Role of Process Systems Engineering in Chemical Engineering

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Chemical Engineering Division's Lectureship Award
ASEE Meeting, Seattle
June 15, 2015
Major Questions

What are major trends in Chemical Engineering?
- Brief historical evolution
- Recent trends and academic/industry disconnect

What is the impact of Process Systems Engineering in Chemical Eng. and major research challenges?
- Process and Product Design
- Energy and sustainability
- Enterprise-wide Optimization
History of Chemical Engineering

George Davis, Manchester 1888

Lewis Norton, MIT 1888

J.W. Gibbs, 1878

H. Helmholtz, 1847

L. Boltzmann, 1866

K.G. Denbigh, Southampton, London, Imperial, 1955

Arthur D. Little, MIT, 1916

William Walker, MIT 1924

Olaf Hougen, Wisconsin 1947

Unit Operations

Chemical Engineering Principles

Thermodynamics
Transport Phenomena

Bird, Stewart, Lightfoot, Wisconsin, 1960

Applied Mathematics/Reaction Engineering

R. Aris, 1962; N. Amundson, 1972; Minnesota

Mass Transfer

P.V. Danckwerts, Cambridge 1965

Polymers

P. Flory, 1969; Dupont, Cornell, Carnegie Mellon

Fluid Mechanics

G. Batchelor, Cambridge, 1967

Catalysis

Michel Boudard, Stanford 1968
Process Systems Engineering

Dale Rudd, Wisconsin 1968  Roger Sargent, Imperial College 1964

Bioengineering


Nanotechnology

Diversification Chemical Engineering

B.S. Job placement (AIChE, 2007)

Chemicals
Fuels ~42%

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Trends in Chemical Engineering
(Last decade)

- Bioengineering area:
  - Has been “hot” area: most new faculty in bio area
  
  New frontier in chemical engineering:
  Bob Langer MIT: Study and development of polymers to deliver drugs, particularly genetically engineered proteins, DNA and RNAi, continuously at controlled rates for prolonged periods of time

- Many new Biomedical Engineering Depts (Whittaker Foundation)
  Job market biomedical engineers?

- Many U.S. departments (~50%) were renamed as:
  Chemical and Biomolecular Engineering
  (e.g. Cornell, U. Penn., Illinois, Georgia Tech)
  Chemical and Biological Engineering
  (e.g. Colorado, Northwestern, Notre Dame, Wisconsin)
Trends in Chemical Engineering
(Last decade)

- Nanotechnology is other “hot” area

- Increasing emphasis on Science in Chemical Eng. Departments
  - Many professors are not chemical engineers
  - Has increased multidisciplinary approach
  - Decreased emphasis on chemical engineering fundamentals (fewer transport courses, one semester Thermo: 1st & 2nd Law, Phase & Chemical Equilibria)
  - Process Design courses largely outsourced to retired industry people
  - Process Control no longer required at several U.S. universities
Many faculty members in US do not publish anymore in chemical engineering journals

Move from Engineering to Science

Impact factors ~2.2

25% US  15% US

Impact factors ~30
## The Industry Connection

### Revenues of major U.S. companies (billions)

<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>ExxonMobil</td>
<td>$365.5</td>
<td>$452.93</td>
</tr>
<tr>
<td>ChevronTexaco</td>
<td>204.9</td>
<td>241.9</td>
</tr>
<tr>
<td>Dow</td>
<td>49.1</td>
<td>56.8</td>
</tr>
<tr>
<td>DuPont</td>
<td>27.4</td>
<td>38.72</td>
</tr>
<tr>
<td>Procter &amp; Gamble</td>
<td>68.2</td>
<td>82.55</td>
</tr>
<tr>
<td>Johnson &amp; Johnson</td>
<td>53.3</td>
<td>67.22</td>
</tr>
<tr>
<td>Merck</td>
<td>22.3</td>
<td>48.05</td>
</tr>
<tr>
<td>Bristol-Myers Squibb</td>
<td>17.9</td>
<td>21.24</td>
</tr>
<tr>
<td>Amgen</td>
<td>13.8</td>
<td>23.6</td>
</tr>
<tr>
<td>Genentech</td>
<td>7.6</td>
<td>17.3</td>
</tr>
</tbody>
</table>

### One trillion dollar industry !!
### Industrial Survey on Importance of Skills

*John Chen (2013)*

<table>
<thead>
<tr>
<th>Skill</th>
<th>Average Relative Importance 1-5</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>UO</strong>: unit operations, transport phenomena, thermodynamics, separation processes *</td>
<td>4.6</td>
</tr>
<tr>
<td><strong>RE</strong>: reaction engineering, catalysis, kinetics.</td>
<td>4.0</td>
</tr>
<tr>
<td><strong>AM</strong>: analysis, modeling, simulation, process control *</td>
<td>4.0</td>
</tr>
<tr>
<td><strong>MAT</strong>: materials, surface science, polymers *</td>
<td>3.2</td>
</tr>
<tr>
<td><strong>BIO</strong>: biotechnology, medical and life sciences</td>
<td>2.1</td>
</tr>
<tr>
<td><strong>NANO</strong>: nanotechnology and its applications</td>
<td>1.8</td>
</tr>
</tbody>
</table>

*main perceived gaps between importance and proficiency by new hires*
Academic Disconnect: Trends Faculty Composition

Unit Operations

Faculty Strength in UO

<table>
<thead>
<tr>
<th>Rank</th>
<th>% in Each Rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emeritus</td>
<td>50%</td>
</tr>
<tr>
<td>Professor</td>
<td>20%</td>
</tr>
<tr>
<td>Associate Prof.</td>
<td>15%</td>
</tr>
<tr>
<td>Assistant Prof.</td>
<td>10%</td>
</tr>
</tbody>
</table>

Evolution over Time --->

Bioengineering

Faculty Strength in Bio

<table>
<thead>
<tr>
<th>Rank</th>
<th>% in Each Rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emeritus</td>
<td>10%</td>
</tr>
<tr>
<td>Professor</td>
<td>30%</td>
</tr>
<tr>
<td>Associate Prof.</td>
<td>35%</td>
</tr>
<tr>
<td>Assistant Prof.</td>
<td>40%</td>
</tr>
</tbody>
</table>

Evolution over Time --->
Dow Decides to Influence the Scientific Funding Environment

AS THE BIGGEST US EMPLOYER IN THE CHEMICAL INDUSTRY DOW HAS TO:

• Partner with strategic universities to:
  • Work on problems relevant to Dow
  • Develop talent with the skills needed
  • Influence the “Influencers”

Commit to Long Term Funding
$25 million/year for next 10 yr in US
$10 million/year for next 10 yr outside US
New emphasis: energy and sustainability

Growing World Energy Demand
Most Energy Growth in Developing Nations

Energy and sustainability likely to swing pendulum away from bio and nano areas in Chemical Engineering

Sheppard, Socolow (2007)
Process Systems Engineering is concerned with the systematic analysis and optimization of decision making processes for the discovery, design, manufacture and distribution of chemical products.

What is science base for PSE?

Process Knowledge => Conceptual design => Process Integration

Numerical analysis => Simulation => Performance process-product

Mathematical Programming => Optimization => Synthesis/design

Systems and Control Theory => Process Control => Manufacture

Computer Science => Advanced Info./Computing => Efficient problem solving

Management Science => Operations/Business => Supply chain
**Mathematical Programming**

**MINLP: Mixed-integer nonlinear programming**

\[
\begin{align*}
    \text{min } Z &= f(x, y) \\
    \text{s.t. } h(x, y) &= 0 \\
    \quad g(x, y) &\leq 0 \\
    x &\in \mathbb{R}^n, \quad y \in \{0,1\}^m
\end{align*}
\]

**MILP**: \( f, h, g \) linear

**LP**: \( f, h, g \) linear, only \( x \)

**NLP**: \( f, h, g \) nonlinear, only \( x \)
Process Systems Engineering Expanded its Scope

(Grossmann & Westerberg, 2000; Marquardt et al, 1998)
Research Challenges in PSE

I. Product and Process Design

II. Energy and Sustainability

III. Enterprise-wide Optimization
I. Product and Process Design: from “Bulk” to “Molecular” Processing

George Stephanopoulos (2004)

Macro-Processing:
Batch or Continuous Chemical Plants

Micro-Processing:
Plant-on-a-Chip

Molecular-Processing:
The Cell

Metabolites

DNA  RNA  Protein

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De Novo Protein Design

Define target template
Backbone coordinates for N, Ca, C, O
and possibly Ca-Cb vectors from PDB

Design folded protein
Which amino acid sequences will stabilize this target structure?

Approach
In silico sequence selection => MILP
Fold specificity => Global optimization

Combinatorial complexity
- Backbone length : n
- Amino acids per position : m
m^n possible sequences

=> New improved inhibitors

(Carlton, Floudas, Lambris, Morikis, 2004)
Metabolic Networks: Inverse Problem

(Hash, Domach, Grossmann, 2005)

Find reaction pathway (linear combination of extreme points for fluxes) that minimizes squared deviation from NMR spectra for given selection of measured metabolites.

MILP for all extreme points
Global optimization inverse problem
A conceptual example

Solvent selection-substitution-design problem

"I want acyclic alcohols, ketones, aldehydes and ethers with solvent properties similar to Benzene"

A set of building blocks: CH3, CH2, CH, C, OH, CH3CO, CH2CO, CHO, CH3O, CH2O, CH-O

A collection of group vectors like: 3 CH3, 1 CH2, 1 CH, 1 CH2O

All group vectors satisfy constraints

Design (Higher levels)

2. order group

Group from other GCA method

Refined property estimation. Ability to estimate additional properties or use alternative methods.

Rescreening against constraints.

Start of Post-design

Method: CAMD (Computer Aided Molecular Design)

Gani et al. (2012)
Multi-Scale Model
Quantum Mechanics
Kinetics
Heat Transfer FEA
Mechanics FEA
Part Design CAD /CAM

Over 1000 rubber parts in failure critical functions

Quantum Chemistry

Ax + S \xrightarrow{k_1} AxS
Ax + R \xrightarrow{k_2} B_x
B_x \xrightarrow{k_3} B^*_x
etc

Polymer Network
Mechanical Response

New Molecules
Material Formulation

Constitutive Model
Spring-Dashpot Approximation with Chemical Aging

Engine
Design & Operation of Complex Sub-Assembly

Part Design CAD /CAM
Part Design & Operation

Mixing + Heat Transfer + Mold Filling
Part Manufacturing

Overcure
Undercure

Time

Constitutive Model
\bar{\tau} = 2\rho R \left[ \frac{\partial \psi}{\partial t_1} + \frac{\partial \psi}{\partial t_2} I - \frac{\partial \psi}{\partial t_2} C + \frac{\partial \psi}{\partial t_3} C^{-1} \right] \frac{\partial C}{\partial C}

Example Process Intensification

Methyl Acetate Flowsheet

Single Reactive Dist Col!

Siirola (1988)
II. Energy and Sustainability

Environmental impact

Renewables: Carbon footprint various Energy Options

Adisa Azapagic (2012)
Depletion of fossil fuels?

Oil Reserves

Year 2000
Total: 1105 thousand million barrels

Year 2010
Total: 1383 thousand million barrels

25% increase!

- Discovery of New Large Oil and Gas Reserves
- New technologies for Offshore oil exploration and production

*Statistical Review of World Energy (June, 2011)
Depletion of fossil fuels?

Growth in Shale Gas

In 2035 close to 50% from Shale Gas

Northeast: from 0.3 trillion scft 2009 to 5.8 trillion scft 2035

Perspectives Article: Jeff Siirola

*The Impact of Shale Gas in the Chemical Industry*

*AIChe Journal, Volume 60, pp 810–819 (2014)*
Design Project:

Preliminary design and cost estimation of Aromatics Plant from Shale Gas

Plant to produce aromatics 500 Mlbs/yr*

Aromatics: Benzene, Toluene, Xylenes (ortho, para, meta)

Plant location: Monaca (next to Shell’s projected cracker)

Feedstocks: methane (1 atm, 60F; 95% methane, 2.5% ethane)?
Price methane: $3.50/MBtu

Price Benzene: $1,400/tonne
Price Toluene: $1,300/tonne
Price Xylenes: $1,200/tonne (higher price if separated into o, m, p)

* M=mega/million
Water scarcity

Two-thirds of the world population will face water stress by year 2025.

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Superstructure for water networks for water reuse, recycle, treatment, and with sinks/sources water

Karuppiah, Grossmann (2008)
Ahmetovic, Grossmann (2010)
Optimization Model

Nonconvex NLP or MINLP

Objective function: \( \text{min Cost} \)

Subject to:

- Splitter mass balances
- Mixer mass balances (bilinear)
- Process units mass balances
- Treatment units mass balances
- Design constraints

0-1 variables for piping sections

Model can be solved to global optimality
Superstructure of the integrated water network

1 feed, 5 process units, 3 treatment units, 3 contaminants

MINLP: 72 0-1 vars, 233 cont var, 251 constr
BARON optcr=0.01 197.5 CPUsec
Optimal design of the simplified water network with 13 removable connections

Optimal Freshwater Consumption

40 t/h

vs

300 t/h

conventional

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Biofuels: Conceptual Design Strategy for Energy and Water Optimization

Energy optimization

*Issue:* fermentation reactions at modest temperatures

=> No source of heat at high temperature as in petrochemicals

Multieffect distillation followed by heat integration process streams

Water optimization

*Issue:* cost contribution is currently still very small

(freshwater contribution < 0.1%)

=> Total cost optimization is unlikely to promote water conservation

Optimal process water networks for minimum energy consumption
Scope of Advanced Process Systems Engineering Tools

### Energy consumption corn-based process

<table>
<thead>
<tr>
<th>Author (year)</th>
<th>Energy consumption (Btu/gal)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pimentel (2001)</td>
<td>75,118</td>
</tr>
<tr>
<td>Keeney and DeLuca (1992)</td>
<td>48,470</td>
</tr>
<tr>
<td>Wang et al. (1999)</td>
<td>40,850</td>
</tr>
<tr>
<td>Shapouri et al. (2002)</td>
<td>51,779</td>
</tr>
<tr>
<td>Wang et al (2007)</td>
<td>38,323</td>
</tr>
</tbody>
</table>

From Karrupiah et al (2007)
24,918 Btu/gal vs 38,323 Btu/gal
Why? Multieffect distillation and heat integration

### Water consumption corn-based process

<table>
<thead>
<tr>
<th>Author (year)</th>
<th>Water consumption (gal/gal ethanol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gallager (2005) First plants</td>
<td>11</td>
</tr>
<tr>
<td>Philips (1998)</td>
<td>5.8</td>
</tr>
<tr>
<td>MATP (2008) Old plants in 2006</td>
<td>4.6</td>
</tr>
<tr>
<td>MATP (2008) New plants</td>
<td>3.4</td>
</tr>
</tbody>
</table>

From Martin and Grossmann (2010)
1.5 gal water/gal ethanol vs 3.4
Why? Integrated process network with reuse and recycle
Superstructure Thermochemical Bioethanol

Ethanol via gasification

Gasification
- Direct Gasification
- Indirect Gasification

Reforming
- Steam Reforming
- Partial Oxidation

Clean up
- Wet solids removal
- Filter
- CO/H2 adjustment
- WGSR
- Bypass
- Membrane/PSA

Sour gases removal:
- MEA
- PSA
- Membrane

Synthesis
- Fermentation
- Rectification
- Adsorption
- Molecular sieves
- Pervaporation

Catalytic
- Direct Sequence
- Indirect sequence

Martin, Grossmann (2010)

Process Design Alternatives:
- Gasification
  - Indirect Low pressure
  - Direct high Pressure
- Reforming
  - Steam reforming
  - Partial oxidation
- CO/H2 adjustment
  - WGSR
  - Bypass
  - Membrane/PSA
- Sour gases removal:
  - MEA
  - PSA
  - Membrane
- Synthesis
  - Fermentation
  - Rectification
  - Adsorption
  - Molecular sieves
  - Pervaporation
- Catalytic
  - Direct Sequence
  - Indirect sequence
Optimal Design of Lignocellulosic Ethanol Plant

$67.5$ Million/yr

1,996 Btu/gal (< 1/10th of corn!)

Each NLP subproblem:  7000 eqs., 8000 var
≈25 min to solve

Ethanol: $0.81$/gal  (no H₂ credits)
$0.41$/gal  (H₂ credits)

Low cost is due to H₂ production

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Biorefinery

Bioethanol, FT-diesel and hydrogen from switchgrass
Biodiesel from cooking oil or algae oil

Martin, Grossmann (2012)
Optimal Development of Oil Fields (deepwater)

Offshore field having several reservoirs (oil, gas, water)

Decisions:
- Number and capacity of FPSO facilities
- Installation schedule for facilities
- Number of sub-seawells to drill
- Oil/gas production profile over time

Objective:
- Maximize the Net Present Value (NPV) of the project

MINLP model
- Nonlinear reservoir behavior
- Three components (oil, water, gas)
- Lead times for FPSO construction
- FPSO Capacity expansion
- Well Drilling Schedule
Example

20 Year Time Horizon
10 Fields
3 FPSOs
23 Wells
3 Yr lead time FPSO
1 Yr lead time expansion

Optimal NPV = $30.946 billion

Oil Flowrate

Discrete Var.  483
SOS1 Var.   0
Continuous Var.  5,684
Constraints  9,877
Solver     DICOPT 2x-C
NPV (billion dollars)  30.946
CPU time(s)      67
Shale Gas Reserves in World

units = trillion cubic feet
Larger circles = technical reserves
Smaller circles = potential reserves
yellow = current usage
blue = estimate for 2035

Optimal Drilling Strategy: Shale Gas

MINLP Optimization Model  
*Cafaro, Grossmann (2013)*

- 9 well-pads
- 20 wells per pad
- 3 potential plants
- 10 years
- 40 periods

**Methane Production**

**Ethane Production**

9 well-pads
20 wells per pad
3 potential plants
10 years
40 periods

Optimal Drilling Strategy: Shale Gas

MINLP Optimization Model  
*Cafaro, Grossmann (2013)*

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**Methane Production**

**Ethane Production**

Optimal Drilling Strategy: Shale Gas

MINLP Optimization Model  
*Cafaro, Grossmann (2013)*

- 9 well-pads
- 20 wells per pad
- 3 potential plants
- 10 years
- 40 periods

**Methane Production**

**Ethane Production**
Water use in hydraulic fracturing large but over short periods

Yang, Grossmann (2013)

Large volume of water (3-5 MM gallons) to complete a well

Well timeline

- Site Preparation: 3 weeks
- Drilling: 4-6 weeks
- Completion: 1-3 months
- Production: 20-40 years

» Most water used (65-80%) in fracking for shale is consumed
  
  > Accounts for 0.3% of all water consumption in the US\(^1\)
  > Accounts for 0.1% of all freshwater withdrawal in the US\(^1\)

Flowback water treated for reuse

1.3 gal/MMBtu for shale gas vs 7 coal/slurry and 50 oil

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Water use logistics in Shale Gas production
Scheduling model: STN discrete-time MILP model (Kondili, Pantelides, Sargent, 1993)

- **Robust source**
- **Intermittent source 1**
- **Intermittent source 2**

### Equations

- \[ V^d_{rt} \text{ Volume} \]
- \[ y^d_{pt} = 1 \]
  - *If pump from the source to impoundment*
- \[ y^d_{scj} = 1 \]
  - *If crew j starts to frac pad s on day d*

### Diagram

- **Frac crew 1**
- **Frac crew 2**
- **Frac pad s**
- **Frac pad s’**
- **Frac pad s”**
- **Pad A**
- **Impoundment 1**
- **Impoundment 2**
- **Pad J**
- **Pad L**
- **Truck**
- **Pipeline**

*Pumping is significantly cheaper than trucking*
Example: results

- **14 well pads**
- **540 time periods**
- **2 impoundments**
- **1 frac crew**

<table>
<thead>
<tr>
<th></th>
<th>Heuristic schedule</th>
<th>MILP schedule ‡</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trucking cost</td>
<td>$5,886,743</td>
<td>$568,827</td>
</tr>
<tr>
<td>Pumping cost</td>
<td>$9,905,219</td>
<td>$12,792,088</td>
</tr>
<tr>
<td>Total expected cost ($)</td>
<td>$15,791,963</td>
<td>$13,360,915</td>
</tr>
</tbody>
</table>

**Trucking cost is reduced by an order of magnitude.**
- 14,010 \(\rightarrow\) 1,350 truck trips.
- CO\(_2\) emissions from trucking reduced from 630 \(\rightarrow\) 60 metric tons
III. Enterprise-wide Optimization

Beyond the plant level/ Integration with business operations

Wellhead
- Trade & Schedule
- Crude and Other Feedstocks

Transfer of Crude and Feedstocks to Refinery

Refinery Optimization

Trade & Schedule Products

Transfer of Products from Refinery to Terminal

Terminal Loading

Pump

Discovery
- Targets
- Hits
- Leads
- Candidate

Development
- Pre-clinical Development
- Phase 1
- Phase 2a/b
- Phase 3

Market
- Submission & Approval
- Lifecycle Management

Colin Gardner (Transform Pharmaceuticals)

Dennis Houston (ExxonMobil)
Integrated Planning and Scheduling Batch Plant

- Batch units operating in parallel
- Sequence-dependent changeovers between products groups
- A subset of products are blended

Bi-level Decomposition

Upper Level Planning (ULP)
Determine upper bound (UB) on profit

Add cuts

Outputs: assignments (fixed for LLS) and number of batches of each product

Lower Level Scheduling (LLS)
Determine lower bound (LB) on profit

UB - LB < tolerance?

no

yes

Stop
Solution = LB

Calfa, Agarwal, Wassick, Grossmann (2013)
Example

- 2 parallel units
- 2 raw materials
- 7 products (6 individual and 1 blended)
- 10 customers
- Time horizon
- 12 weeks

Optimal Schedule (week 1)

Bilevel decomposition converged in one iteration!

*Upper level MILP*: 1,032 0-1  1,800 cont.v.  3,300 constr.  2.5 sec

*Lower level MILP*: 19,600 0-1  23,100 cont.v.  15,300 constr  479 sec
Given:
- Power-intensive plant
- Products $g \in G$ (Storable and Nonstorable)
- Product demands $d^t_g$ for season $t \in T$
- Seasonal electricity prices on an hourly basis $e^{t,h}$, $t \in T$, $h \in H$
- Upgrade options $u \in U$ of existing equipment
- New equipment options $n \in N$
- Additional storage tanks $s \in ST$

Determine:
- Production levels $Pr^{t,h}_g$
- Mode of operation $y^{t,h}_{m,o}$
- Sales
- Inventory levels $s^{t,h}_g$
- Upgrades for equipment $VU^{t}_{m,u}$
- Purchase of new equipment $VN^{t}_{n}$
- Purchase of new tanks $VS^{t}_{n,g}$

With minimum investment and operating costs
Incorporating design decisions: seasonal variations drive the development of a seasonal model

- Horizon: 5-15 years, each year has 4 periods (spring, summer, fall, winter)
- Each period is represented by one week on an hourly basis
- Each representative week is repeated in a cyclic manner (13 weeks reduced to 1 week) (8736 hr vs. 672 hr)
- Design decisions are modeled by discrete equipment sizes
### MILP model for multi-scale capacity planning

#### Objective

![Objective](image1.png)

<table>
<thead>
<tr>
<th>Operational</th>
<th>Strategic</th>
<th>Terms for the objective function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Disjunction over the modes that describe the feasible region</td>
<td>Additional storage</td>
<td>Idea: additional modes for which all variables are controlled by the corresponding binary investment variable</td>
</tr>
<tr>
<td>Operational Logic constraints for transitions (e.g. minimum uptime/downtime)</td>
<td>Additional equipment</td>
<td>Idea: the corresponding mode has an alternative feasible region</td>
</tr>
<tr>
<td>Operational Mass balances for inventory, constraints related to demand</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
\text{min} \quad \text{OBJ} = \sum_t (\text{Cost}_{\text{ops}}^t + \text{Cost}_{\text{invest}}^t) \quad (37)
\]
Retrofitting an air separation plant

Superstructure

- Existing equipment
  - Option A
  - Option B? (upgrade)
- Additional Equipment

Air Separation Plant

- LIN 1.Tank
- LIN 2.Tank?
- Liquid Nitrogen
- LIN 1.Tank
- LIN 2.Tank?
- Liquid Argon
- LAR 1.Tank
- LAR 2.Tank?
- Liquid Oxygen
- LOX 1.Tank
- LOX 2.Tank?
- Gaseous Oxygen
- Gaseous Nitrogen
- Pipelines

Time

- Spring - Investment decisions: (yes/no)
  - Option B for existing equipment?
  - Additional equipment?
  - Additional Tanks?
- Fall - Investment decisions: (yes/no)
  - Option B for existing equipment?
  - Additional equipment?
  - Additional Tanks?

- Spring
- Summer
- Fall
- Winter

- The resulting MILP has **191,861 constraints** and **161,293 variables** (18,826 binary.)
- Solution time: **38.5 minutes** (GAMS 23.6.2, GUROBI 4.0.0, Intel i7 (2.93GHz) with 4GB RAM).
Investments increase flexibility help realizing savings

Remarks on case study

- **Annualized costs:** $5,700,000/yr
- **Annualized savings:** $400,000/yr

- **Buy new liquefier** in the first time period (annualized investment costs: $300k/a)
- **Buy additional LN2 storage tank** ($25k/a)
- **Don’t upgrade existing equipment** ($200k/a) equipment: 97%.

---

**Power consumption**

- Power consumption w/ investment
- Power consumption w/o investment
- Summer prices in $/MWh

**LN2 inventory profile**

- Outage level
- LN2-w/ investment
- 2-tanks capacity
- LN2-w/o investment
- 1-tank capacity

---

**Hour of a typical week in the summer season**

<table>
<thead>
<tr>
<th>1</th>
<th>25</th>
<th>49</th>
<th>73</th>
<th>97</th>
<th>121</th>
<th>145</th>
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</thead>
<tbody>
<tr>
<td>Power consumption</td>
<td>Power consumption w/ investment</td>
<td>Power consumption w/o investment</td>
<td>Summer prices in $/MWh</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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**Price in $/MWh**

- 0
- 50
- 100
- 150
- 200
Optimal Design of Responsive Process Supply Chains

Objective: design supply chain polystyrene resins under responsive and economic criteria

You, Grossmann (2008)
Potential Network Superstructure

 Suppliers Plant Sites Distribution Centers Customers

Max: Net present value Max: Responsiveness Demand uncertainty ⇒ Responsiveness

Expected Lead Time
Example Bi-criterion Multiperiod MINLP

Pareto Curves – with and without safety stock

Best Choice

Expected Lead Time (day)

NPV (M$)

with safety stock
without safety stock
Network Structure at Location Map

You, Grossmann (2009)
Optimal Planning of Sustainable Chemical Supply Chains

Guillen, Grossmann (2010)

Life Cycle Analysis

Bicriterion optimization
Max Net Present Value
Min Environmental Impact

Eco-Indicator 99 for LCA
(Health, Ecosystem, Resources)

Uncertainty in emissions

Parametric programming
Concluding Remarks

Major challenges in Process Systems Engineering

- Product and Process Design
- Energy and Sustainability
- Enterprise-wide Optimization

+ Fundamentals of Process Systems Engineering
  - Modeling
  - Optimization
  - Process Synthesis
  - Process Operations
  - Process Control

Challenge for Process Systems community:
- Communicate importance of area to rest of Chemical Engineering
- Driven by Industrial Needs!!
- Chemical Engineering Community needs recognize value of PSE
Remarks on Education

1. Need to keep core Chemical Engineering Knowledge
   Need to emphasize fundamentals: basis life-long learning

2. Need to modernize curriculum and add flexibility
   • Increase exposure molecular level
   • Increase exposure to energy (alternative/renewable) and sustainability issues
   • Expose students to new process technology
   • Introduce product design as complement of process design
   • Emphasize process operations, enterprise planning
   • Increase link to other industrial sectors (pharma, electronics)

3. Need to recognize that “bio-area” will be important but not dominant force in Chemical Engineering; similarly “nano area”

4. Environmental Engineering increasingly important and requires chemical engineering (water use efficiency, pollution control.) Civil Eng. ownership?

5. Need closer interaction with industry; otherwise risk being irrelevant

6. Need to provide excitement to recruit the very best young people to join Chemical Engineering

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