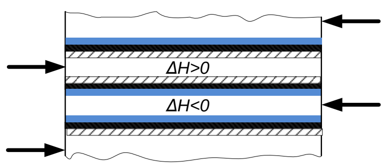
BUT

- Reduced number of degrees of freedom for design and control

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

Heat Integration vs. Intensification

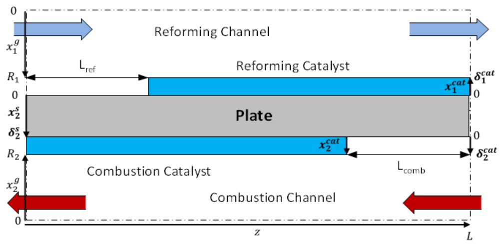




- Often safety-critical
- Ample instrumentation and actuation
- Multiple design DOF, several possible control configurations

- **Microchannel reactors**
- Exothermic and endothermic reactions occur in parallel channels

Prototype System: Methane Steam Reformer



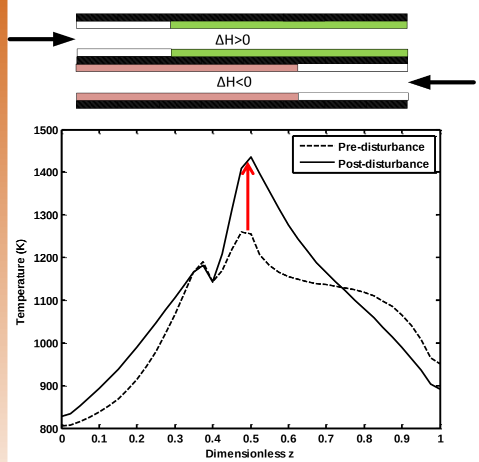
Assumptions Zanfir and Gavriilidis, 2003, Zanfir et al., 2011, Pattison and Baldea, 2013

- **Gas phase:** 2D convection-diffusion-reacting flow (laminar)
- **Wall:** 2D heat conduction
- **Catalyst layers:** 1D reaction-diffusion
- **Boundary conditions:** no flux (outlet), equal flux (fluid-solid interface), symmetry (channel center)

Implementation: gPROMS

- **Discretization:** axial: finite differences, radial: OCFEM

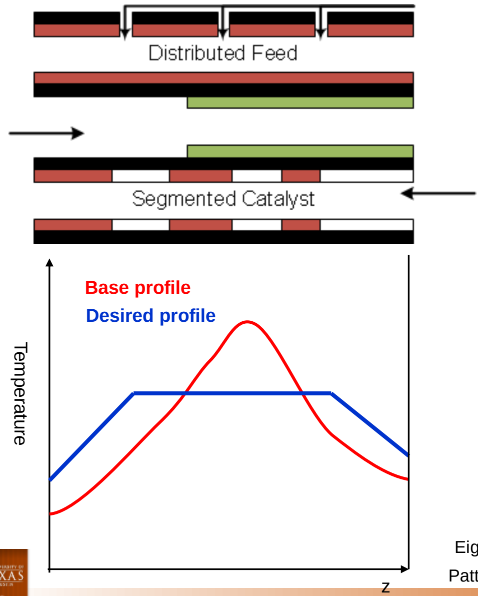
Temperature Control Problem



- Reactor subject to operational disturbances:
  - Flow rate
  - Pressure
  - Temperature
  - Composition
- May result in formation of “hotspots” that damage the reactor or catalysts
- **Goal: develop distributed control concepts that prevent the formation of hotspots**

Pattison, R.C. and Baldea, M., *AIChE J., 2013*

Concept 1: Segmented Catalyst

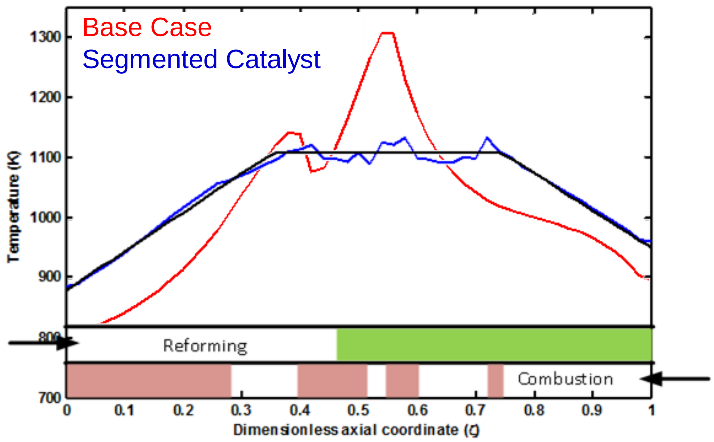


- Alternating catalytically active and inactive segments
- Emulates a distributed feed system : increase number of design degrees of freedom
- Modulates the rate of heat generation axially
- Formulate optimization to select:
  - the optimal parametric temperature trajectory and
  - the optimal catalyst segmentation to track the trajectory

Eigenberger et al., CES, 2000

Pattison, R.C. and Estep, F.E. and Baldea, M., *IECR., 2013*

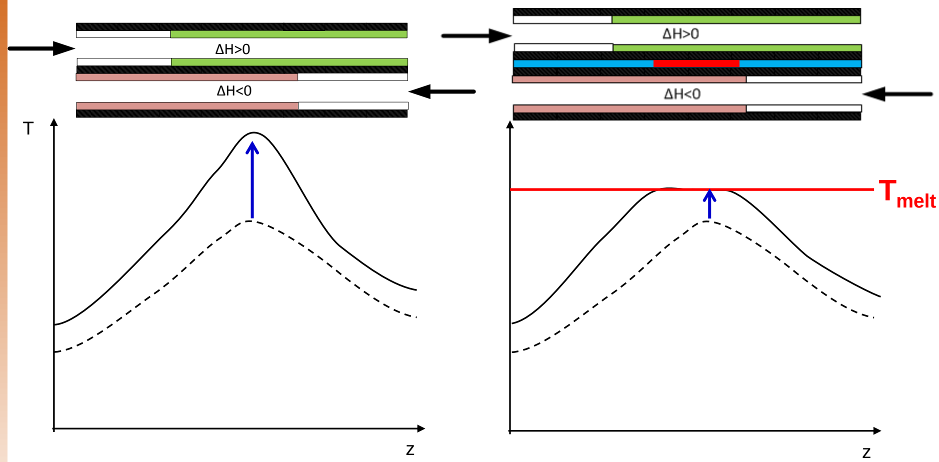
Catalyst Segmentation Results



Pattison, R.C. and Estep, F.E. and Baldea, M., *IECR., 2013*

- 200ºC reduction in maximum temperature
- Higher average temperature
- Increase methane conversion in both sets of channels

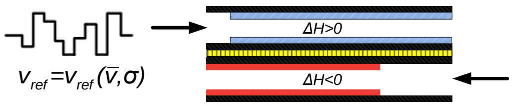
Concept 2: Thermal Fuse



- Phase change material (PCM) layer absorbs heat at constant temperature when melting, prevents formation of hotspots

Pattison, R.C. and Baldea, M., *AIChE J., 2013; Patent* **WO2014042800 A1**

PCM Controller Tuning



Single degree of freedom: PCM layer thickness

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

Model-based controller design:

- Shape dynamic behavior (melting/solidification time) via stochastic optimization of PCM size
- Identification-based optimization: represent disturbances as multi-level random signals, impose on system model during dynamic optimization iterations

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

Optimization Under Uncertainty

- Problem Pistikopoulos, 1995

$$\min_{\boldsymbol{u},\boldsymbol{d}} \; E(J(\dot{\boldsymbol{x}},\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta}(t),t))$$

$$\text{s.t.} \quad \boldsymbol{h}(\dot{\boldsymbol{x}},\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta}(t),t) = \boldsymbol{0}$$

$$\boldsymbol{g}(\dot{\boldsymbol{x}},\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta}(t),t) \leq \boldsymbol{0}$$

θ: Uncertain variables

d: design variables

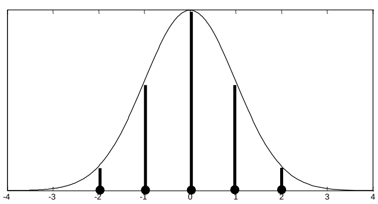
u: controls

Infinite-dimensional problem due to $\boldsymbol{\theta}, \boldsymbol{u}$

- Discretization to convert to finite-dimensional (MI)NLP
- Problem solution:
  - Multi stage (design vs. resource variables), generalized Benders decomposition
- Chance constrained formulation, parametric programming

Acevedo and Pistikopoulos, 1997, Clay and Grossmann, 1997, Dua et al., 2002, Benerjee and Ierapetritou, 2002, Li et al., 2008, Faisca et al., 2008

Discretization



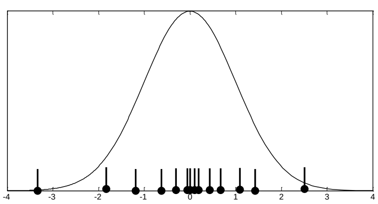
- Multiperiod

Ierapetritou et al., 1996, Acevedo and Pistikopoulos, 1998

$$\min_{\boldsymbol{u},\boldsymbol{d}} \sum_{p=1}^{P} w^p J(\dot{\boldsymbol{x}},\boldsymbol{x},\boldsymbol{u},\boldsymbol{d},\boldsymbol{\theta}^p,t)$$

$$\text{s.t.} \;\; \forall p \;\; \boldsymbol{h}(\dot{\boldsymbol{x}},\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta}^p,t) = \boldsymbol{0}$$

$$\boldsymbol{g}(\dot{\boldsymbol{x}},\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta}^p,t) \leq \boldsymbol{0}$$



- Sample Average Approximation (SAA)

Linderoth et al.2006, Constantinescu et al., 2008

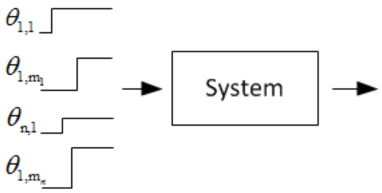
$$\min_{\boldsymbol{u},\boldsymbol{d}} \frac{1}{N} \sum_{k=1}^{N} J(\dot{\boldsymbol{x}},\boldsymbol{x},\boldsymbol{u},\boldsymbol{d},\boldsymbol{\theta}^k,t)$$

$$\text{s.t.} \; \forall k \quad \boldsymbol{h}(\dot{\boldsymbol{x}},\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta}^k,t) = \boldsymbol{0}$$

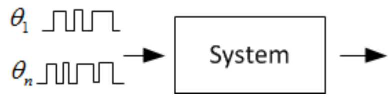
$$\boldsymbol{g}(\dot{\boldsymbol{x}},\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta}^k,t) \leq \boldsymbol{0}$$

- Infinite-dimensional problem converted to (MI)NLP
- Computationally expensive when number of scenarios increases
- Similar to a system identification experiment

Identification-Based Optimization



Step testing: generate scenarios to quantify input/output relationship



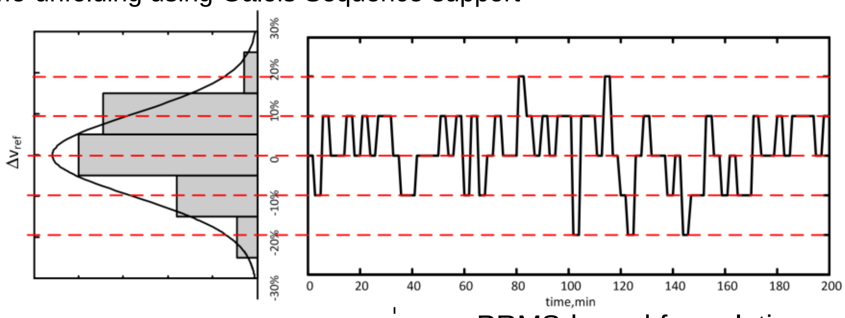
Train of signal changes (e.g.: PRBS): increase efficiency

- Nonlinear systems: pseudo-random *multi-level* signal (PRMS) Godfrey, 1993, Barker., 2004
- IBO concept:
  - represent uncertain variables as pseudo-random multi-level signals (PRMS)
  - apply PRMS to efficiently evaluate the response of the system to fluctuations in uncertain variables.

Problem Reformulation

Pseudo-Random Multi-Level Signal representation:

- time-unfolding using Galois Sequence support



$$h_{PCM} = \arg\min \frac{1}{N}\sum_{j=1}^{N}\int_{0}^{t_s}(T_{max,wall,j}-T_{melt})ds$$

s.t. reactor model equations

$$v_{ref,j}=v_{ref}(\bar{v},\sigma)$$

$$Nt_s \le t_{MPRS}$$

$$\equiv$$

PRMS-based formulation

$$h_{PCM} = \arg\min \int_{0}^{t_{MPRS}}(T_{max,wall}-T_{melt})d\tau$$

s.t. reactor model equations

$$v_{ref}(t)=v_{MPRS}$$

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

Identification-Based Optimization: Algorithm

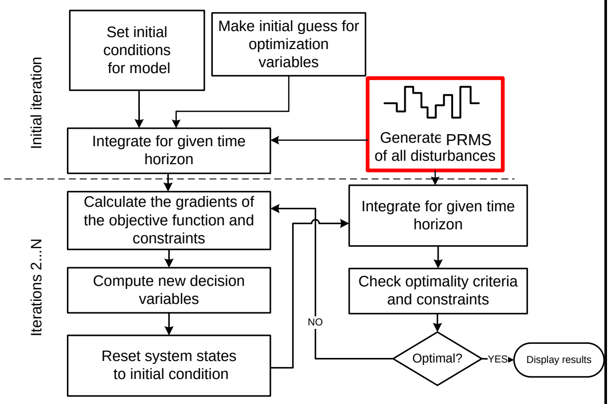
$$\min_{d,k} J(\dot{x}, x, u, d, \theta^{PRMS}(t), t)$$

s.t. $h(\dot{x}, x, u, d, \theta^{PRMS}(t), t) = 0$

$u = k(x)$

$g(\dot{x}, x, u, d, \theta^{PRMS}(t), t) \leq 0$

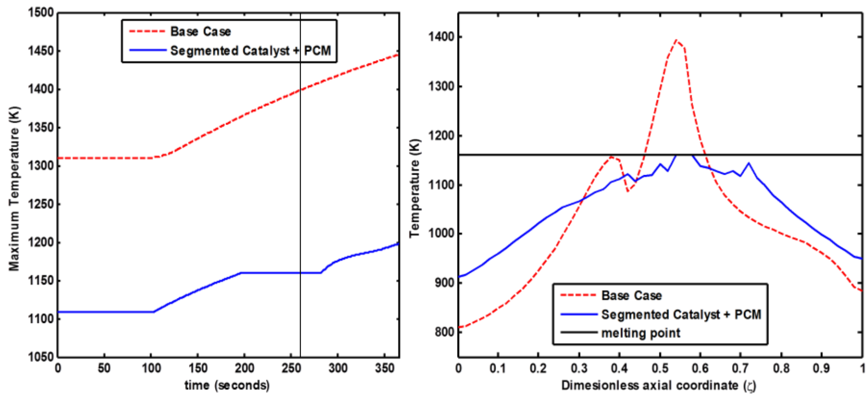
$0 < t < T$



- Assumptions
  - Time horizon T is sufficiently long
  - System is feedback stabilizable
  - Disturbance distributions known

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

Thermal Fuse: Results



- Segmented Catalyst: reduced nominal temperature profile
- 0.8 mm Thermal Fuse: prevents the formation of hotspots
- Cannot account for sustained disturbances

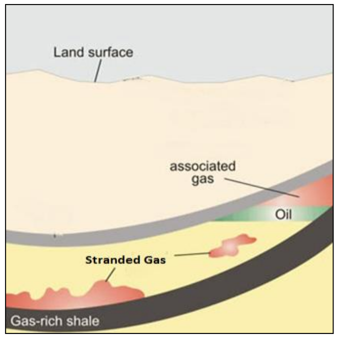
Pattison and Baldea, *AICHE J.* 2013

Application: Stranded and Associated Gas

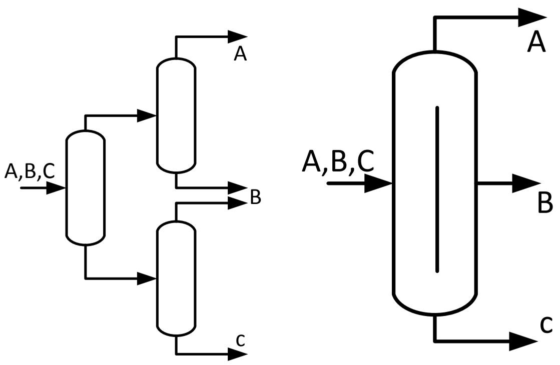
- **Stranded gas**: Small remote deposits that are too expensive to extract & transport to consumers
  - 7000 tcf worldwide
- **Associated gas**: found with oil, typically flared or reinjected
  - 4.5 trillion megajoules wasted in 2011
- **Monetization**: pipeline, liquefaction, Gas-To-Liquids (GTL):
  - Not viable at small scales

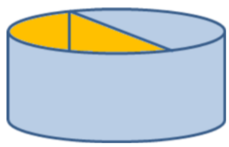
Microchannel reactor-based systems can have large impact

image source: www.gereports.com



Intensification of Systems without Recycle





Courtesy of Bailee Roach

- Dividing wall column (DWC): separate ternary mixture using a single physical device

DWC at the University of Texas at Austin

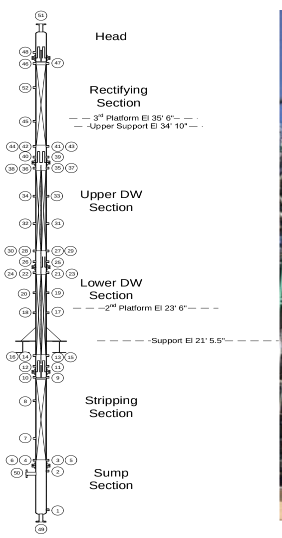
University of Texas at Austin
Pickle Research Center

August 2014

Project Partners:
UT, Eastman, Emerson,
Packing from Sulzer, Koch-Glitsch

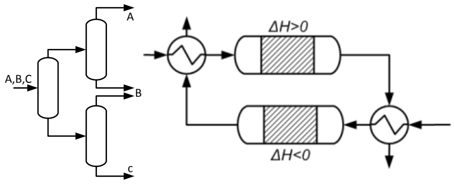
Courtesy of Bailee Roach

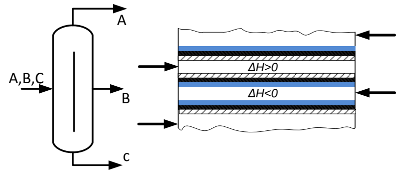
DWC Pilot Plant



Courtesy of Bailee Roach

PI: Future Challenges





Models readily available in process simulator "parts bin"

?

Theory: break unit ops paradigm

Synthesis of intensified processes: Phenomena-based Superstructure? (Ismail et al., 2001, Arizmendi-Sánchez and Sharratt, 2008, Lutze et al., 2013)

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

Embed control capability

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

Acknowledgements

- Students, in particular R.C. Pattison and S. Wang
- American Chemical Society- Petroleum Research Fund
- US Department of Energy, Advanced Manufacturing Office
- W.A. "Tex" Moncrief Grand Challenges Award
- Eastman Chemical, Emerson Process Management, ABB, Dow Chemical, Corning, Center for Operator Performance, Texas Wisconsin California Control Consortium