Role of Process Systems Engineering in Chemical Engineering

Ignacio E. Grossmann
Center for Advanced Process Decision-making (CAPD)
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213, U.S.A.

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

Chemstations Focused on process simulation

Seattle ASEE's 122nd Annual Conference & Exposition Washington Convention Center Seattle, WA June 14 – 17, 2015 Making Value for Society

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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

Unit Operations

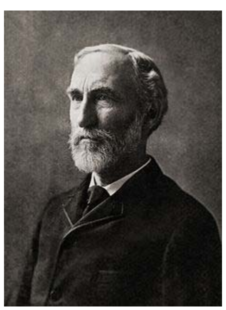
Arthur D. Little, MIT,1916

Chemical Engineering Principles

William Walker, MIT 1924

Olaf Hougen, Wisconsin 1947

Thermodynamics



J.W. Gibbs, 1878

H. Helmholtz, 1847

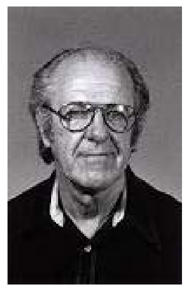
L. Boltzmann, 1866

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

Transport Phenomena

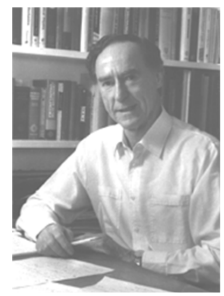
Bird, Stewart, Lightfoot, Wisconsin, 1960

Applied Mathematics/Reaction Engineering



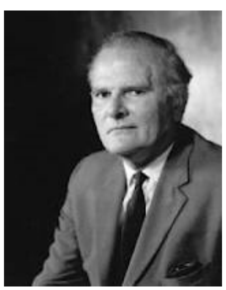
R. Aris, 1962; N. Amundson, 1972; Minnesota

Fluid Mechanics



G. Batchelor, Cambridge, 1967

Mass Transfer

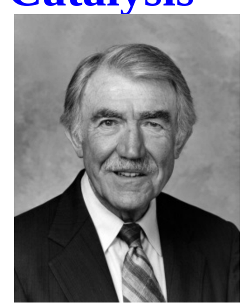


P.V. Danckwerts, Cambridge 1965

Polymers

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

Catalysis

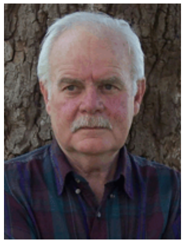


Michel Boudard, Stanford 1968

Chemical ENGINEERING

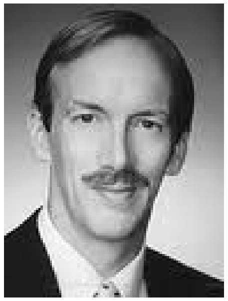
Process Systems Engineering

CAPD CENTER



Dale Rudd, Wisconsin 1968 **Roger Sargent, Imperial College1964**

Bioengineering



Robert Langer, MIT 1977 **Jay Bailey, Caltech 1986** **Michael Shuler, Cornell, 1984**

Nanotechnology

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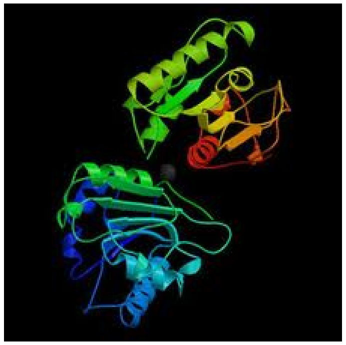
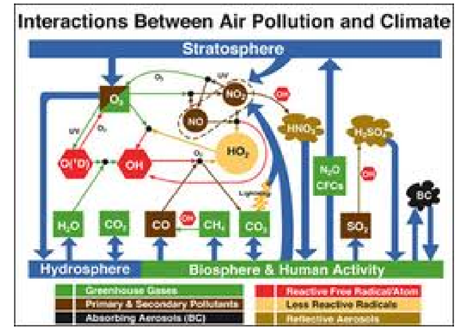
Richard Feyman, Caltech 1968 **George Whitesides, Harvard 1968**

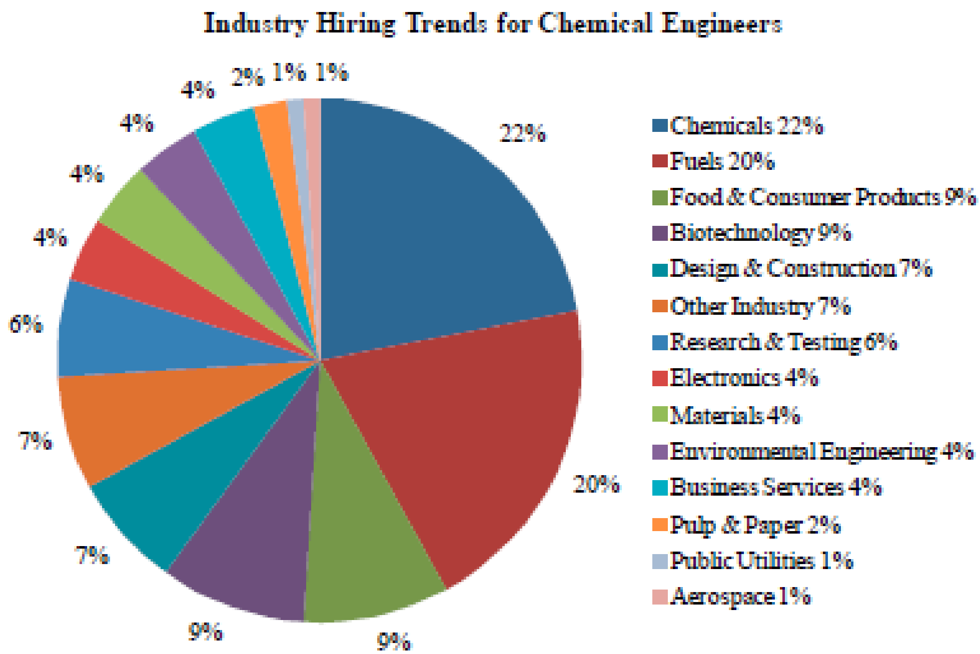
Diversification Chemical Engineering



Chemical Engineers work in a variety of manufacturing operations including oil refineries like this one.



B.S. Job placement (AIChE, 2007)



Chemicals
Fuels ~42%

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: 1^{st}&2^{nd} Law, Phase & Chemical Equilibria)

  - Process Design courses largely outsourced to retired industry people

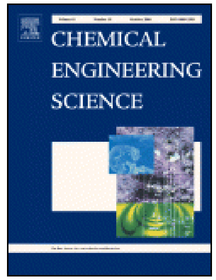
  - Process Control no longer required at several U.S. universities

Many faculty members in US *do not publish anymore* *in chemical engineering journals*

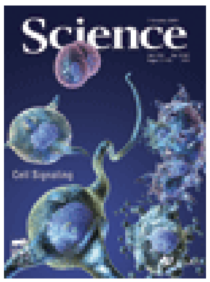
Move from Engineering to Science

25% US

15% US



Impact factors ~2.2



Impact factors ~30

The Industry Connection

Revenues of major U.S. companies (billions)

	(2006)	*(2012)*
ExxonMobil	$365.5	$452.93
ChevronTexaco	204.9	241.9
Dow	49.1	56.8
DuPont	27.4	38.72
Procter & Gamble	68.2	82.55
Johnson & Johnson	53.3	67.22
Merck	22.3	48.05
Bristol-Myers Squibb	17.9	21.24
Amgen	13.8	23.6
Genentech	7.6	17.3

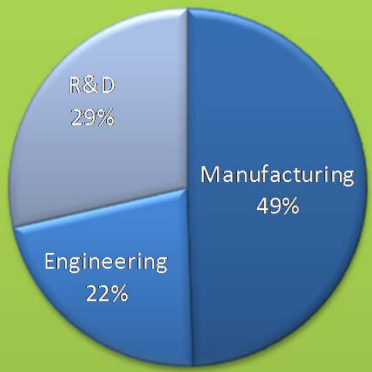
One trillion dollar industry !!

Industrial Survey on Importance of Skills

John Chen (2013)

13AIChE Annual Meeting, San Francisco, CA

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



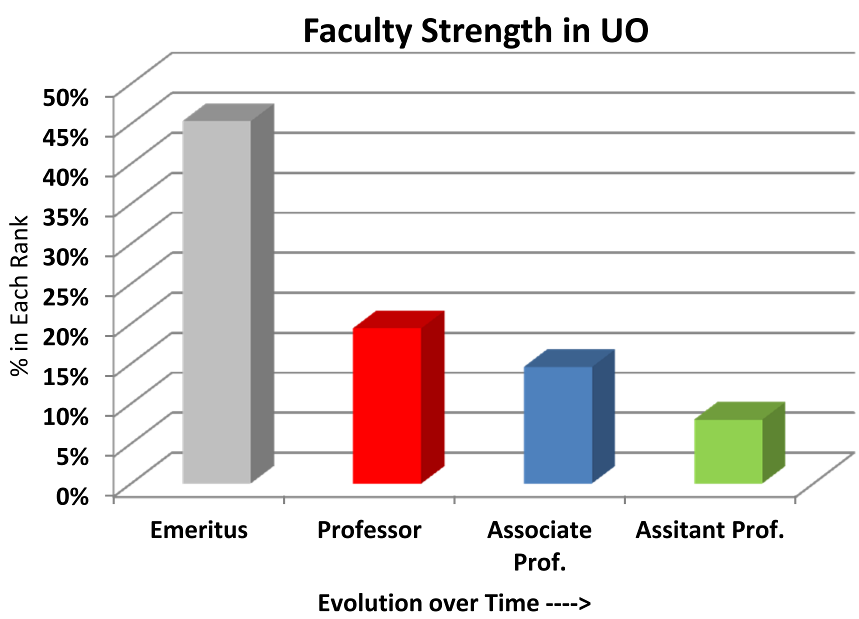
93 respondents (ChemE recruiters and leaders)

* *main perceived gaps between importance and proficiency by new hires*

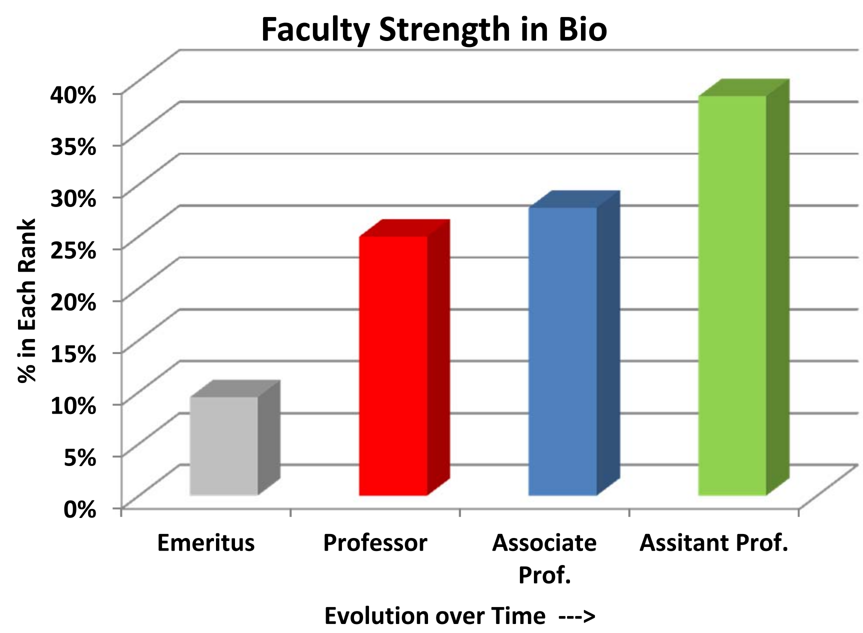
Academic Disconnect: Trends Faculty Composition

13AIChE Annual Meeting, San Francisco, CA

Unit Operations



Bioengineering



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

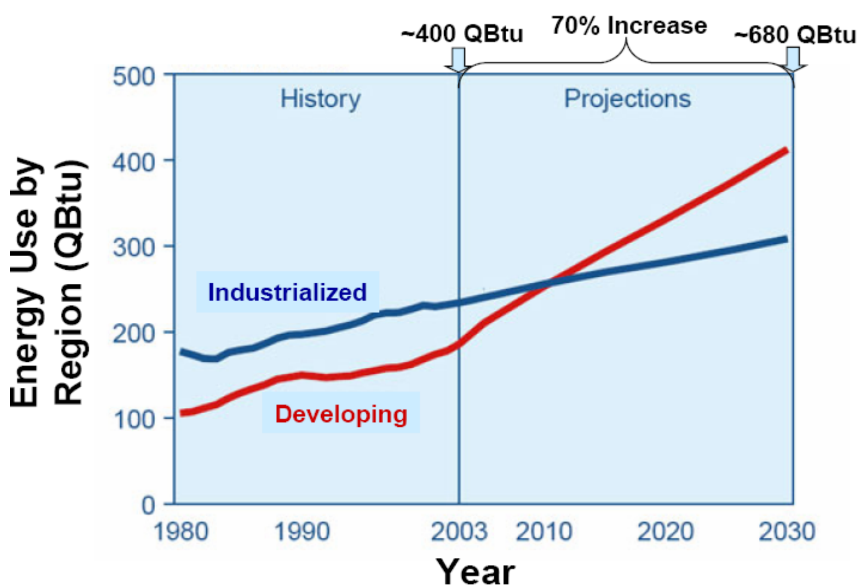
$25 million/year for next 10 yr in US

$10 million/year for next 10 yr outside US

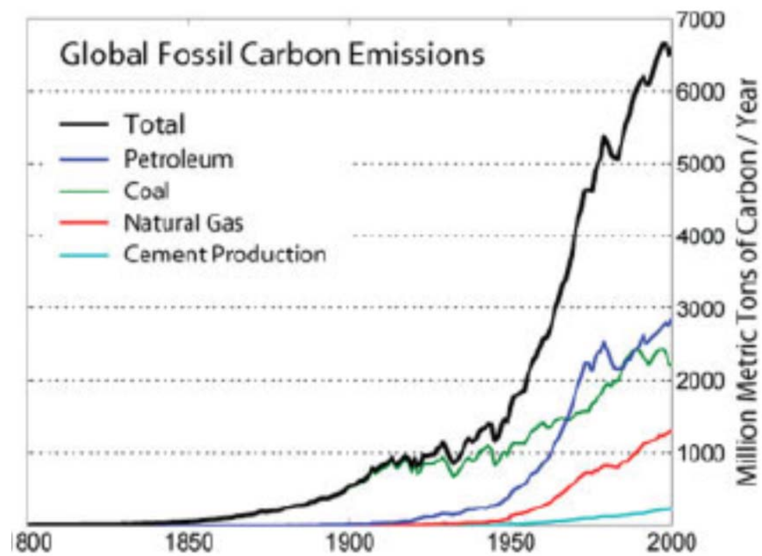
R&D
Dow Research & Development

New emphasis: energy and sustainability

Growing World Energy Demand
Most Energy Growth in Developing Nations



DOE EIA, International Energy Outlook 2006, Figure 8



Sheppard, Socolow (2007)

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

*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***

$$\min Z = f(x, y)$$
$$s.t. \quad h(x, y) = 0$$
$$g(x, y) \le 0$$
$$x \in R^n, \quad y \in \{0,1\}^m$$

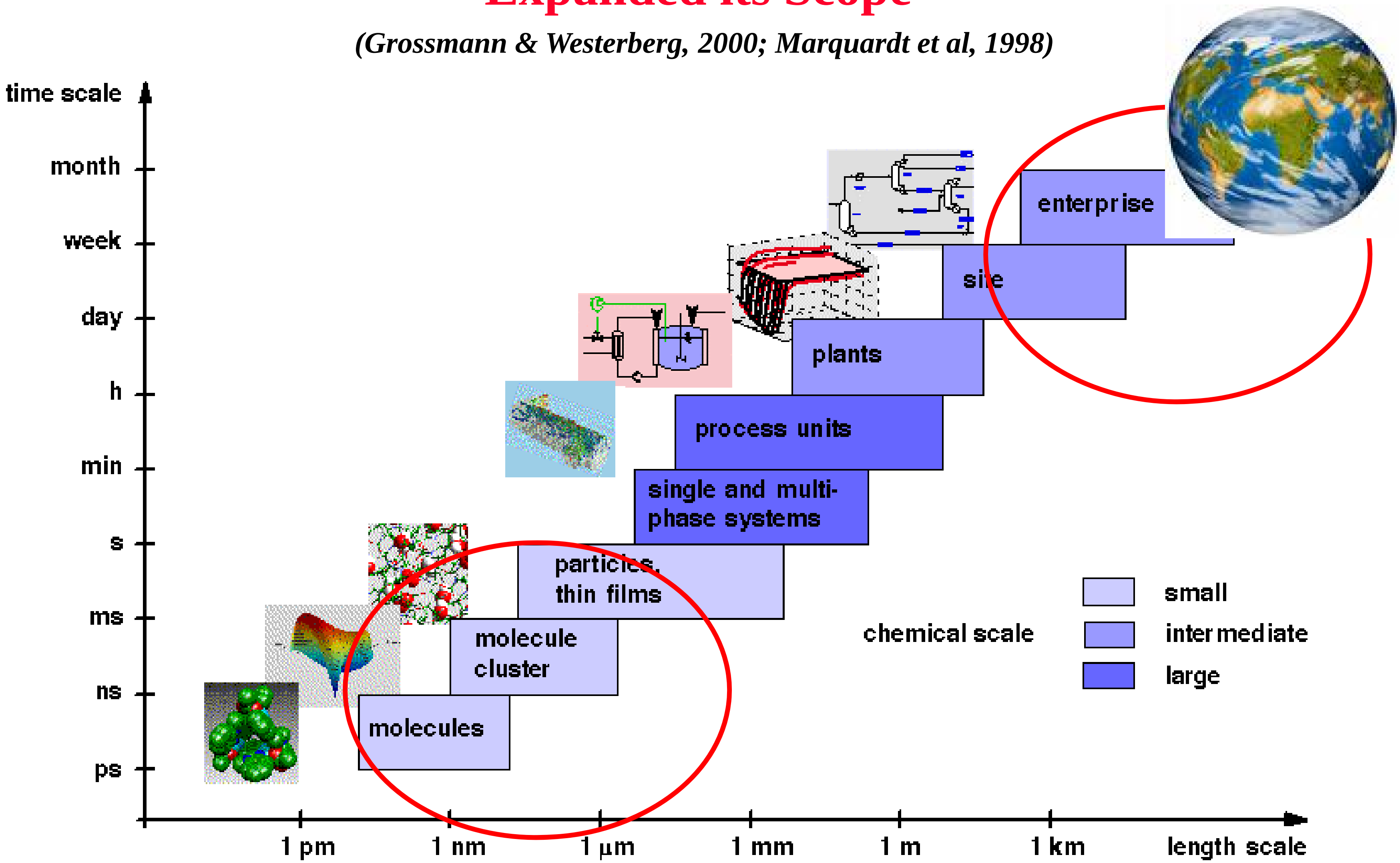
MILP: *f, h, g* linear

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)



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Research Challenges in PSE

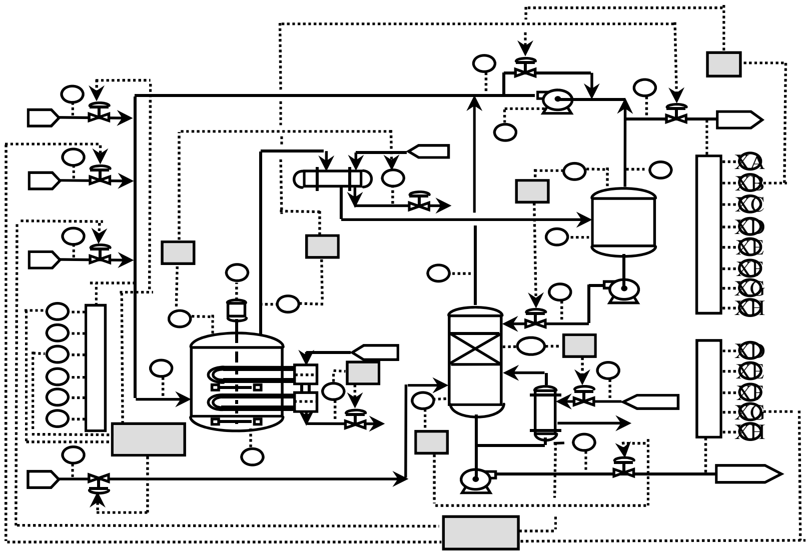
I. Product and Process Design

II. Energy and Sustainability

III. Enterprise-wide Optimization

I. Product and Process Design: from “Bulk” to “Molecular” Processing

George Stephanopoulos (2004)

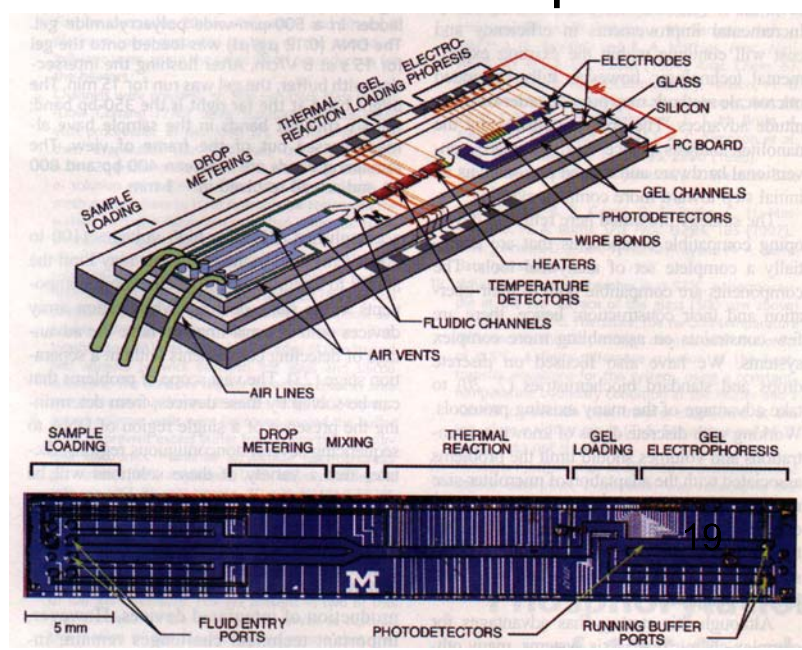


Macro-Processing:

Batch or Continuous Chemical Plants

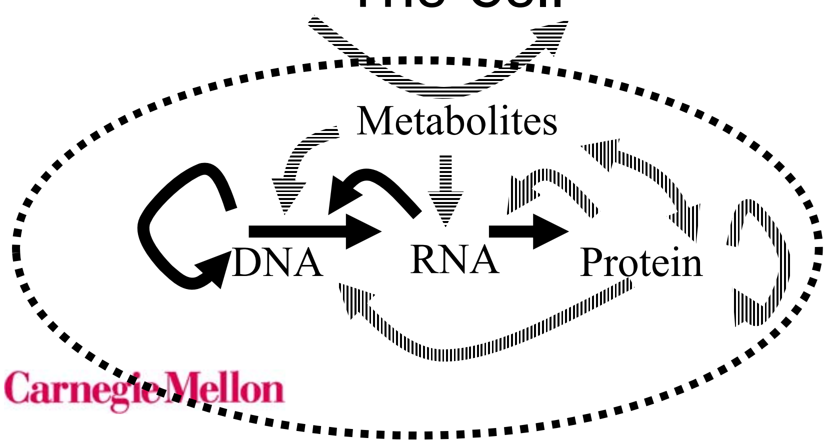
Micro-Processing:

Plant-on-a-Chip



Molecular-Processing:

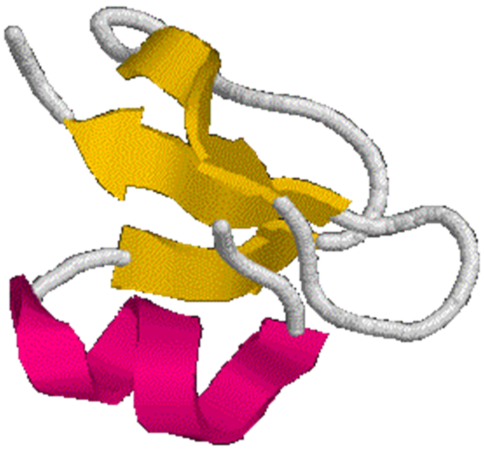
The Cell



De Novo Protein Design *(Chris Floudas, Princeton)*

Define target template

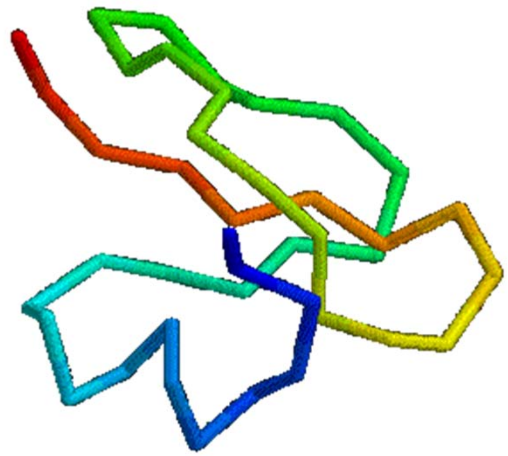
Backbone coordinates for N,Ca,C,O
and possibly Ca-Cb vectors from PDB



Human b-Defensin-2
hbd-2 (PDB: 1fqq)

Design folded protein

Which amino acid sequences will stabilize this target structure ?



Full sequence design

Combinatorial complexity

-Backbone length : n

-Amino acids per position : m

m^n possible sequences

Approach

In silico sequence selection => MILP

Fold specificity => Global optimization

=> New improved inhibitors

(Klapeis, Floudas, Lambris, Morikis, 2004)

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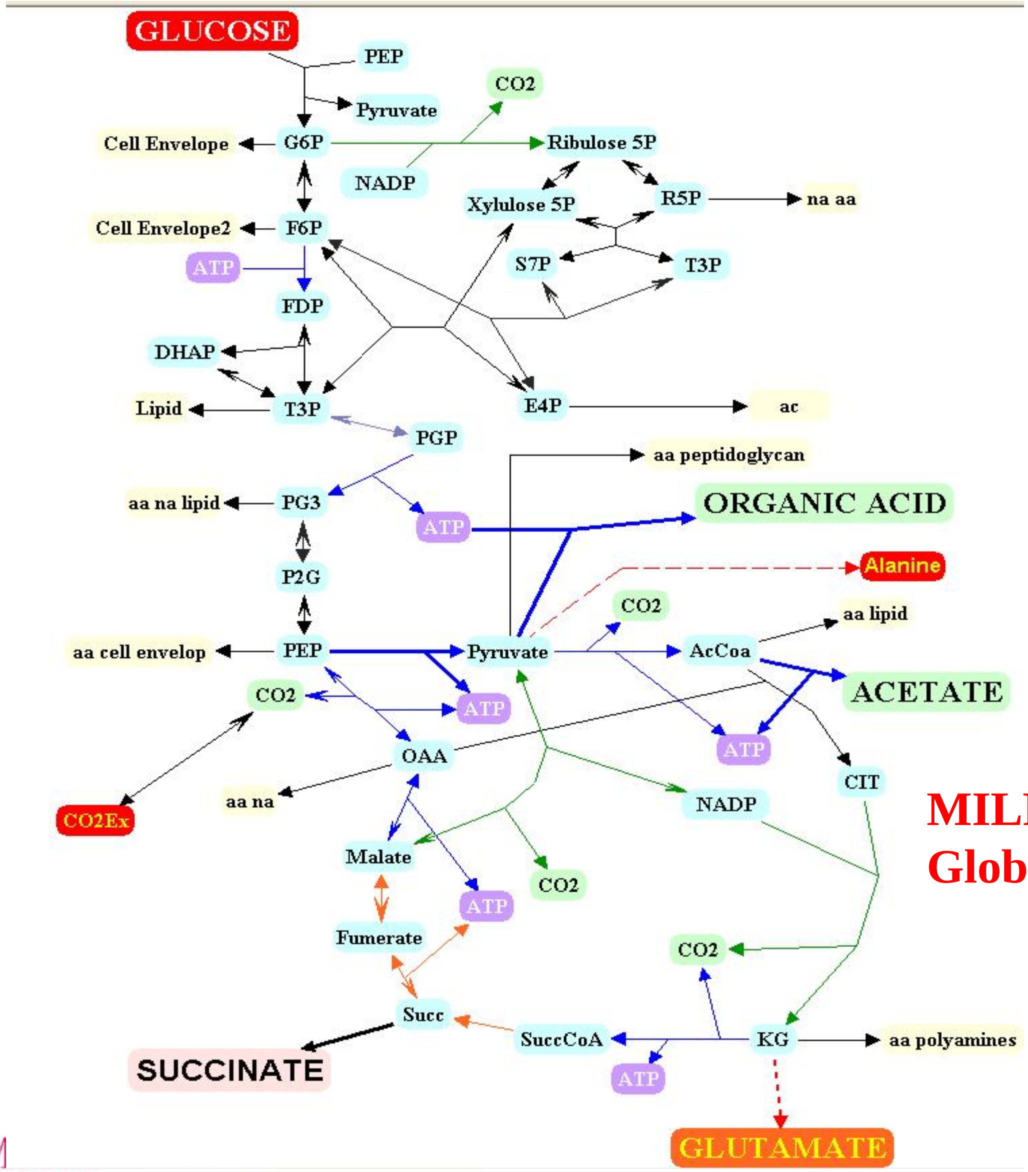
Metabolic Networks: Inverse Problem



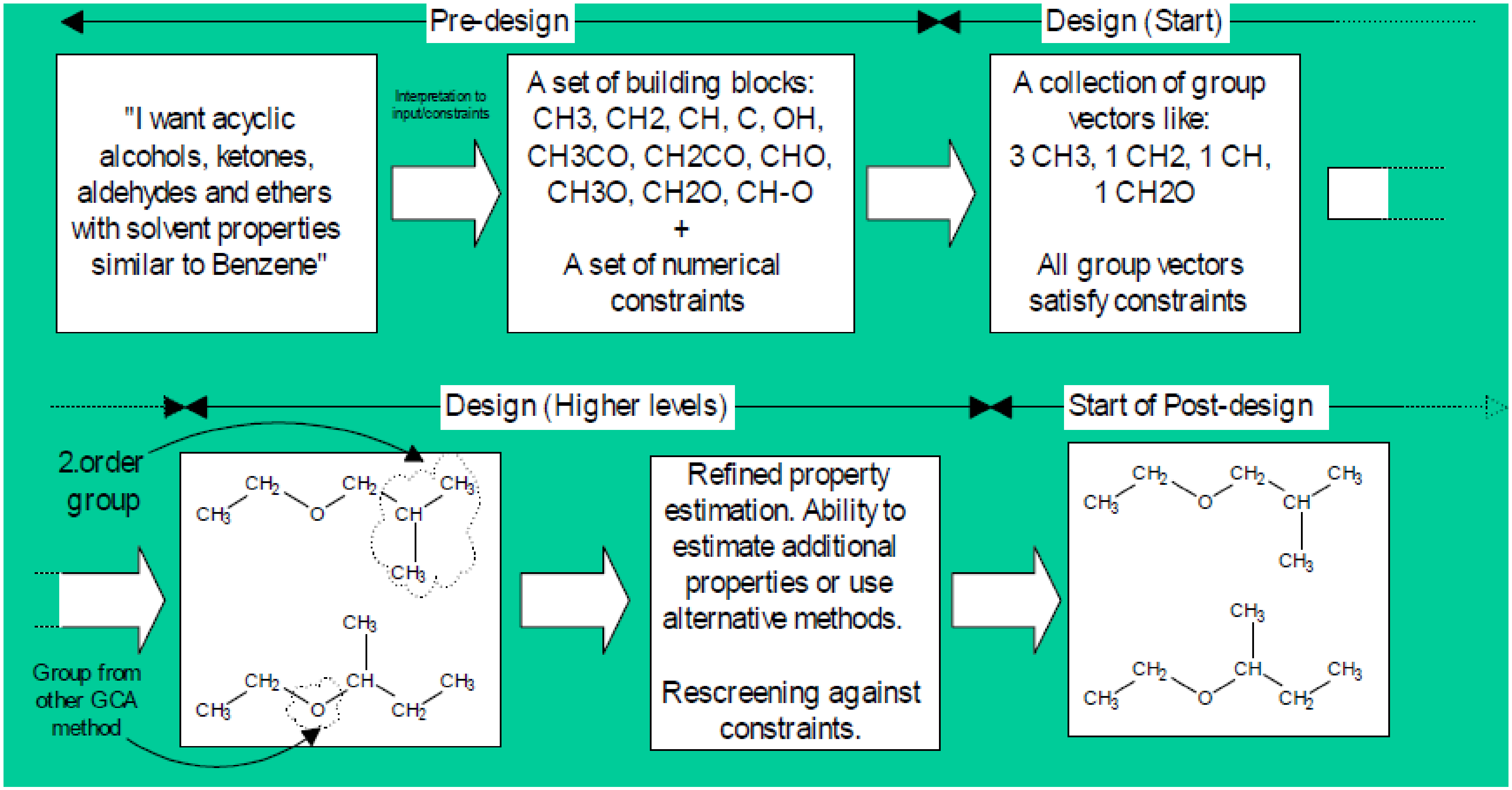
(Ghosh, Domach, Grossmann, 2005)

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



Method: CAMD (Computer Aided Molecular Design)

Gani et al. (2012)

CATERPILLAR®

Integrated Design of Formulated Rubber Parts

Venkat Venkatasubramanian

Multi-Scale Model

Quantum Mechanics

↓

Kinetics

↓

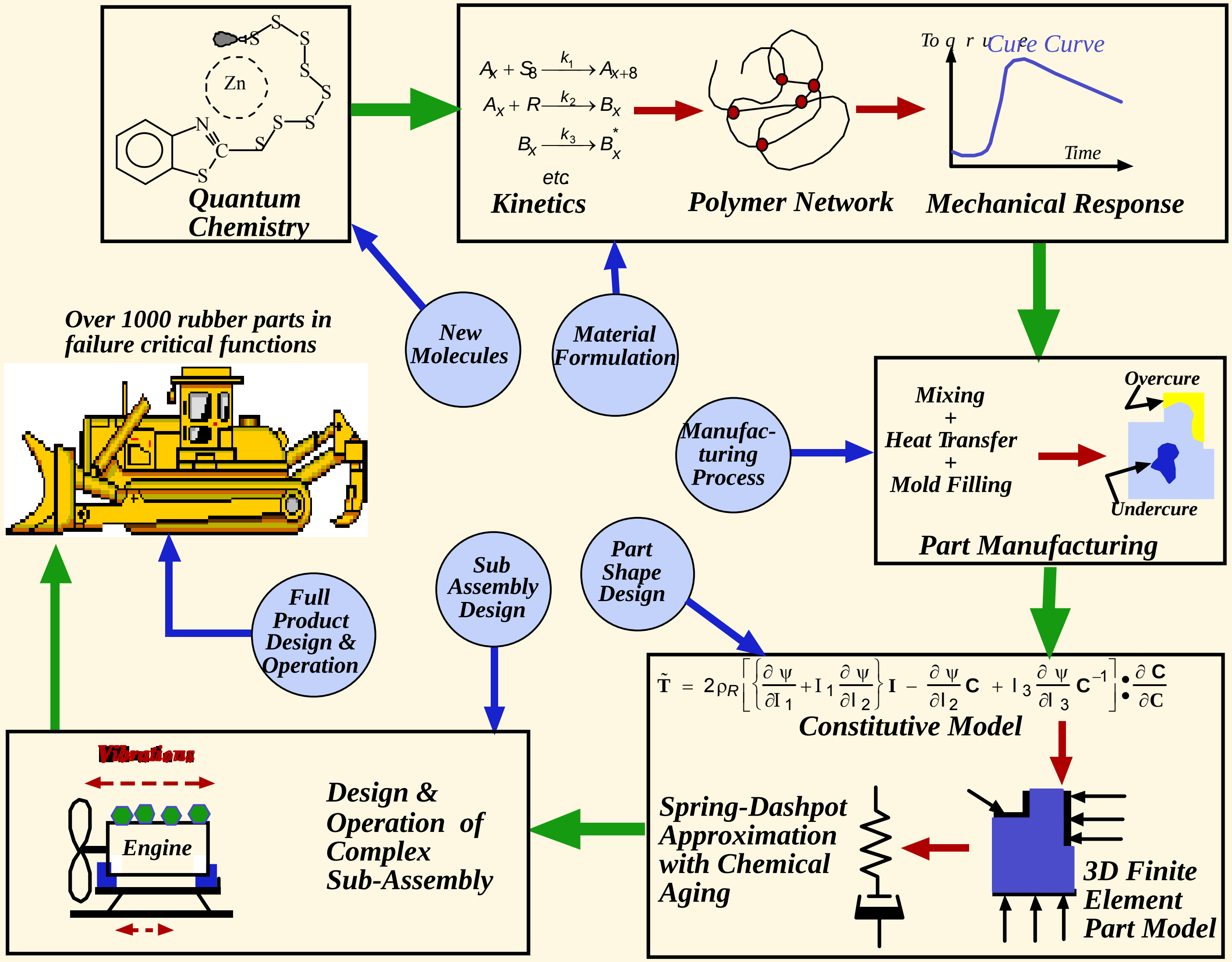
Heat Transfer FEA

↓

Mechanics FEA

↓

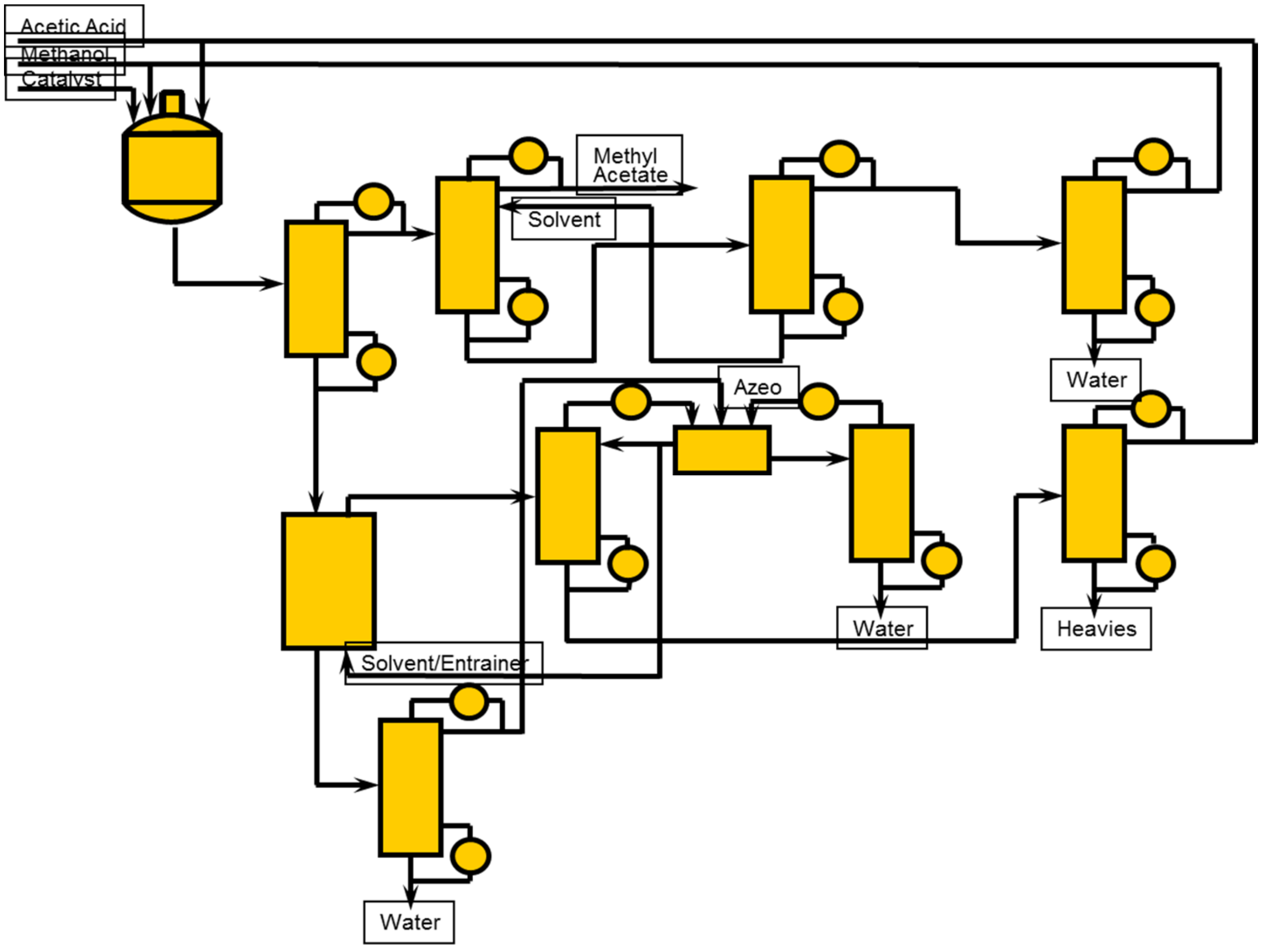
Part Design CAD /CAM



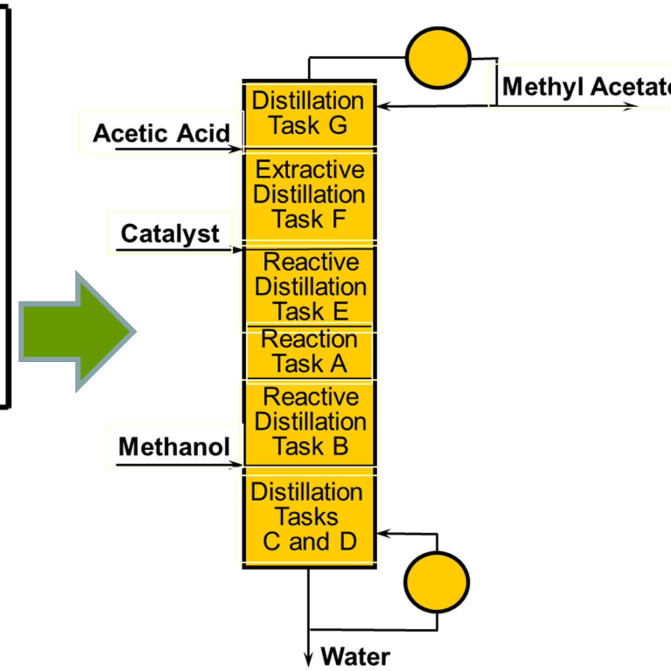
PURDUE UNIVERSITY

Example Process Intensification

Methyl Acetate Flowsheet



Single Reactive Dist Col!

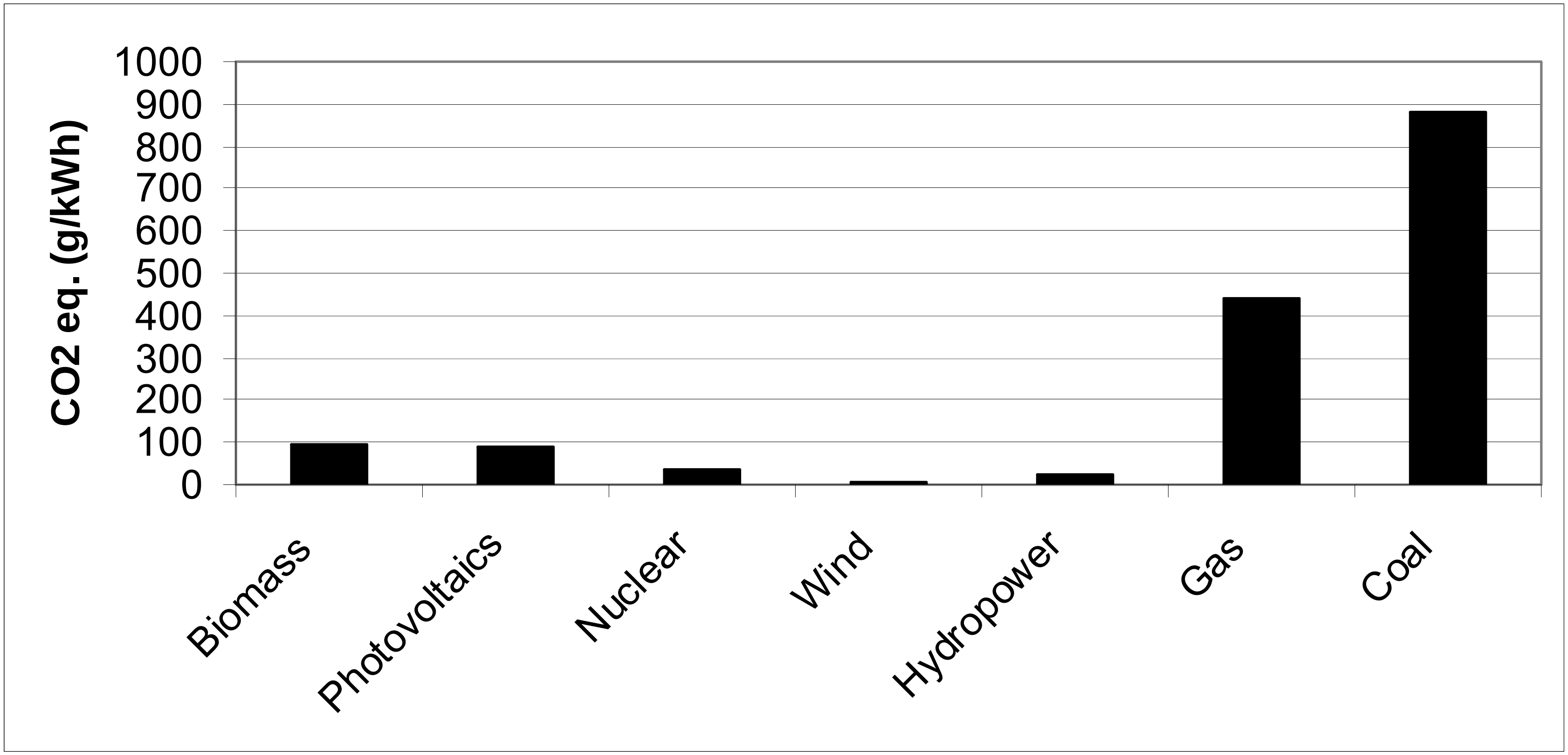


EASTMAN *Siirola (1988)*

II. Energy and Sustainability

Environmental impact

Renewables: Carbon footprint various Energy Options



Adisa Azapagic (2012)

Oil Reserves

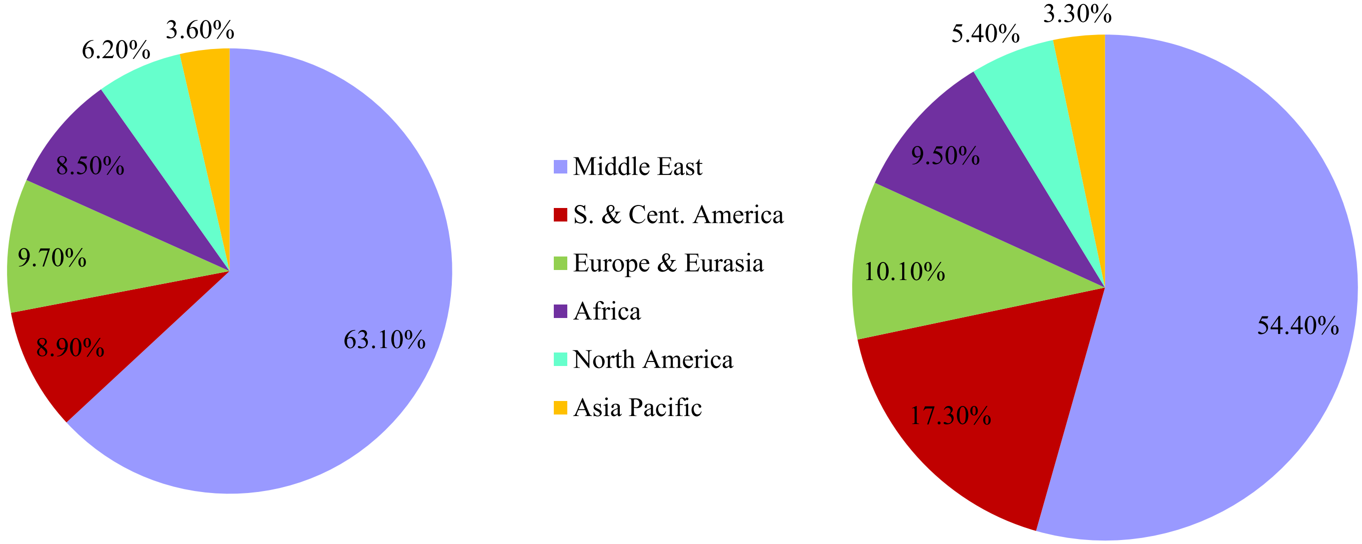
Year 2000

Total: 1105 thousand million barrels

Year 2010

Total: 1383 thousand million barrels

25% increase!

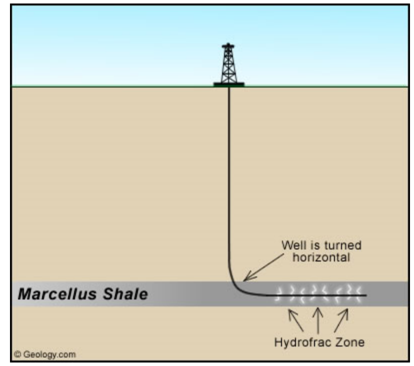


- ***Discovery of New Large Oil and Gas Reserves***
- ***New technologies for Offshore oil exploration and production***

Statistical Review of World Energy (June, 2011)

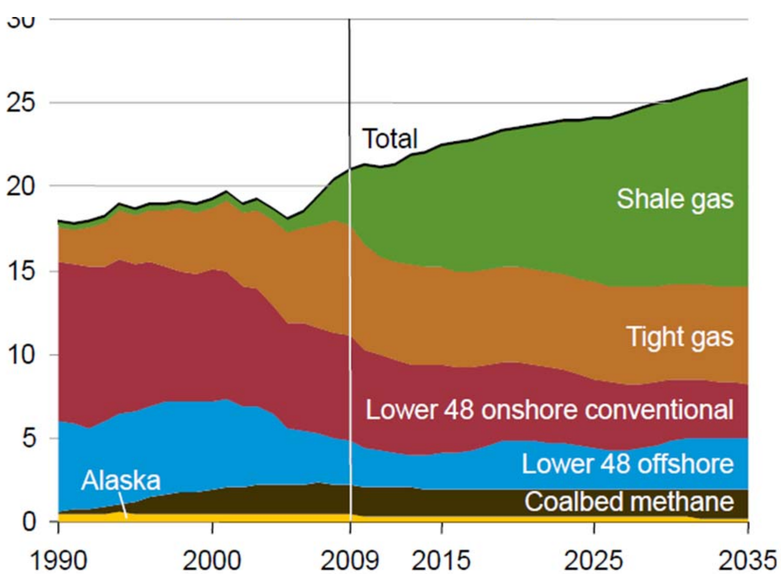
Depletion of fossil fuels?

Growth in Shale Gas

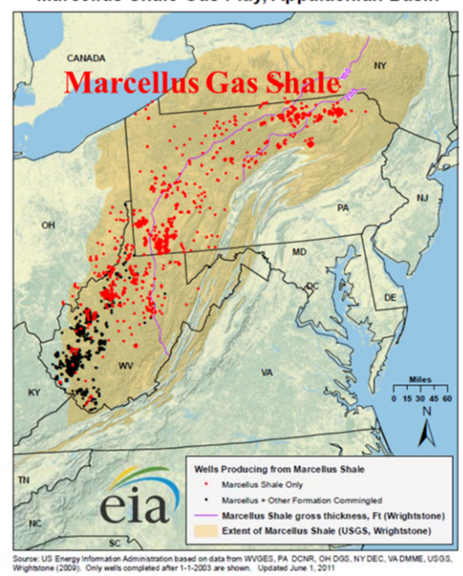


Horizontal drilling
Hydraulic fracking

Figure 89. Natural gas production by source, 1990-2035



Marcellus Shale Gas Play, Appalachian Basin



Large amount "wet 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)**

06-421 Chemical Process Systems Design
Carnegie Mellon University

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)*

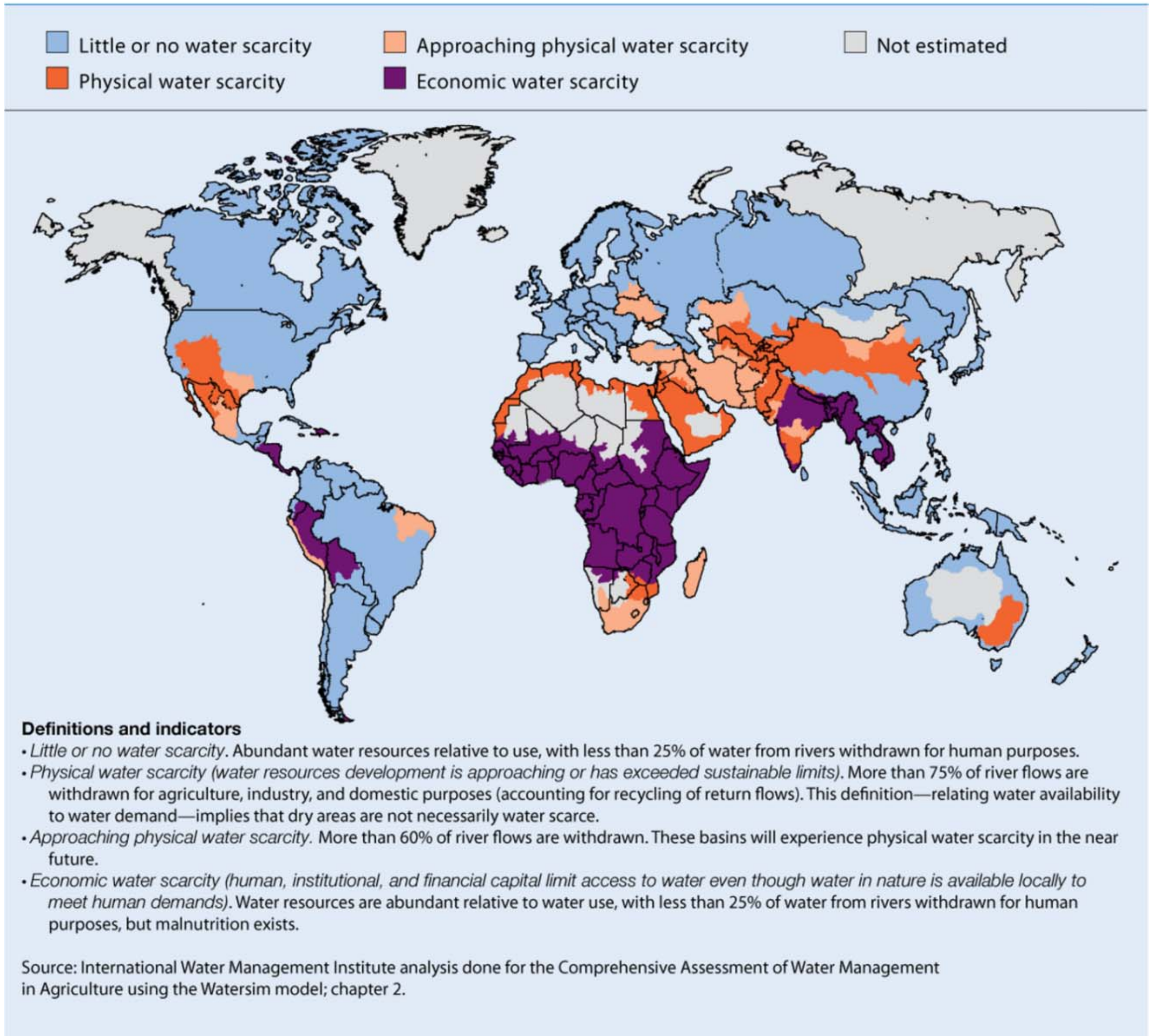
Plant location: Monaca (next to Shell's projected cracker)

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**

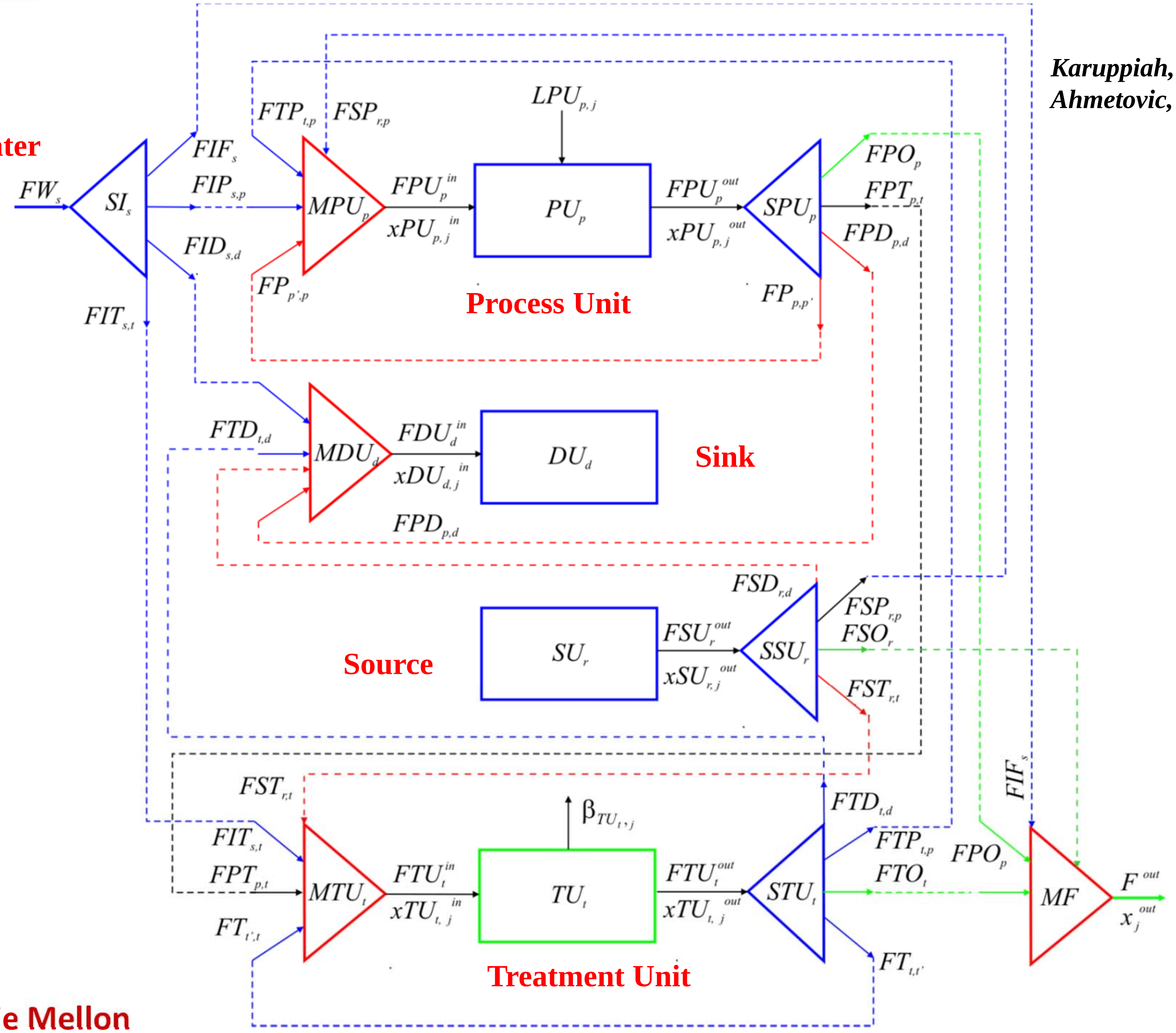
Water scarcity



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

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: ***min Cost***

Subject to:

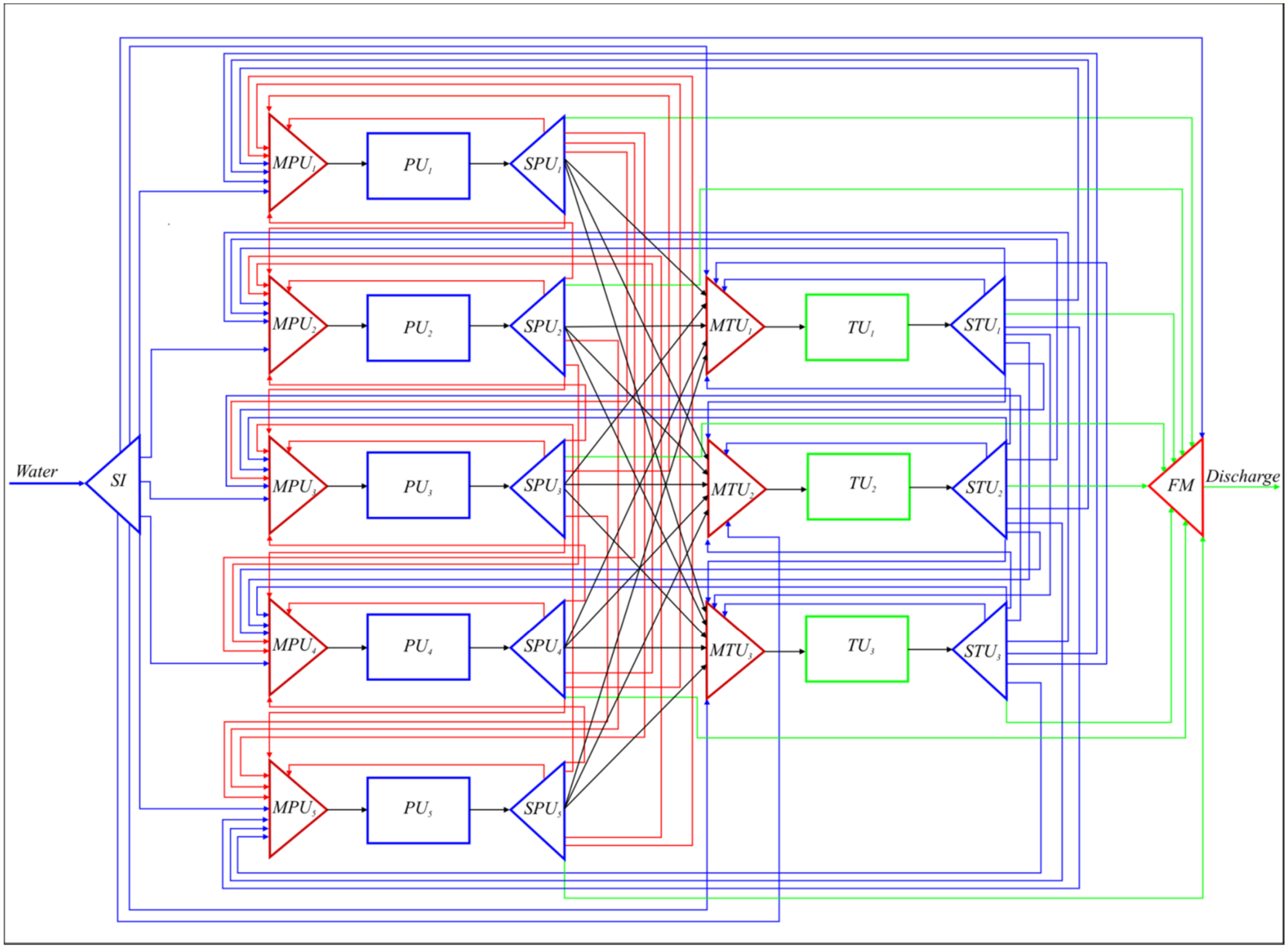
Splitter mass balances
Mixer mass balances (bilinear)
Process units mass balances
Treatment units mass balances
Design constraints

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

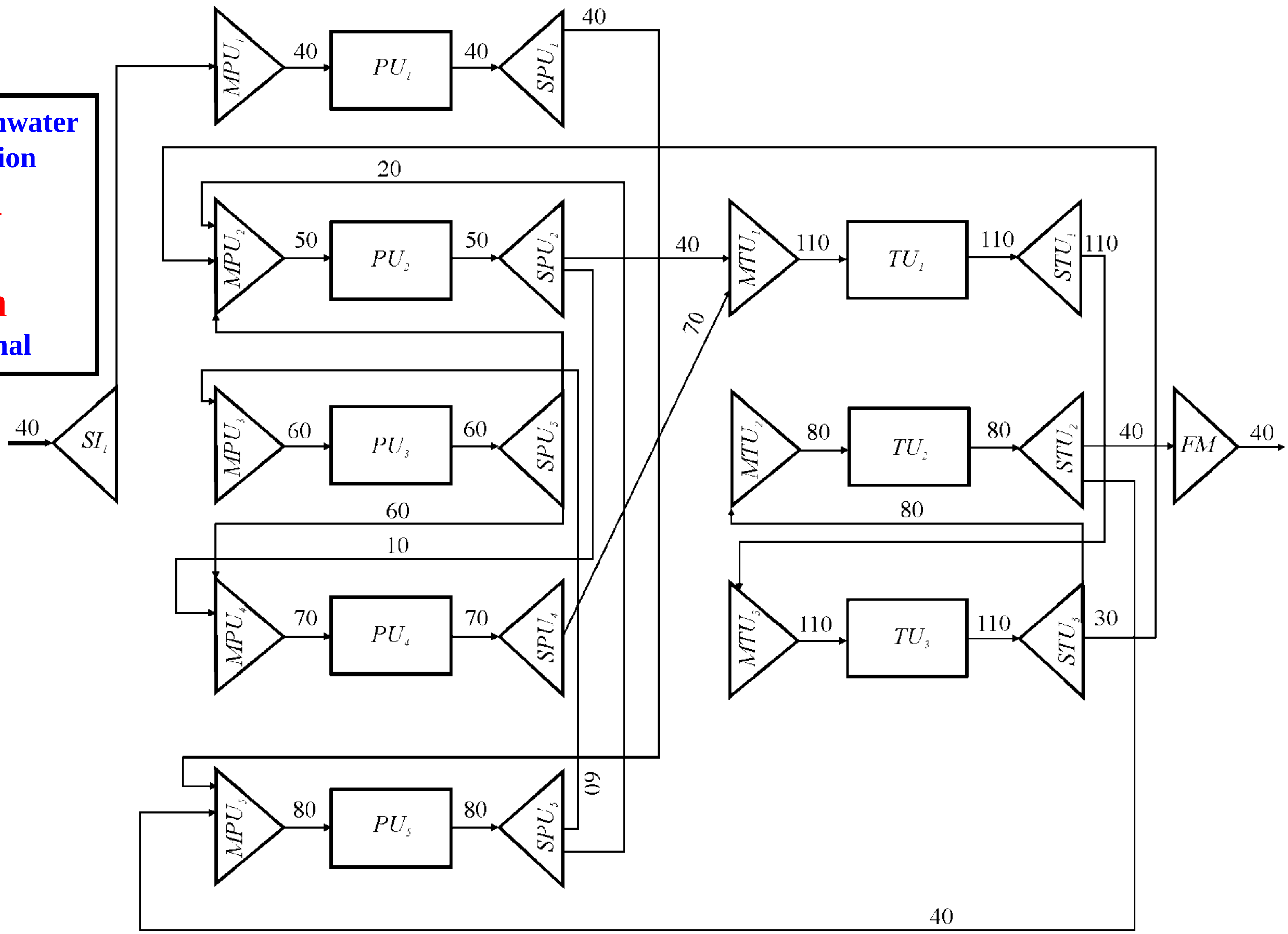
Optimal Freshwater Consumption

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

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

Water consumption corn-based process

Author (year)	Water consumption (gal/gal ethanol)
Gallager (2005) First plants	11
Philips (1998)	5.8
MATP (2008) Old plants in 2006	4.6
MATP (2008) New plants	<u>3.4</u>

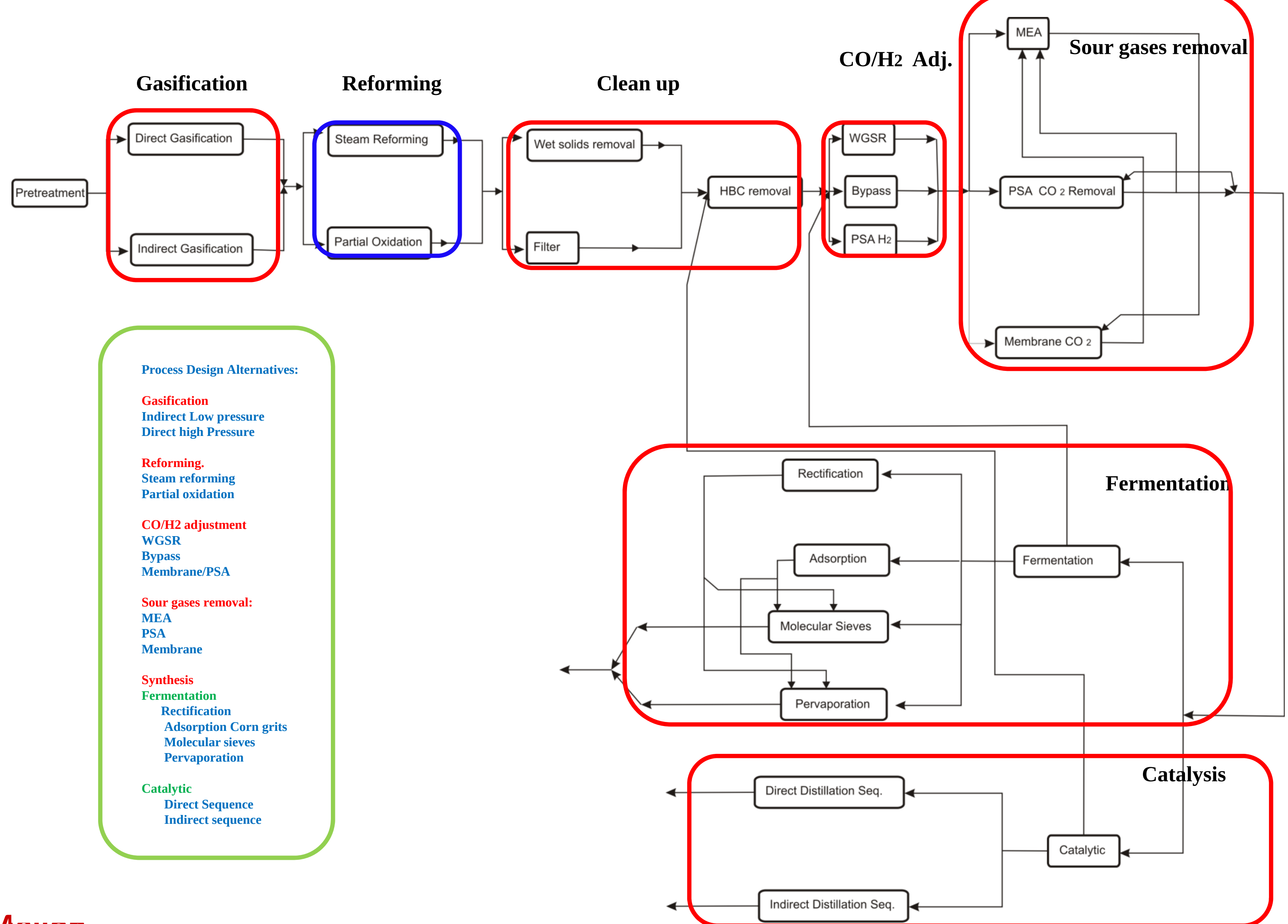
From Karrupiah et al (2007)
<u>24,918 Btu/gal</u> vs 38,323 Btu/gal
Why? ***Multieffect distillation and heat integration***

From Martin and Grossmann (2010)
<u>1.5 gal water/gal ethanol</u> vs 3.4
Why? ***Integrated process network with reuse and recycle***

Superstructure Thermochemical Bioethanol

Martin, Grossmann (2010)

Ethanol via gasification



Process Design Alternatives:

Gasification
Indirect Low pressure
Direct high Pressure

Reforming.
Steam reforming
Partial oxidation

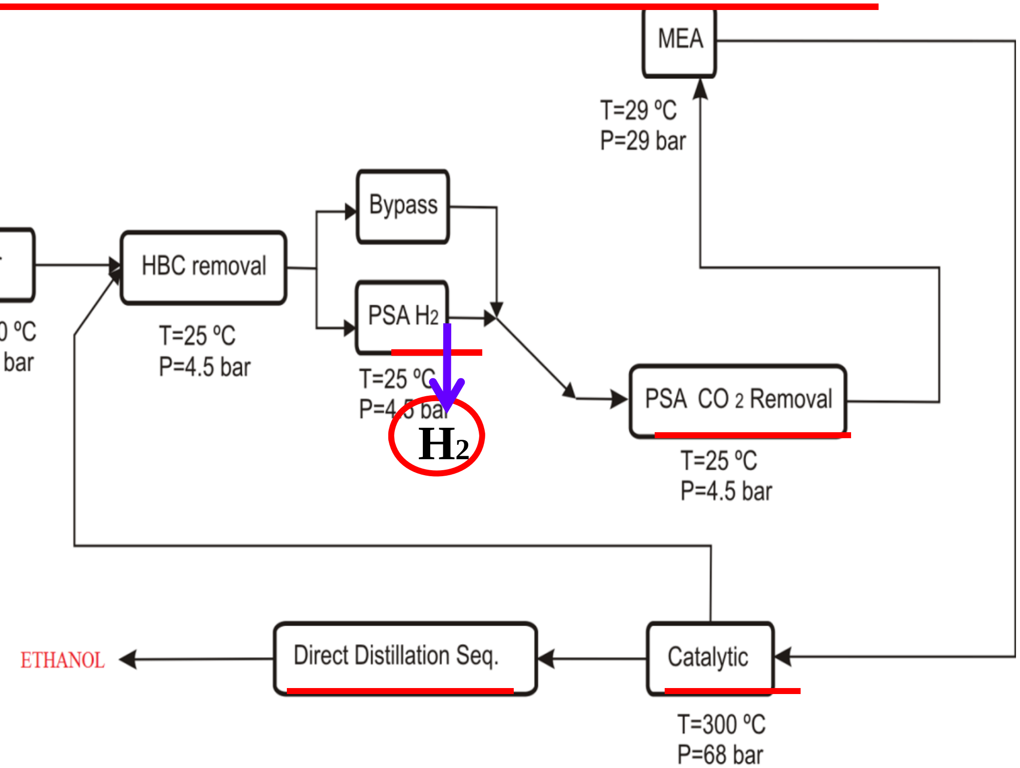
CO/H2 adjustment
WGSR
Bypass
Membrane/PSA

Sour gases removal:
MEA
PSA
Membrane

Synthesis
Fermentation
- **Rectification**
  - **Adsorption Corn grits**
  - **Molecular sieves**
  - **Pervaporation**

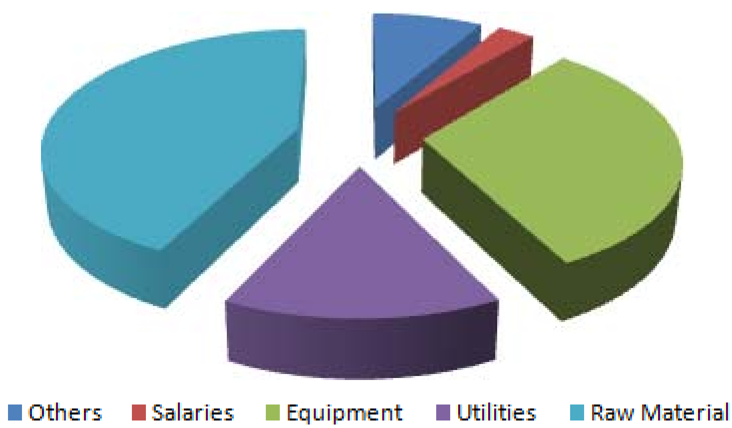
Catalytic
- **Direct Sequence**
- **Indirect sequence**

Optimal Design of Lignocellulosic Ethanol Plant



$67.5 Million/yr

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



Ethanol: \$0.81 /gal *(no H_2 credits)*
\$ 0.41/gal *(H_2 credits)*

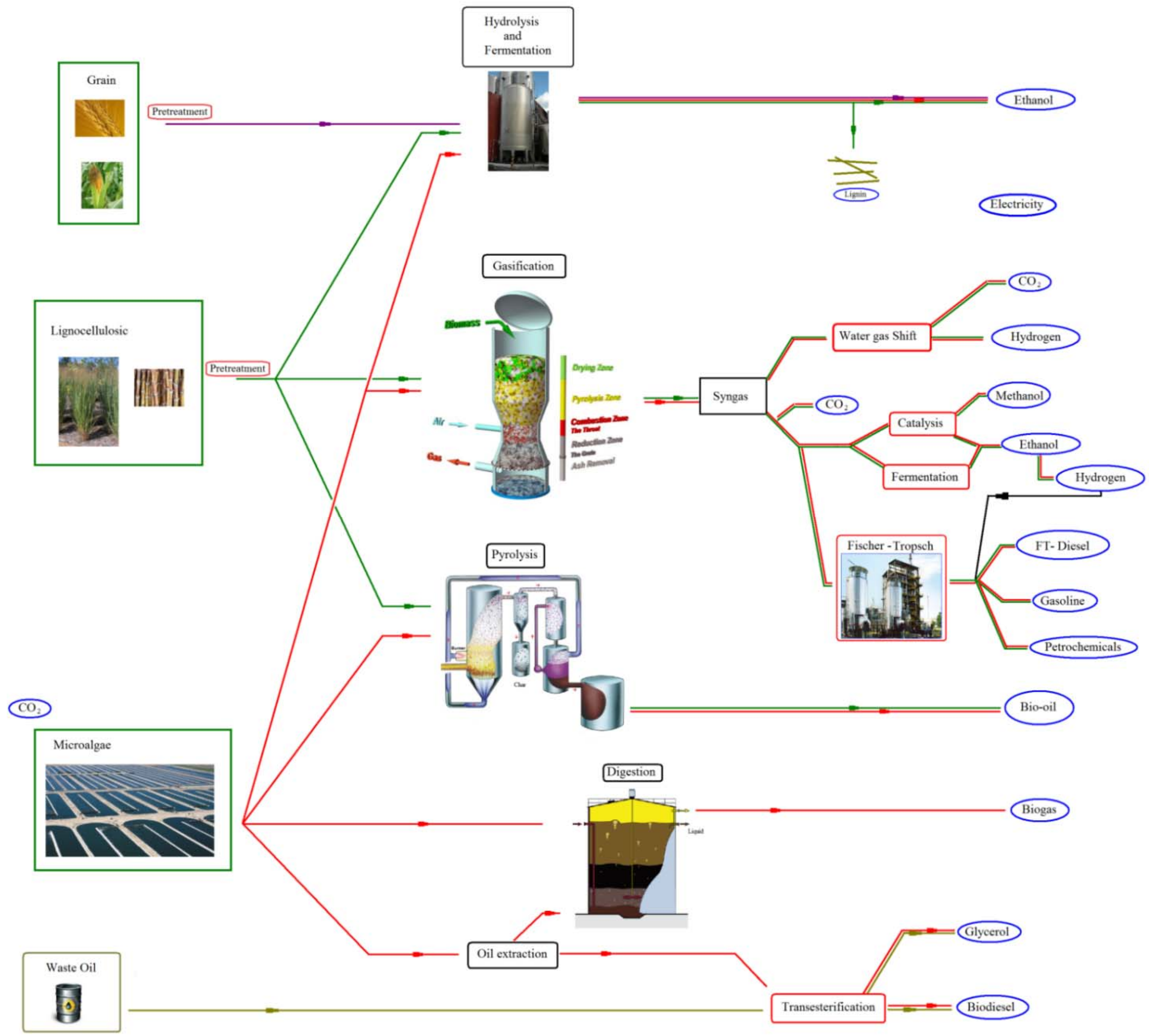
Each NLP subproblem: 7000 eqs., 8000 var
~25 min to solve

Low cost is due to H_2 production

Biorefinery

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

Martin, Grossmann (2012)



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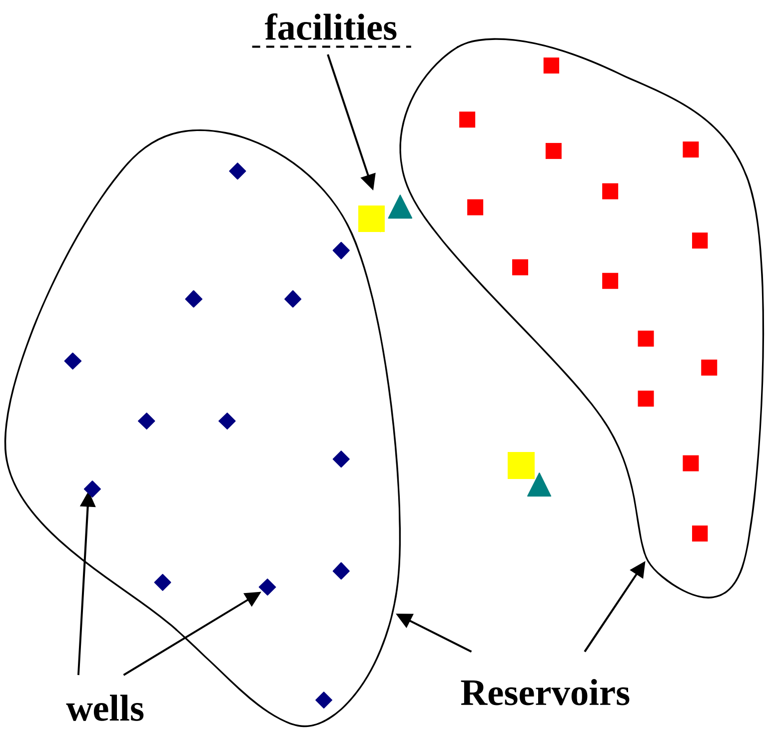
Optimal Development of Oil Fields *(deepwater)*

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

ExxonMobil



Gupta, Grossmann (2011)

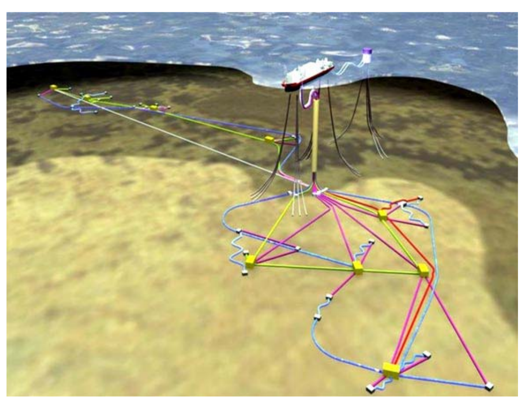
Decisions:

- 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**

FPSO ***(Floating Production Storage Offloading)***



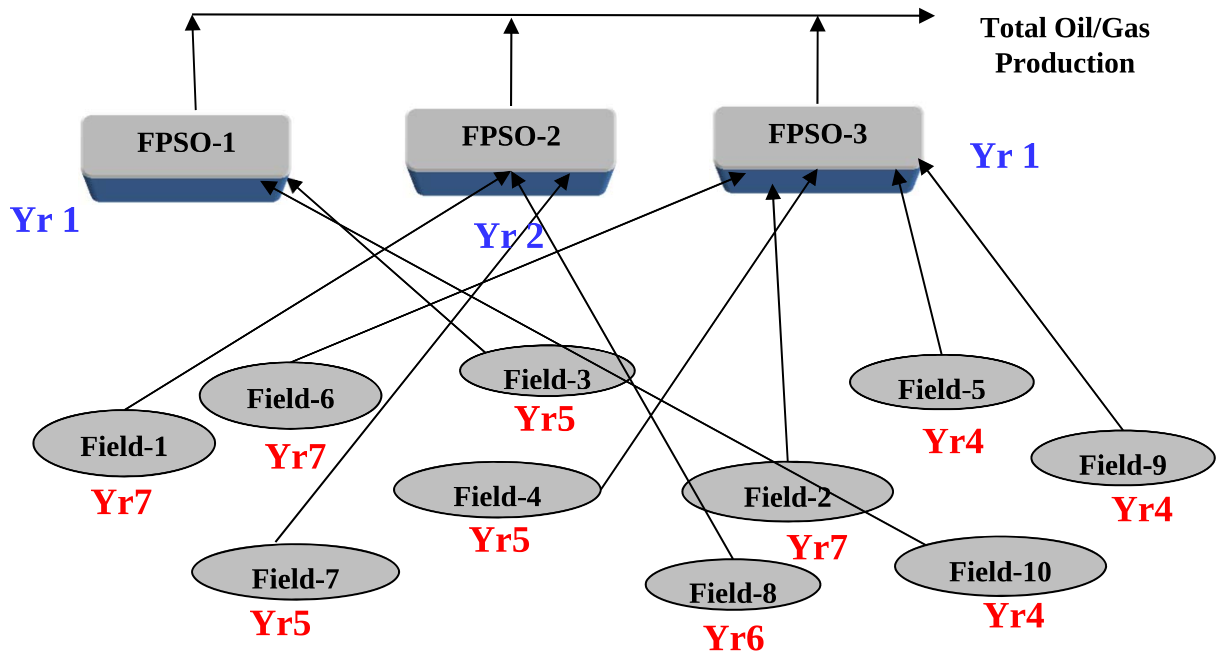
MINLP model

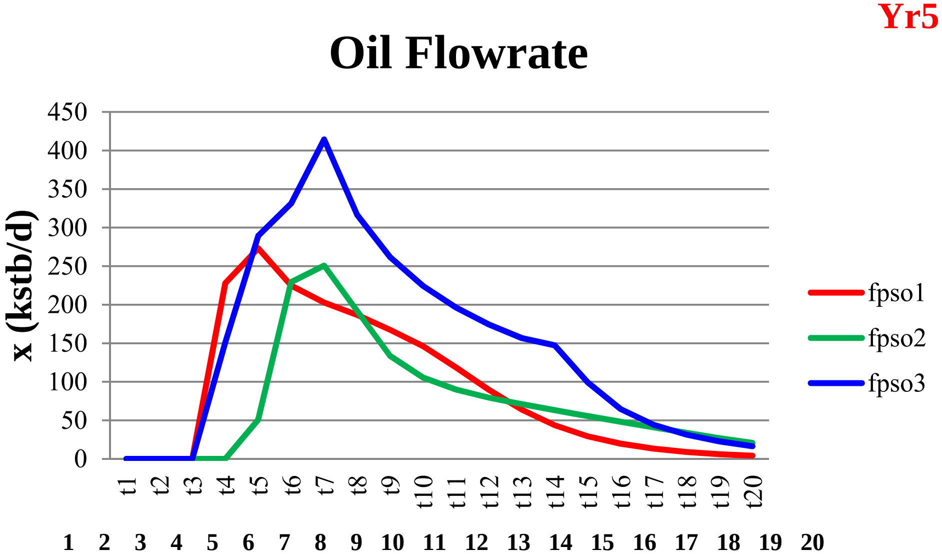
- **Nonlinear reservoir behavior**
- **Three components (oil, water, gas)**
- **Lead times for FPSO construction**
- **FPSO Capacity expansion**
- **Well Drilling Schedule**

Example

Optimal NPV = ***$30.946 billion***

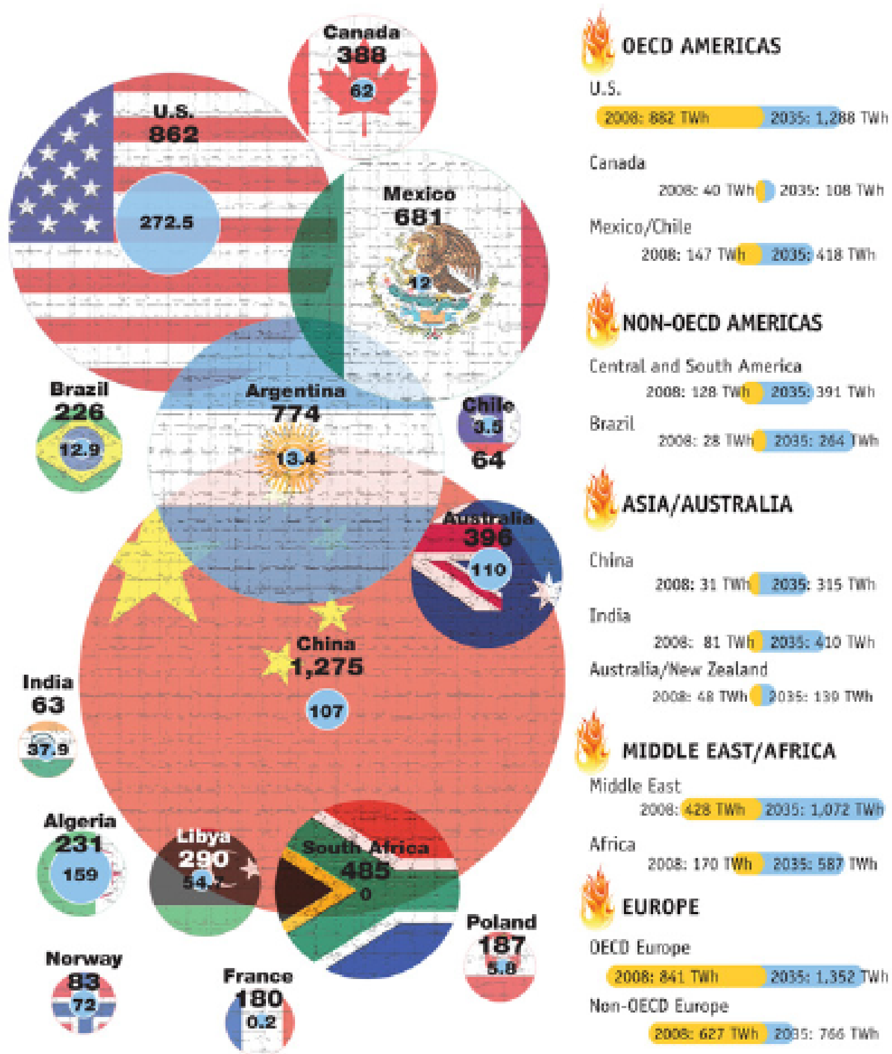
20 Year Time Horizon
10 Fields
3 FPSOs
23 Wells
3 Yr lead time FPSO
1 Yr lead time expansion





	MINLP
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 useage
blue = estimate for 2035

Sonal Patel, "THE BIG PICTURE: A Shale Gas Revolution", Power, June 2012

Carnegie Mellon

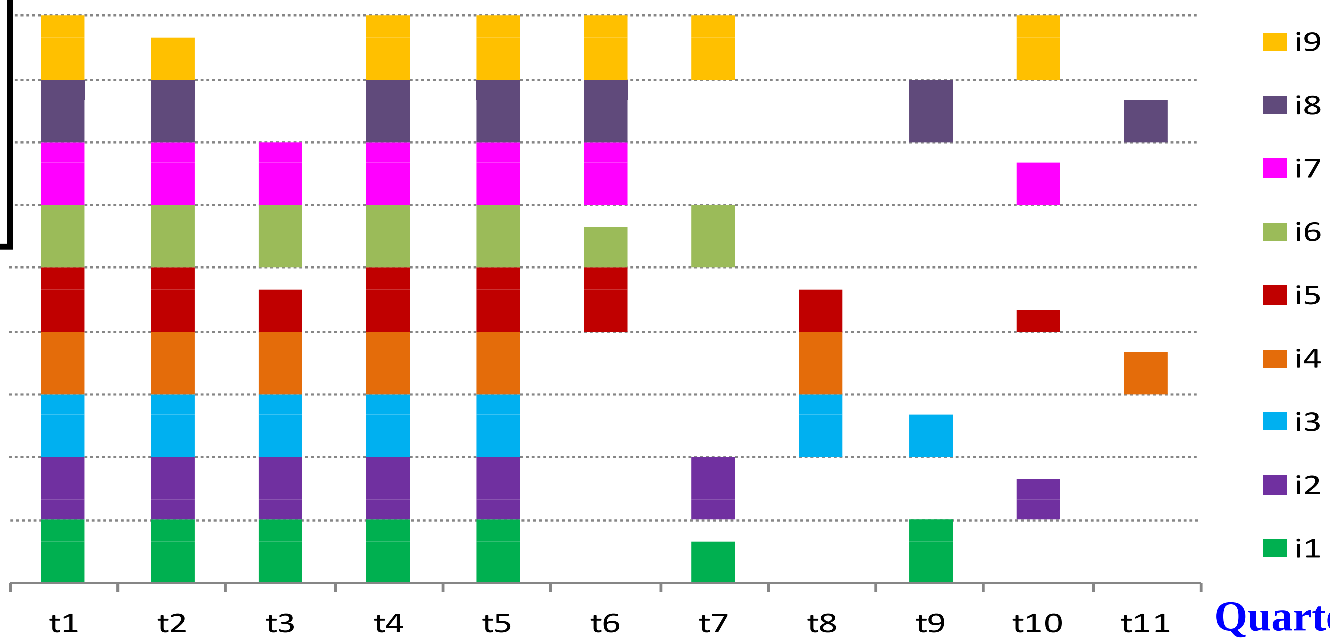
Optimal Drilling Strategy: Shale Gas

CAPD CENTER

MINLP Optimization Model

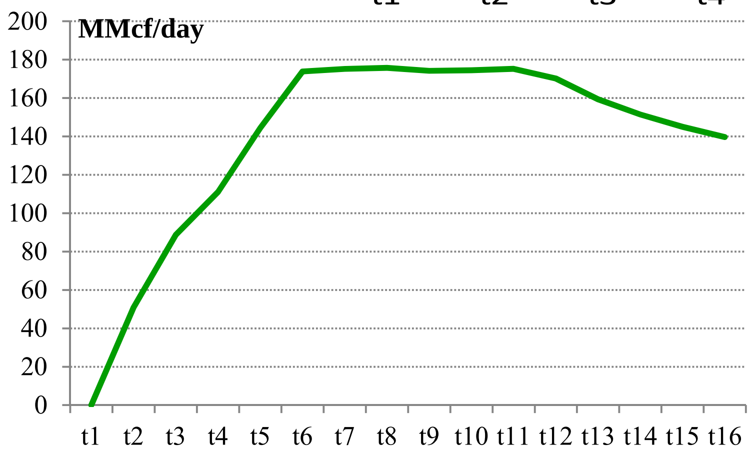
Cafaro, Grossmann (2013)

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

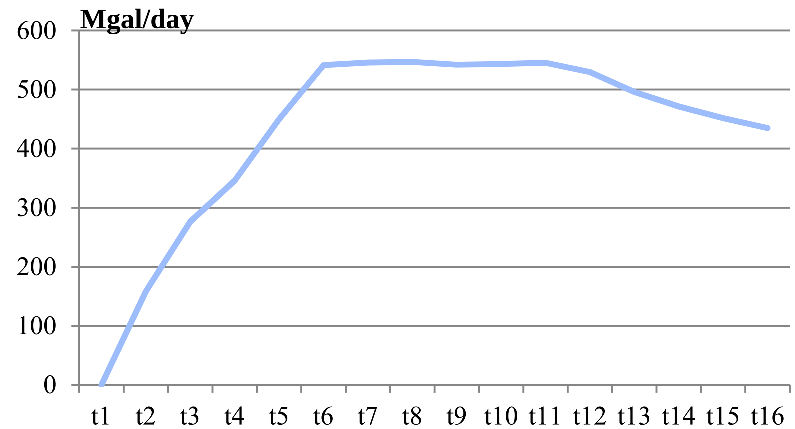


Well pads

Quarters



Methane Production

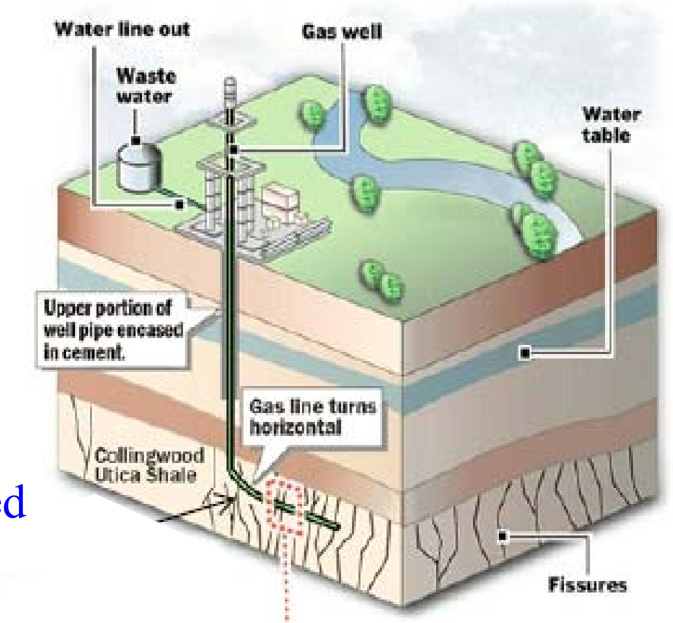


Ethane Production

Water use in hydraulic fracturing large but over short periods

Yang, Grossmann (2013)

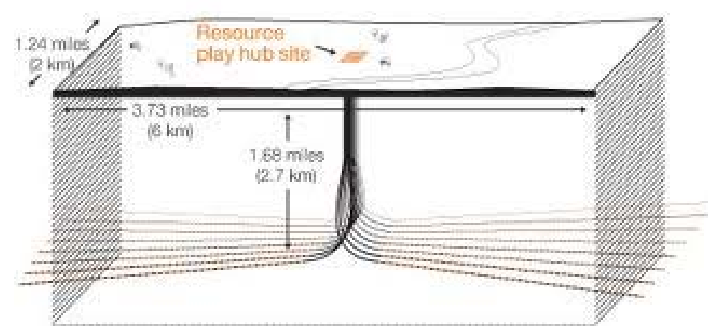
Large volume of water (3-5 MM gallons) to complete a well



- 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]

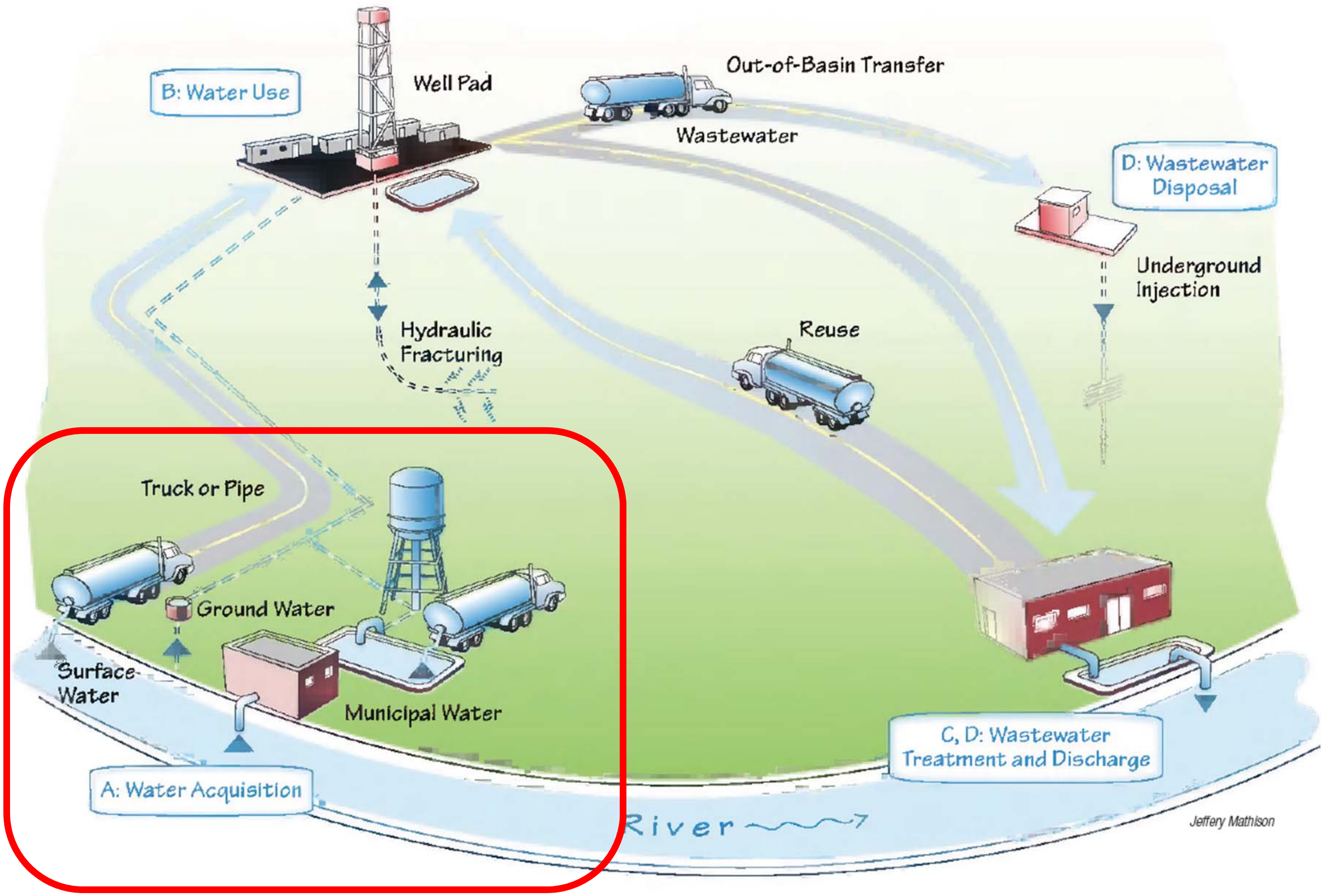
Flowback water treated for reuse

Multi-well pads

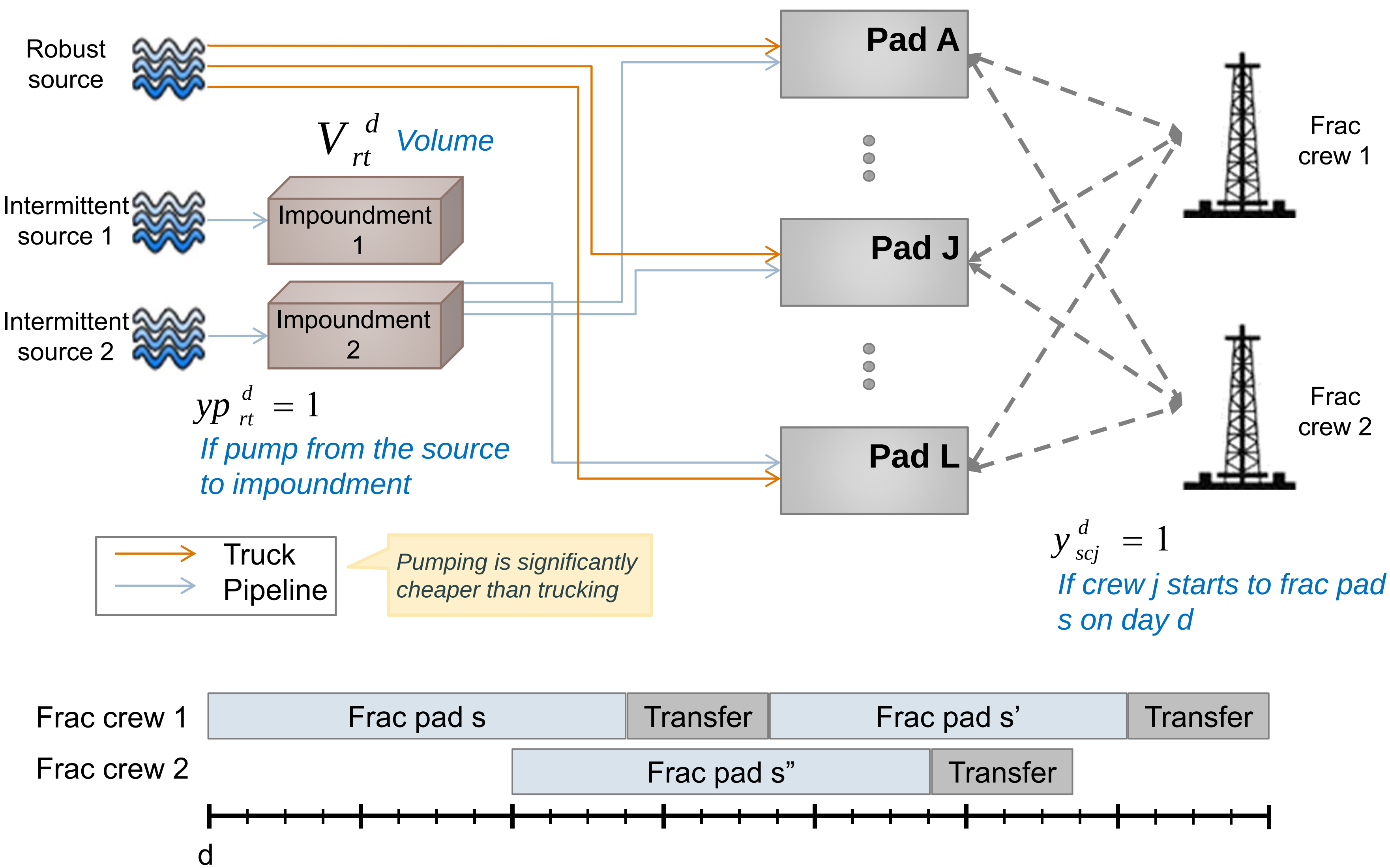


1.3 gal/MMBtu for shale gas vs 7 coal/slurry and 50 oil

Water use logistics in Shale Gas production



Scheduling model: STN discrete-time MILP model *(Kondili, Pantelides, Sargent, 1993)*



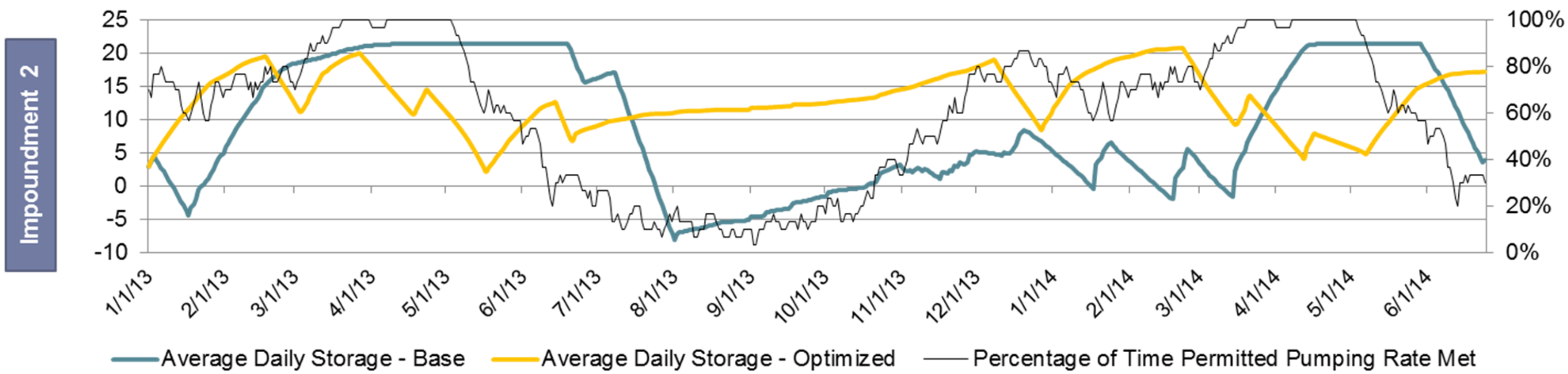
Example: results

14 well pads
540 time periods
2 impoundments
1 frac crew

	Heuristic schedule	MILP schedule‡
Trucking cost	$5,886,743	$568,827
Pumping cost	$9,905,219	$12,792,088
Total expected cost ($)	**$15,791,963**	**$13,360,915**

Trucking cost is reduced by an order of magnitude.

- **14,010 → 1,350 truck trips.**
- **CO_2 emissions from trucking reduced from 630 → 60 metric tons**

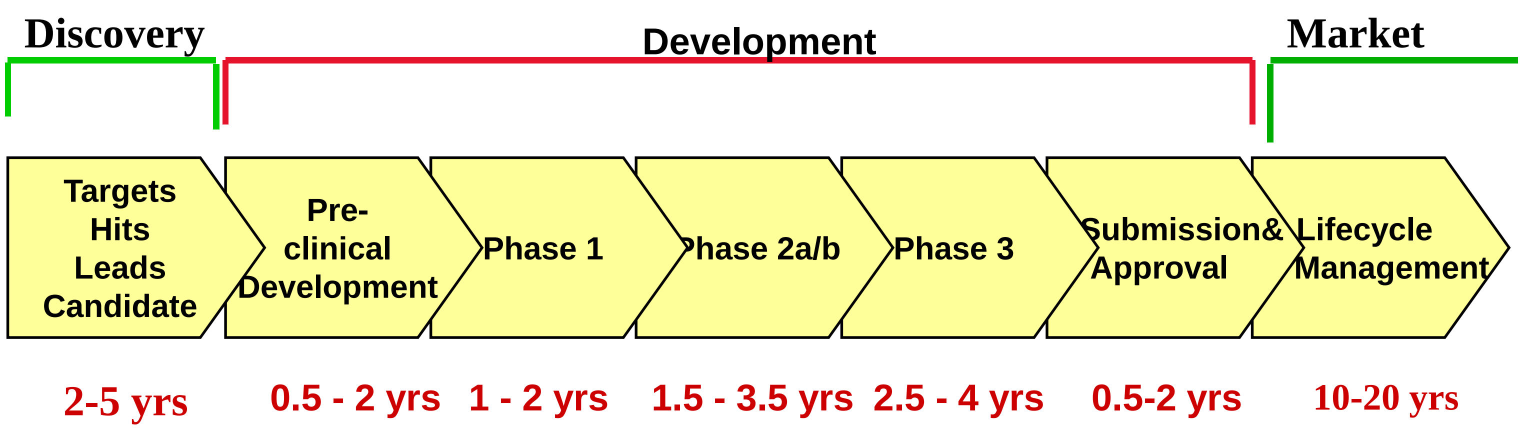


III. Enterprise-wide Optimization

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

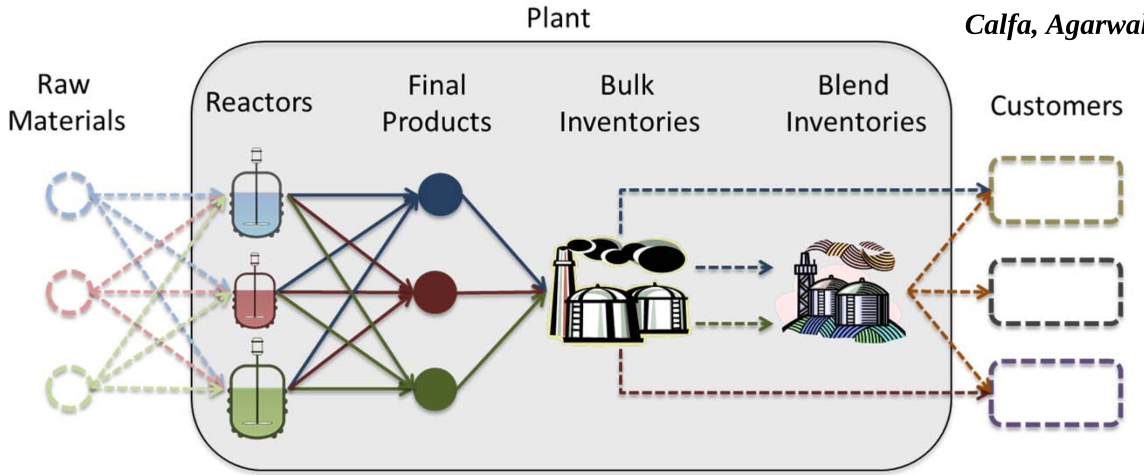
Dennis Houston (ExxonMobil)



Colin Gardner (Transform Pharmaceuticals)

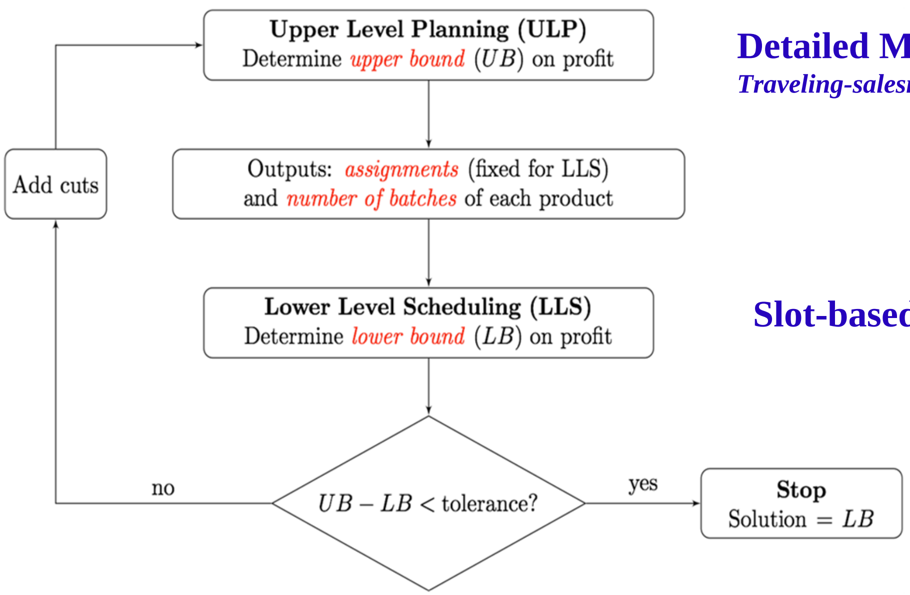
Integrated Planning and Scheduling Batch Plant

Calfa, Agarwal, Wassick, Grossmann (2013)



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

Bi-level Decomposition



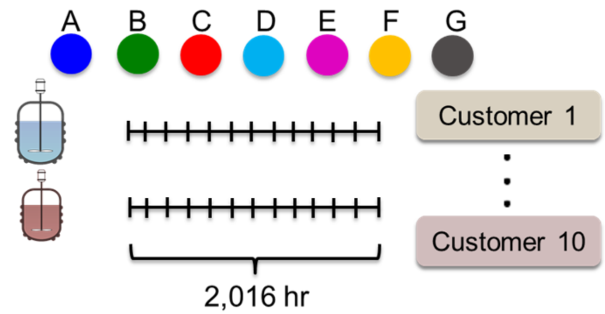
Detailed MILP Planning

Traveling-salesman constraints

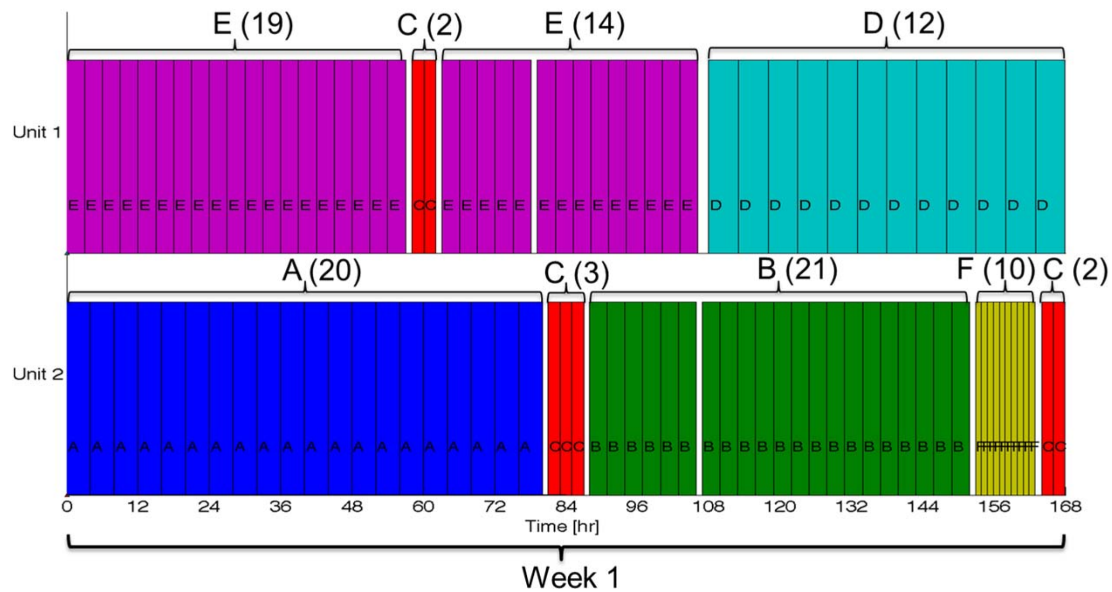
Slot-based MILP model

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**

Optimal Multi-scale Capacity Planning under Hourly Varying Electricity Prices

Mitra, Grossmann (2012)

Price forecast **Demand Side Management**

Given:

- Power-intensive plant
- Products $g \in G$ (Storable and Nonstorable)
- Product demands d_g^t for season t□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 $st \in ST$

Determine:

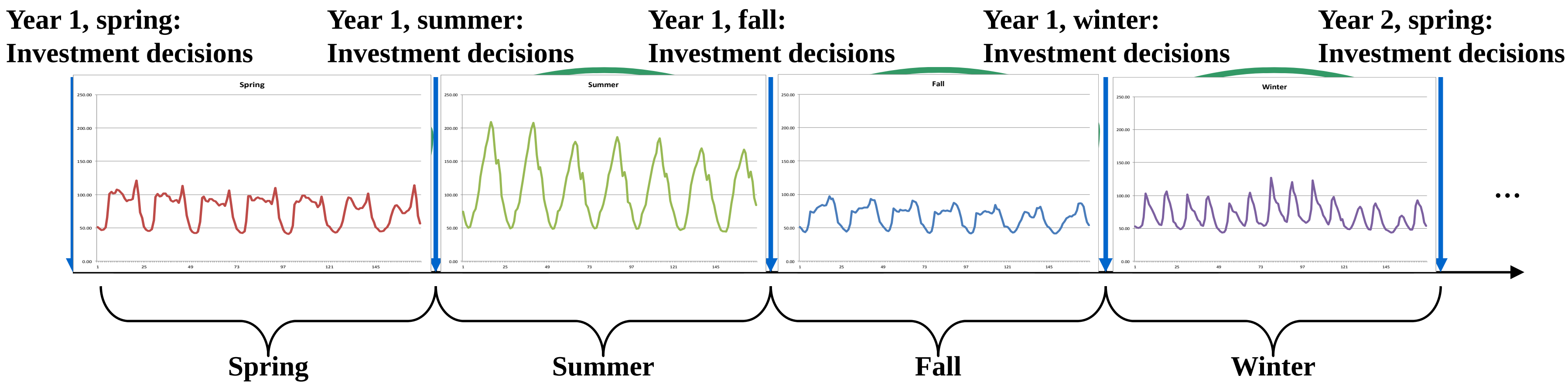
- Production levels $Pr_g^{t,h}$
- Mode of operation $\tilde{y}_{m,o}^{t,h}$, $y_m^{t,h}$
- Sales $S_g^{t,h}$
- Inventory levels $INV_g^{t,h}$

for each season on an hourly basis

- Upgrades for equipment $VU_{m,u}^t$
- Purchase of new equipm. VN_n^t
- Purchase of new tanks $VS_{st,g}^t$

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**

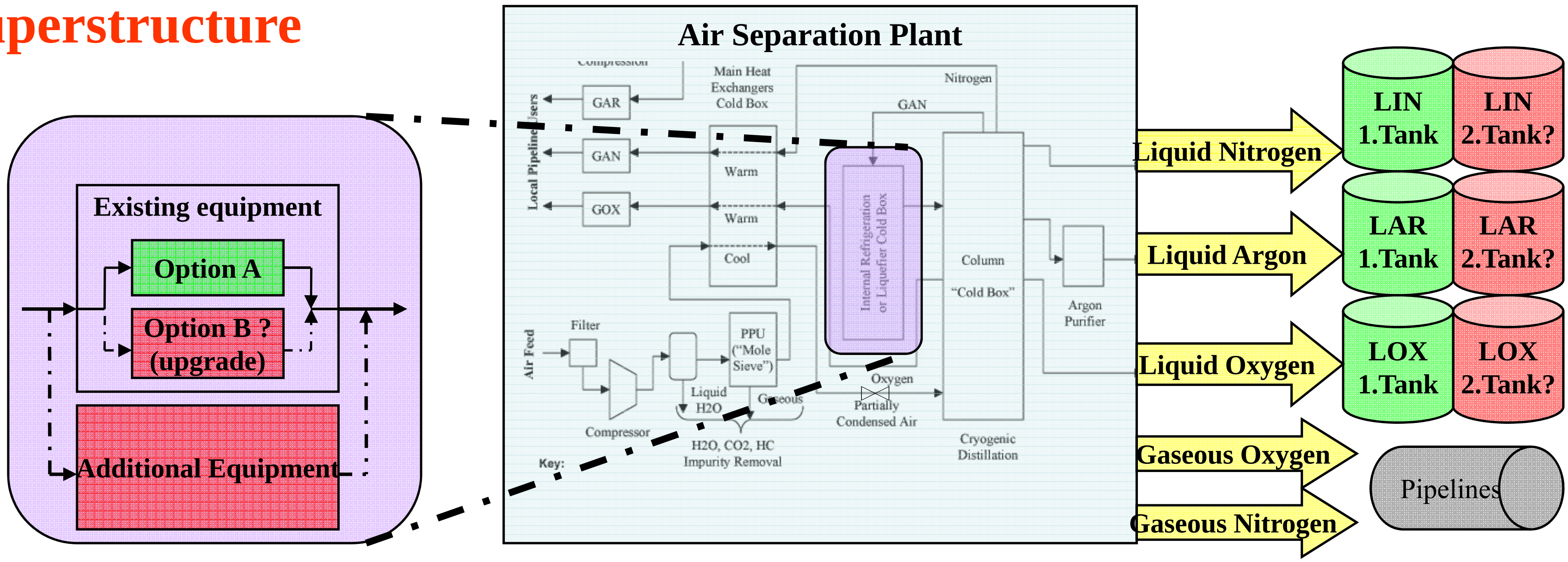
MILP model for multi-scale capacity planning

min $$OBJ = \sum_t (Cost^t_{ops} + Cost^t_{invest}) \quad (37)$$

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

Retrofitting an air separation plant

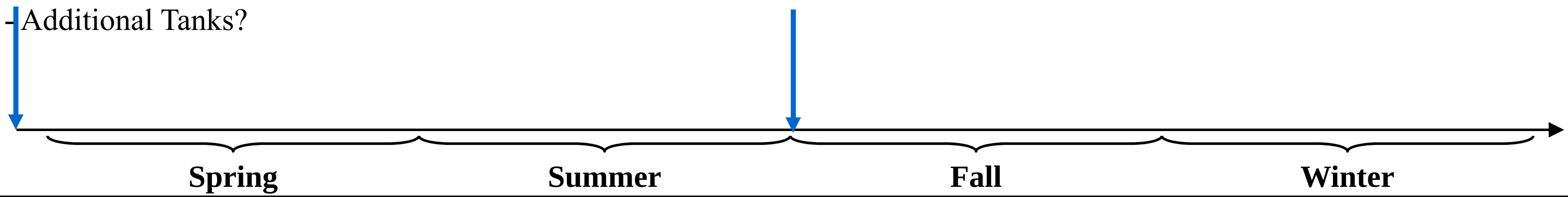
Superstructure



Time

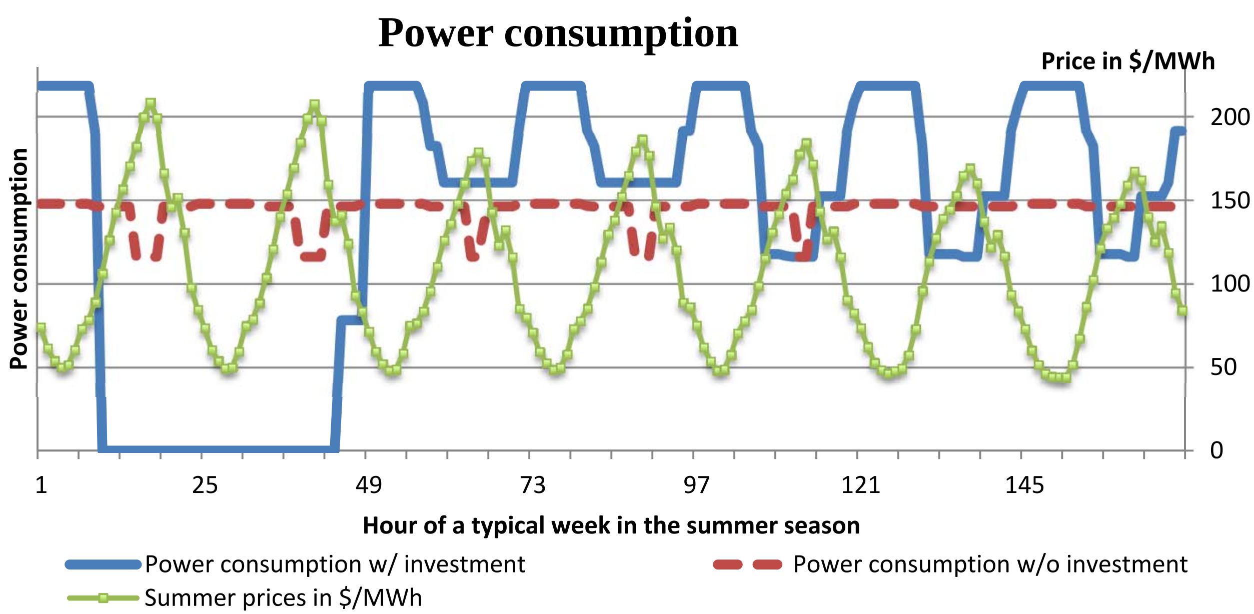
Spring - Investment decisions: (yes/no)
- Option B for existing equipment?
- Additional equipment?
- Additional Tanks?

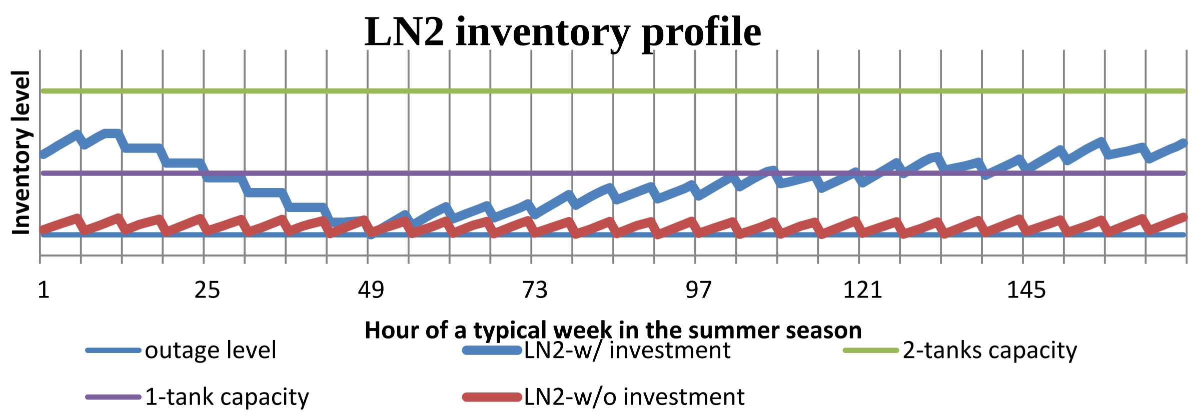
Fall - Investment decisions: (yes/no)
- Option B for existing equipment?
- Additional equipment?
- Additional Tanks?



- 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**

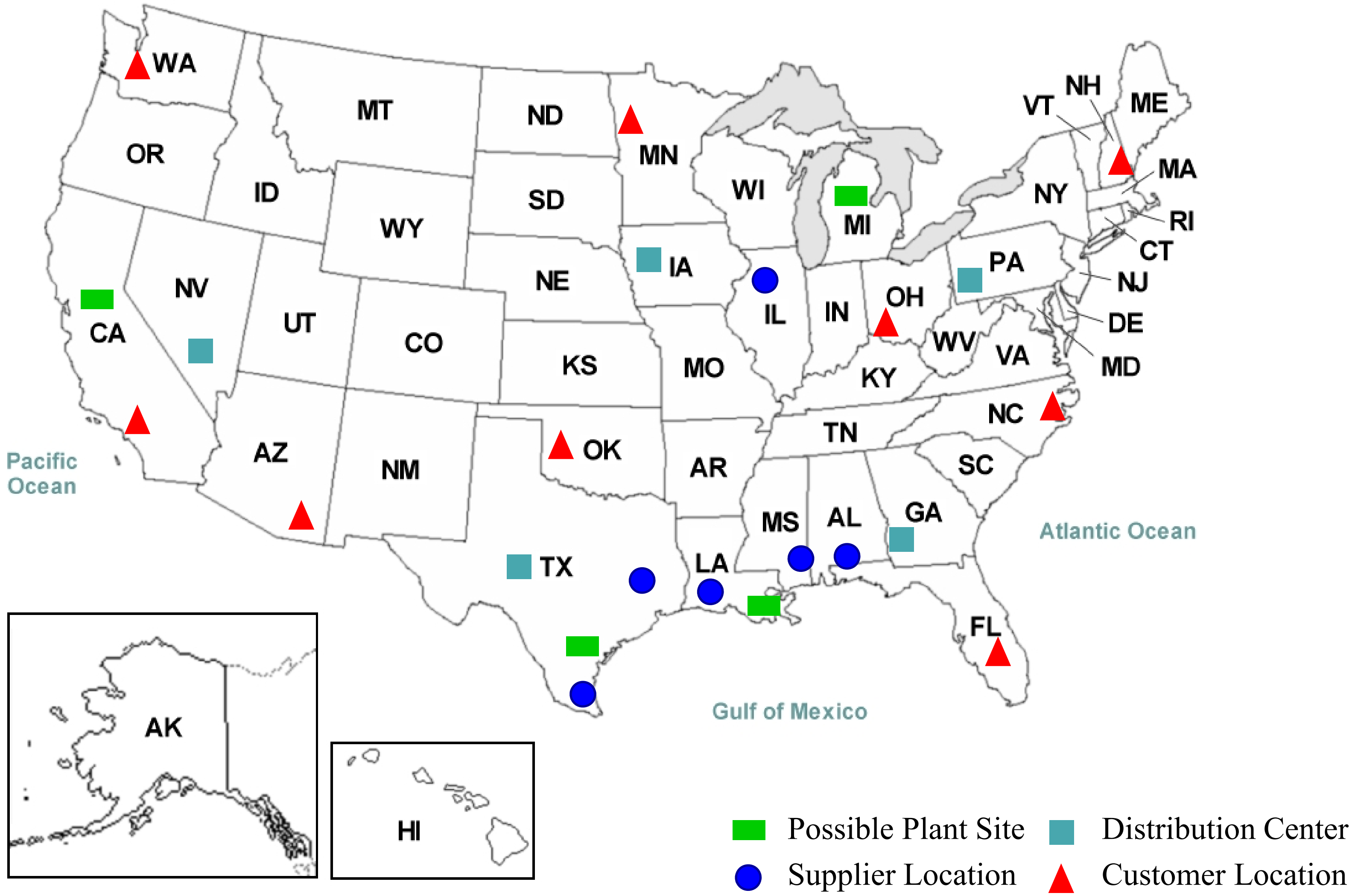
- Buy new liquefier in the first time period (annualized investment costs: $300k/a)
- Buy additional LN2 storage tank ($25k/a)
- Don't upgrade existing equipment ($200k/a) equipment: 97%.

Optimal Design of Responsive Process Supply Chains

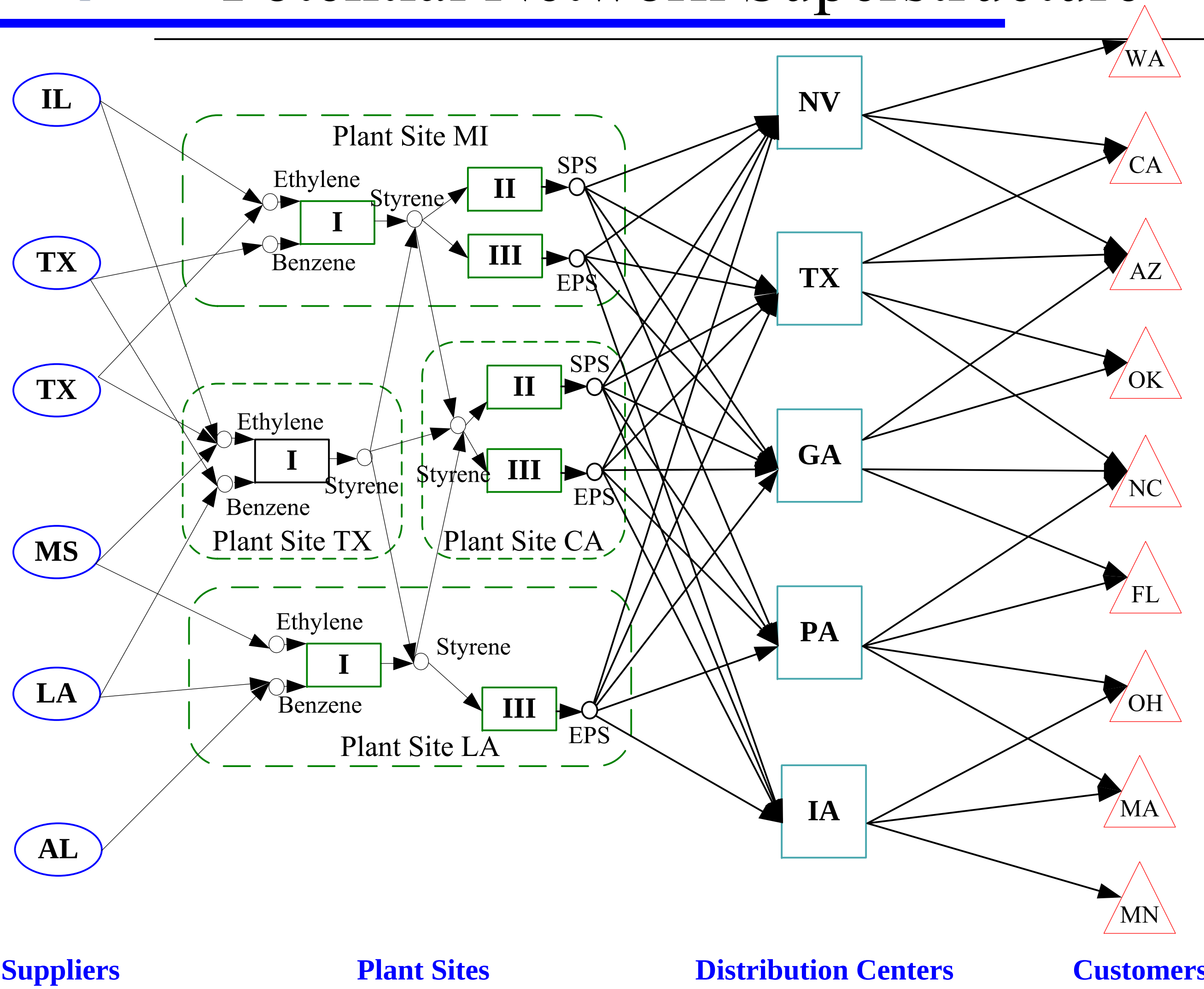
Carnegie Mellon

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

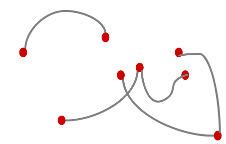
You, Grossmann (2008)



Potential Network Superstructure



Network Structure



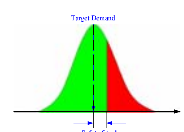
Operational Plan

Production Schedule

Max: Net present value

Max: Responsiveness

Demand uncertainty

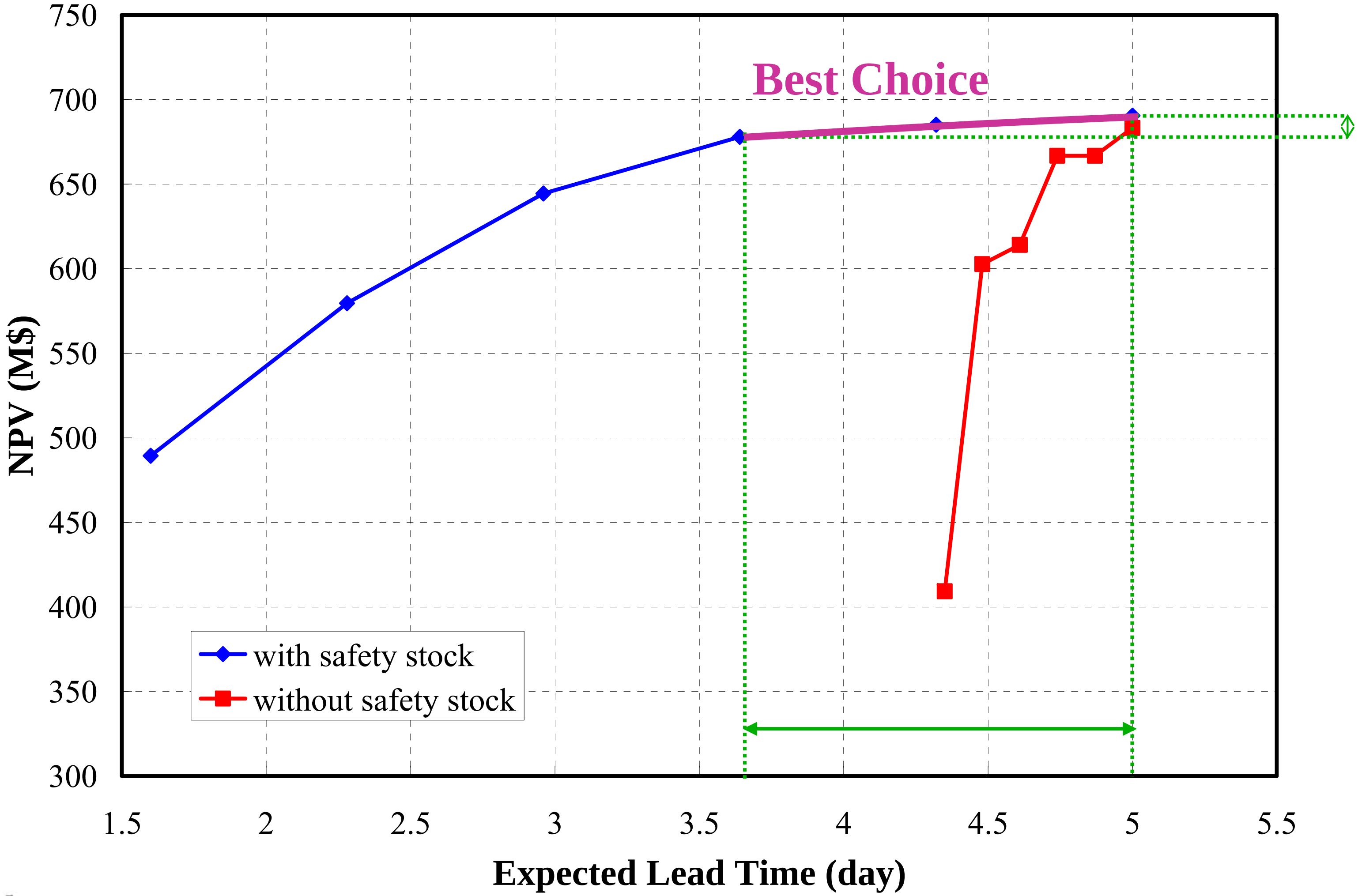


⇒ Responsiveness
Expected Lead Time

Chemical ENGINEERING
Carnegie Mellon

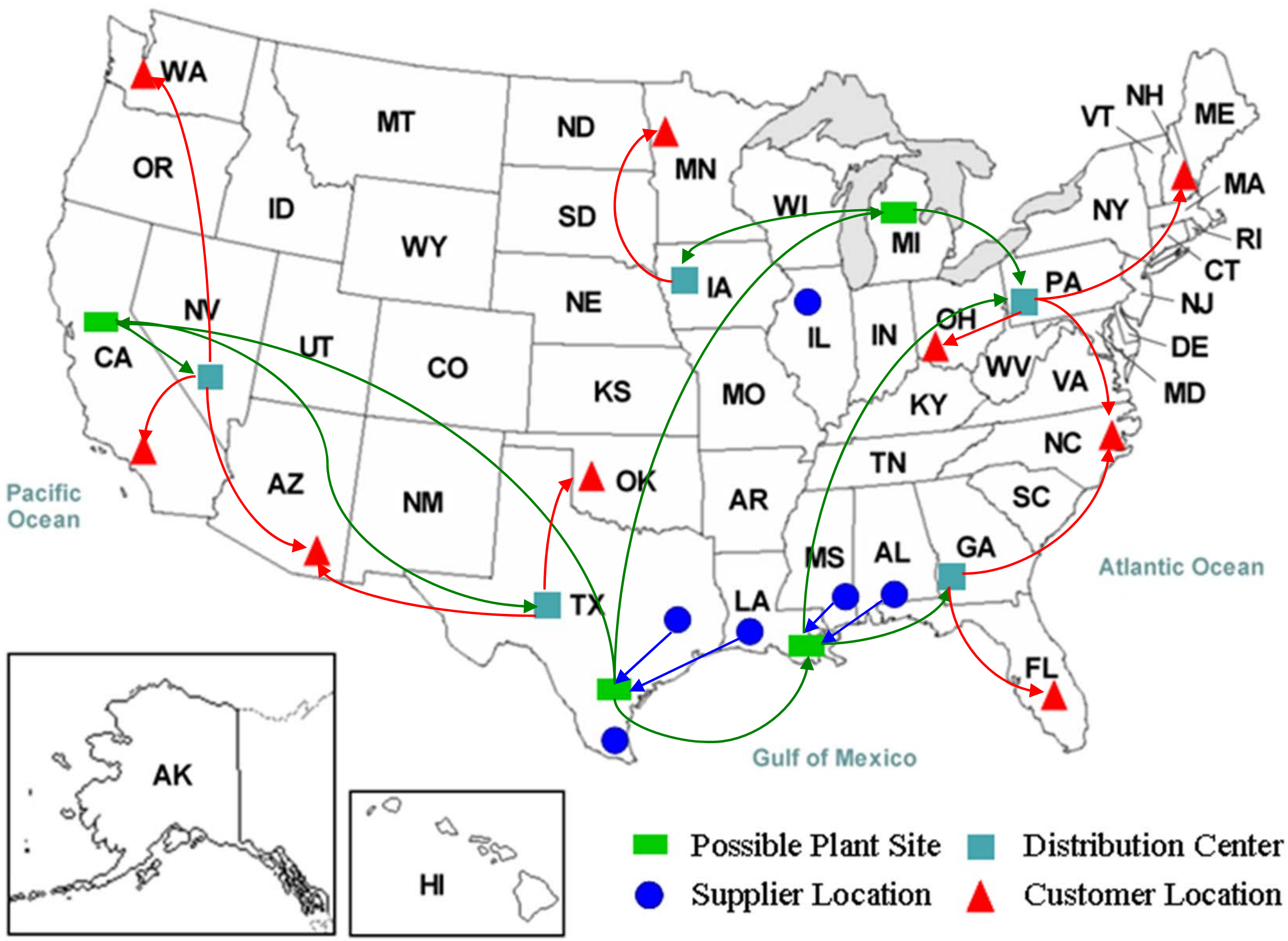
Bi-criterion Multiperiod MINLP

Pareto Curves – with and without safety stock



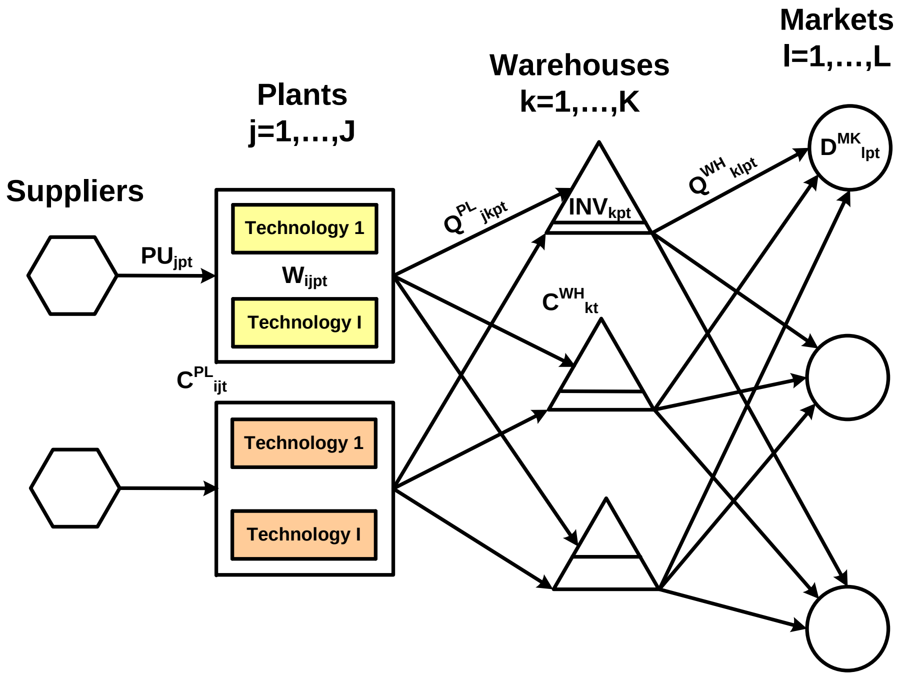
Network Structure at Location Map

You, Grossmann (2009)

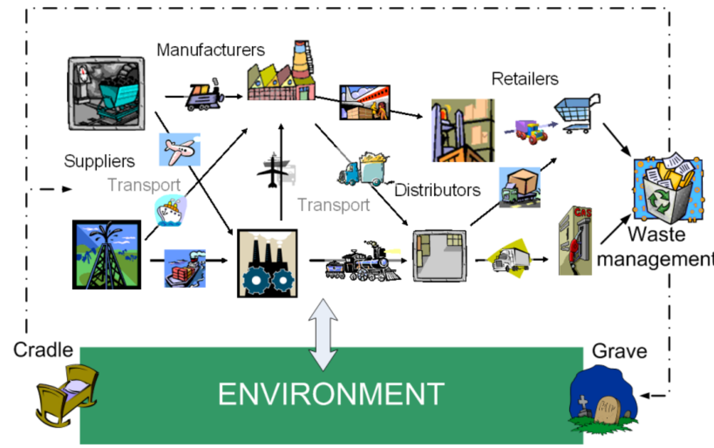


Optimal Planning of Sustainable Chemical Supply Chains

Guillen, Grossmann (2010)



Life Cycle Analysis



Bicriterion optimization

Max Net Present Value

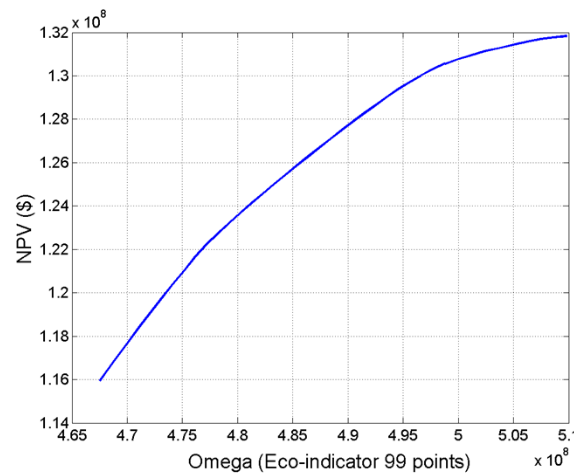
Min Environmental Impact

Eco-Indicator 99 for LCA

(Health, Ecosystem, Resources)

Uncertainty in emissions

Pareto-Optimal Solutions



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**