

Discrete and Continuous Optimization Models for the Design and Operation of Sustainable and Robust Process Systems

Ignacio E. Grossmann
Center of Advanced Process Decision-making
Carnegie Mellon University
Pittsburgh, PA 15217
U.S.A.

OSE, Abo Akademi, Turku
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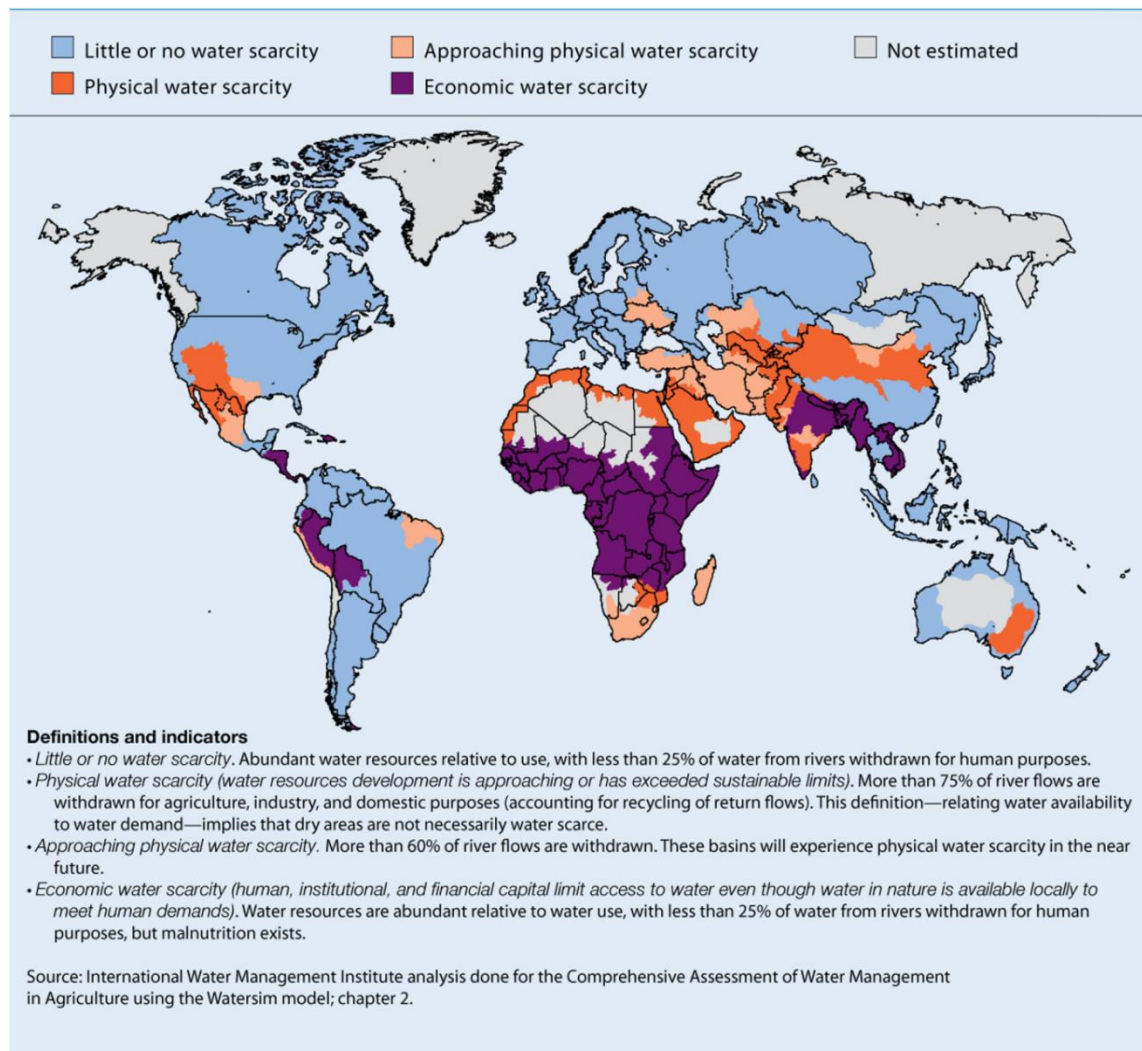
Motivation

1. Increasing interest in **energy systems and supply chains**
2. Need to address design of **sustainable chemical processes**
 - Minimize **energy use**
 - Minimize **water consumption**
3. Need to introduce robustness to account for **uncertainties**

Goal: Systematic Optimization Approaches for **Sustainable and Robust**
Optimization Process Design and Planning Operations Problems

Challenges: *Nonconvexities in MINLP/GDP models*
Large-scale stochastic optimization problems

Water scarcity



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



- **Given is:**
 - a set of single/multiple water sources with/without contaminants,
 - a set of water-using, water pre-treatment, and wastewater treatment operations, sinks and sources of water
- **Synthesize** an integrated process water network
 - **interconnection** of process and treatment units (**reuse, recycle**)
 - the flow rates and contaminants concentration of each stream
 - **minimum total annual cost of water network**

Synthesis Integrated Process Water Networks

- **Pinch analysis** and **mathematical programming** models
- *Reviews in Bagajewicz (2000), Jeřowski (2008), Bagajewicz and Faria (2009), and Foo (2009).*

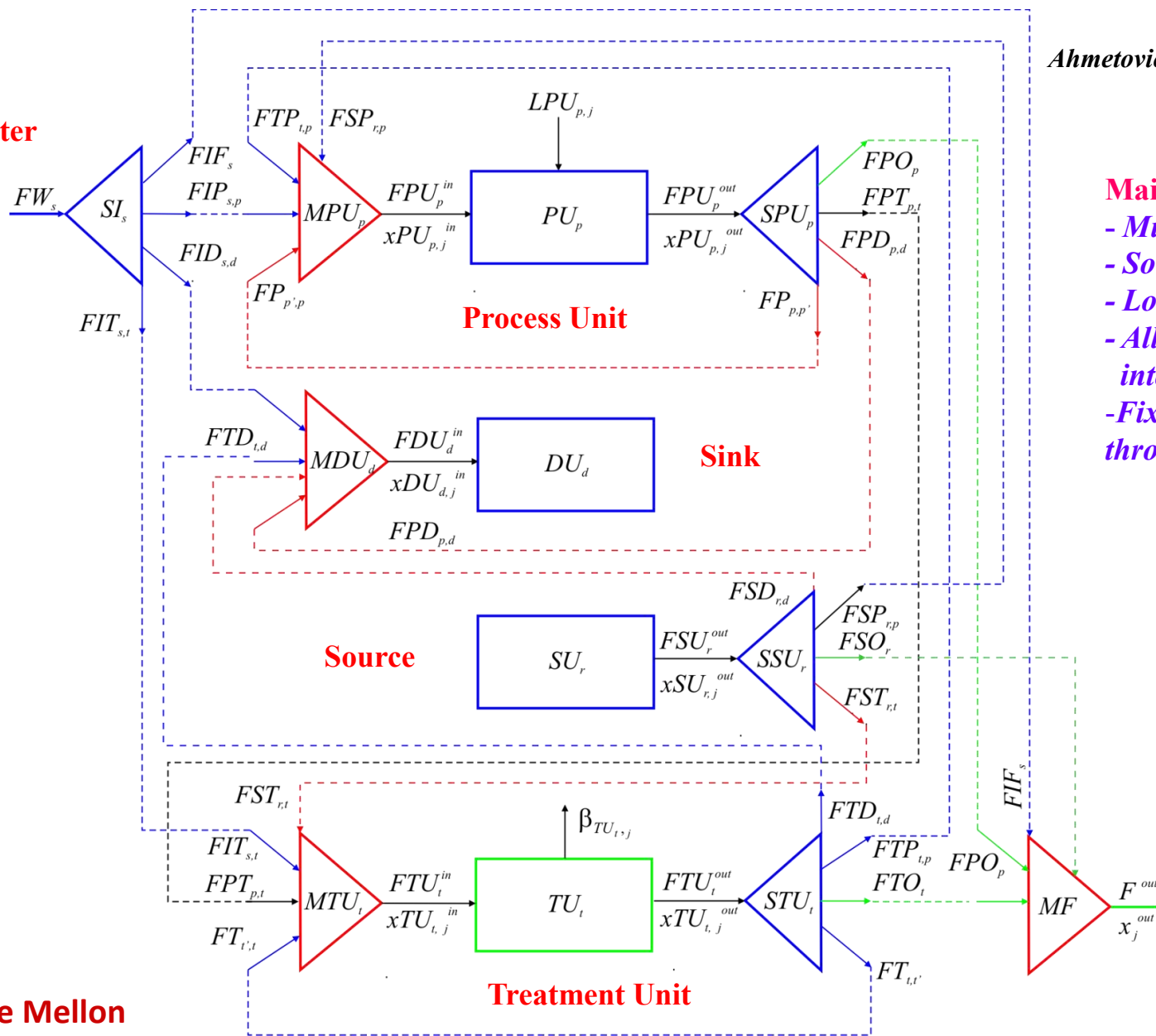
Approach: Global NLP or MINLP superstructure optimization model

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

Ahmetovic, Grossmann (2010)

Main features:

- Multiple feeds
- Source/Sink units
- Local recycles
- All possible interconnections
- Fixed and variable flows through process units



Optimization Model

Nonconvex NLP or MINLP

Objective function: *min Cost*

Subject to:

Splitter mass balances

Mixer mass balances (bilinear)

Process units mass balances

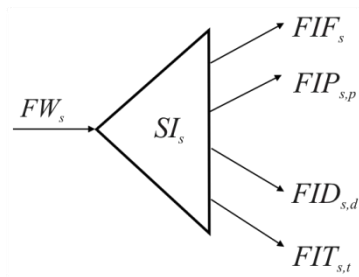
Treatment units mass balances

Design constraints

0-1 variables for piping sections

Model can be solved to global optimality

Splitter



$$FW_s = FIF_s + \sum_{p \in PU} FIP_{s,p} + \sum_{d \in DU} FID_{s,d} + \sum_{t \in TU} FIT_{s,t} \quad \forall s \in SW$$

linear

$$FIF_s^L \cdot y_{FIF_s} \leq FIF_s \leq FIF_s^U \cdot y_{FIF_s} \quad \forall s \in SW$$

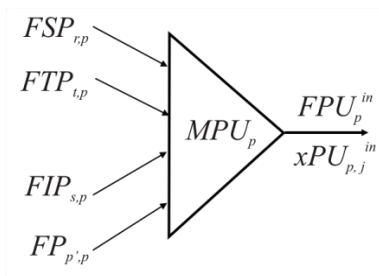
$$FIP_{s,p}^L \cdot y_{FIP_{s,p}} \leq FIP_{s,p} \leq FIP_{s,p}^U \cdot y_{FIP_{s,p}} \quad \forall s \in SW, \forall p \in PU$$

$$FID_{s,d}^L \cdot y_{FID_{s,d}} \leq FID_{s,d} \leq FID_{s,d}^U \cdot y_{FID_{s,d}} \quad \forall s \in SW, \forall d \in DU$$

$$FIT_{s,t}^L \cdot y_{FIT_{s,t}} \leq FIT_{s,t} \leq FIT_{s,t}^U \cdot y_{FIT_{s,t}} \quad \forall s \in SW, \forall t \in TU$$

**0-1
optional**

Mixer

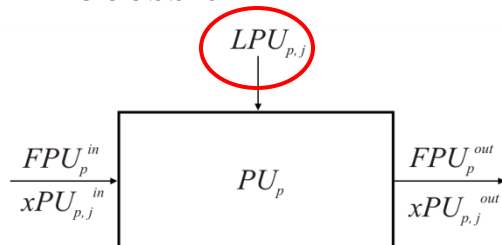


$$FPU_p^{in} = \sum_{r \in SU} FSP_{r,p} + \sum_{t \in TU} FTP_{t,p} + \sum_{s \in SW} FIP_{s,p} + \sum_{\substack{p' \in PU \\ p \neq p', R_p=0}} FP_{p',p} + \sum_{\substack{p' \in PU \\ R_p=1}} FP_{p',p}, \quad \forall p \in PU$$

$$FPU_p^{in} \cdot xPU_{p,j}^{in} = \sum_{r \in SU} FSP_{r,p} \cdot xSU_{r,j}^{out} + \sum_{t \in TU} FTP_{t,p} \cdot xSTU_{t,j}^{out} + \sum_{s \in SW} FIP_{s,p} \cdot xW_{s,j}^{in} \\ + \sum_{\substack{p' \in PU \\ p \neq p', R_p=0}} FP_{p',p} \cdot xSPU_{p',j}^{out} + \sum_{\substack{p' \in PU \\ R_p=1}} FP_{p',p} \cdot xSPU_{p',j}^{out}, \quad \forall p \in PU, \forall j$$

bilinear

Process unit



$$FPU_p^{in} = FPU_p^{out} \quad \forall p \in PU$$

**linear if
flowrate is fixed**

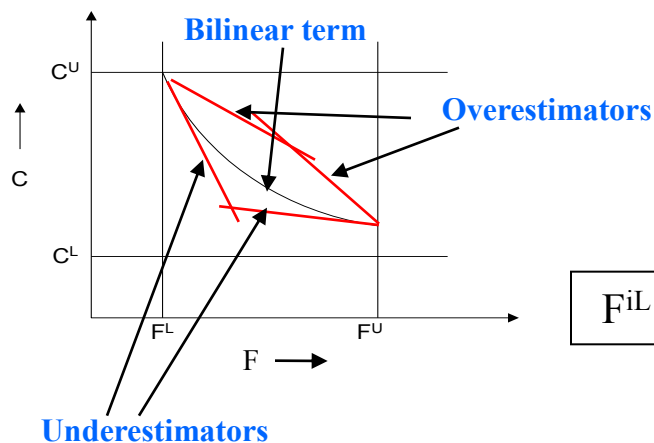
$$FPU_p^{in} \cdot xPU_{p,j}^{in} + LPU_{p,j} \cdot 10^3 = FPU_p^{out} \cdot xPU_{p,j}^{out} \quad \forall p \in PU, \forall j$$

bilinear if the flow treated as cont. variable

Cost function **linear** in feedwater, **concave** in treatment unit,
linear in operating cost, pipe section **fixed charge (0-1)**

$$\min Z = H \cdot \sum_{s \in SW} FW_s \cdot CFW_s + AR \cdot \sum_{t \in TU} IC_t \cdot (FTU_t^{out})^\alpha + H \cdot \sum_{t \in TU} OC_t \cdot FTU_t^{out}$$

Convex Envelopes for Bilinear Terms F^*C



$$\begin{aligned} f_j^i &\geq F^{iL} C_j^i + C_j^{iL} F^i - F^{iL} C_j^{iL} \\ f_j^i &\geq F^{iU} C_j^i + C_j^{iU} F^i - F^{iU} C_j^{iU} \\ f_j^i &\leq F^{iL} C_j^i + C_j^{iU} F^i - F^{iL} C_j^{iU} \\ f_j^i &\leq F^{iU} C_j^i + C_j^{iL} F^i - F^{iU} C_j^{iL} \end{aligned}$$

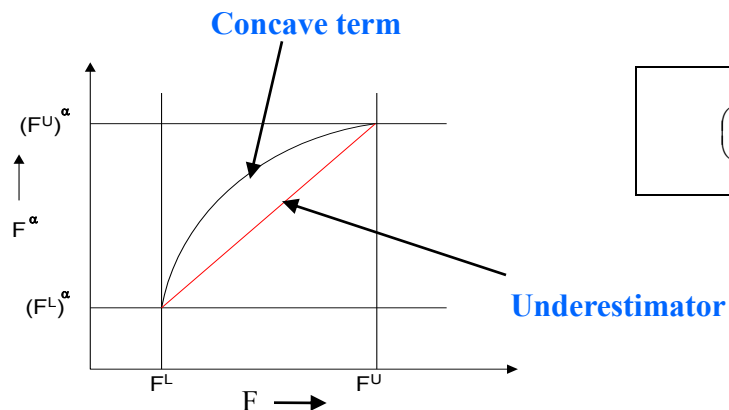
McCormick (1976)

Under- and over-estimators
(Linear Inequalities)

$$F^{iL} \leq F^i \leq F^{iU}$$

$$C_j^{iL} \leq C_j^i \leq C_j^{iU}$$

Underestimation of Concave functions



$$\left(\overline{F}^i \right) \geq \left(F^{iL} \right)^\alpha + \left(\frac{(F^{iU})^\alpha - (F^{iL})^\alpha}{F^{iU} - F^{iL}} \right) \times (F^i - F^{iL})$$

(Secant line)

$$F^{iL} \leq F^i \leq F^{iU}$$

- The cut proposed by Karuppiyah and Grossmann (2006) is incorporated to significantly improve the **strength of the lower bound** for the global optimum: contaminant flow balances for the overall water network system

$$\sum_{s \in SW} FW_s \cdot xW_{s,j}^{in} + \sum_{p \in PU} LPU_{p,j} \cdot 10^3 + \sum_{r \in SU} FSU_r^{out} \cdot xSU_{r,j}^{out} = \sum_{t \in TU} (1 - \beta_{TU,t,j}) \cdot FTU_t^{in} \cdot xTU_{t,j}^{in} + F_j^{out} \cdot x_j^{out} + \sum_{d \in DU} FDU_d^{in} \cdot xDU_{d,j}^{in} \quad \forall j$$

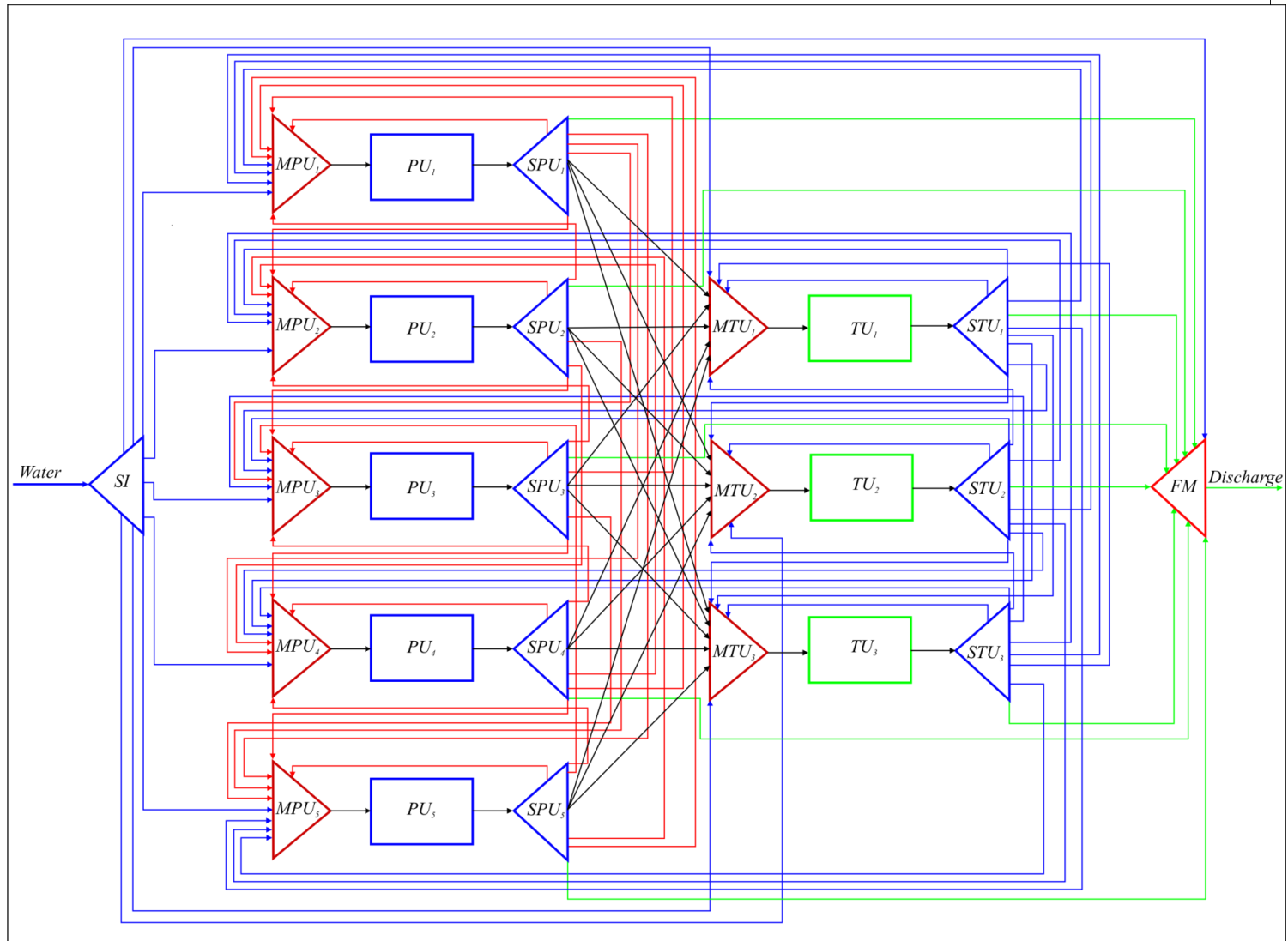
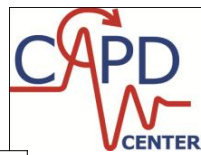
bilinear terms for the **treatment units** and **final mixing points**

Cut is **redundant** for original problem
Non-redundant for relaxation problem

- **Tight bounds on the variables** are expressed as general equations obtained by physical inspection of the superstructure and using logic specifications

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

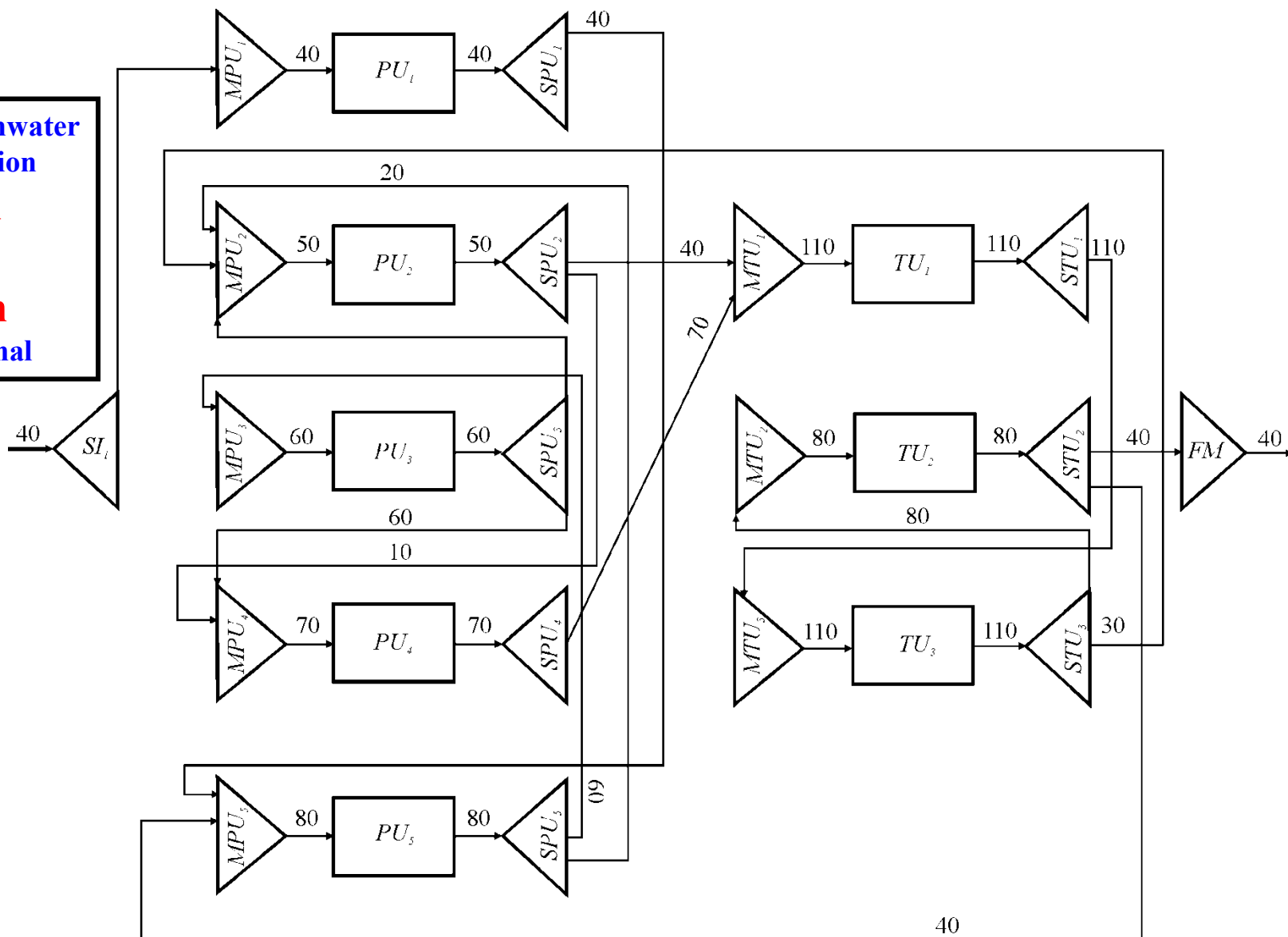
BARON

optcr=0.01

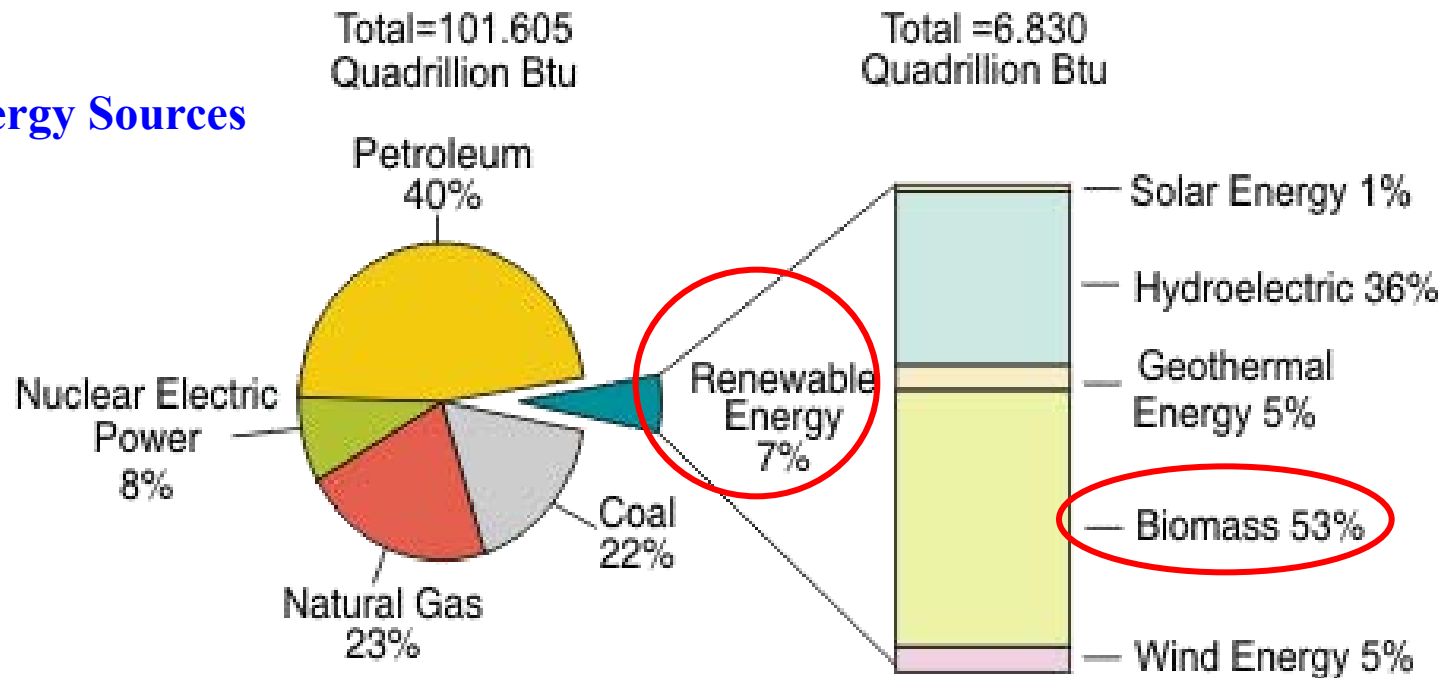
197.5 CPUsec

Optimal design of the simplified water network with 13 removable connections

**Optimal Freshwater
Consumption
40 t/h**
VS
300 t/h
conventional



US Energy Sources



Note: Sum of components may not equal 100 percent due to independent rounding.

Source: EIA, *Renewable Energy Consumption and Electricity Preliminary 2007 Statistics*, Table 1: U.S. Energy Consumption by Energy Source, 2003-2007 (May 2008).

Process Design Challenges in Bioethanol

Energy consumption corn-based process level:

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 level:

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>

Proposed 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

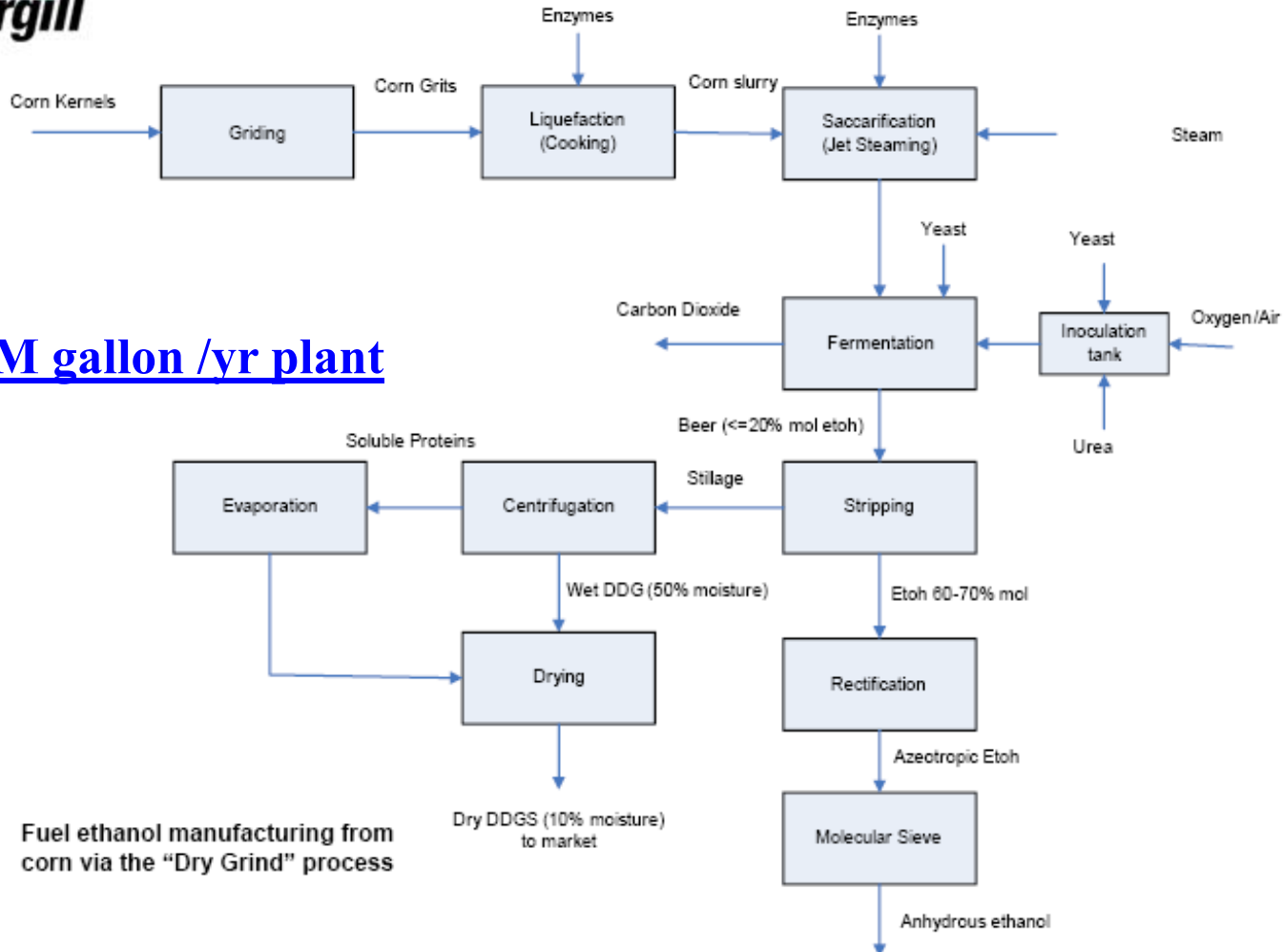
*Issue: cost contribution is currently still very small
(freshwater contribution < 0.1%)*

=> Total cost optimization is unlikely to promote water conservation

Optimal process water networks for minimum energy consumption

Energy Optimization of Corn-based Bioethanol

Peschel, Martin, Karuppiah, Grossmann, Zullo, Martinson (2007)

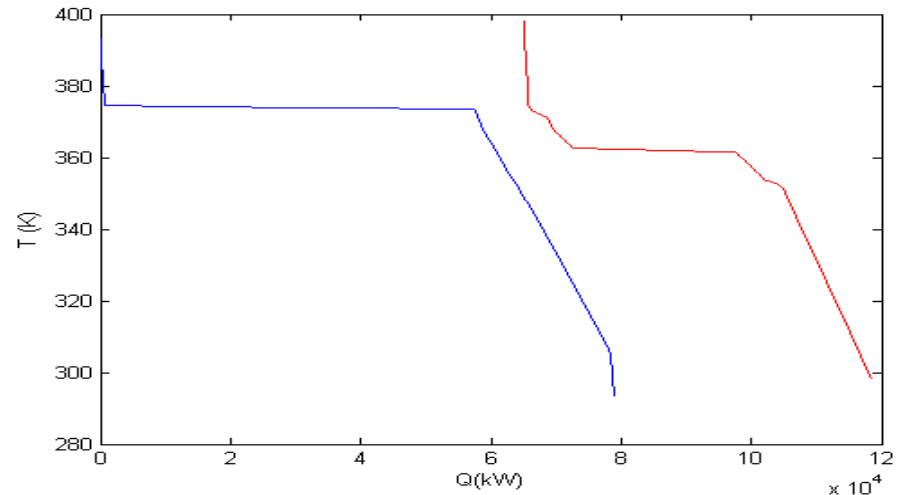


Equipment cost = M\$ 18.4

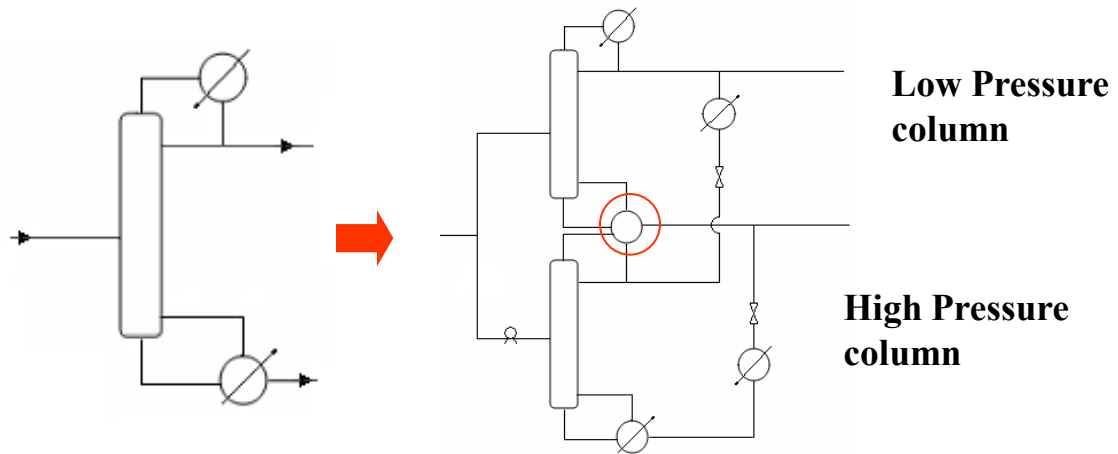
Steam cost = M\$ 21/yr

Prod. cost = 1.50 \$/gal

Heat Integration process streams:



Multieffect columns:

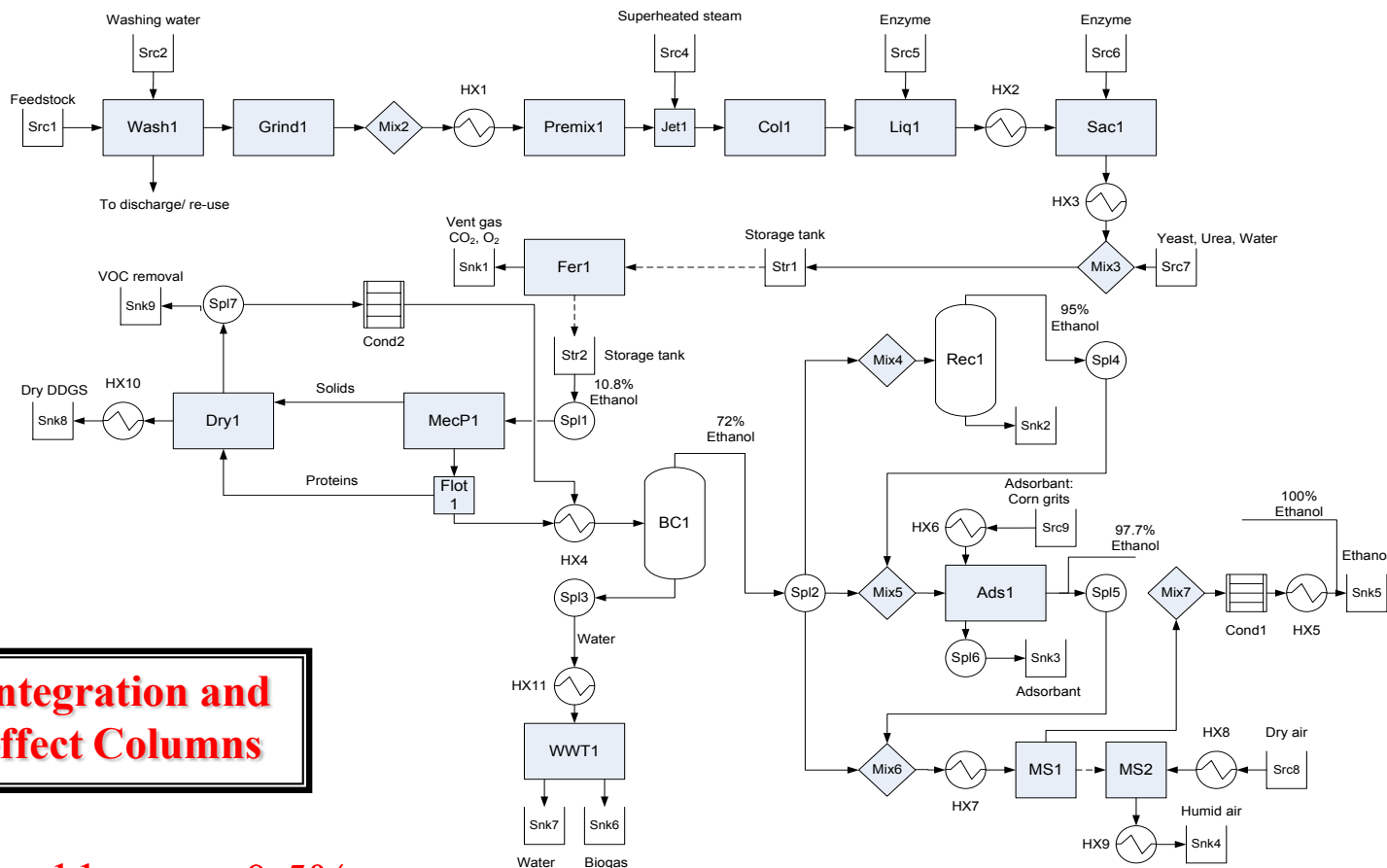


GDP model comprises mass, energy balances, design equations (*short cut*)

2,922 variables (2 Boolean) 2,231 constraints

Energy Optimal Design

60 M gallon /yr plant



**Heat Integration and
Multieffect Columns**

Ethanol losses : 0.5%

Equipment cost = **M\$ 20.7**

Steam cost = **M\$ 7.1/yr (-66%)**

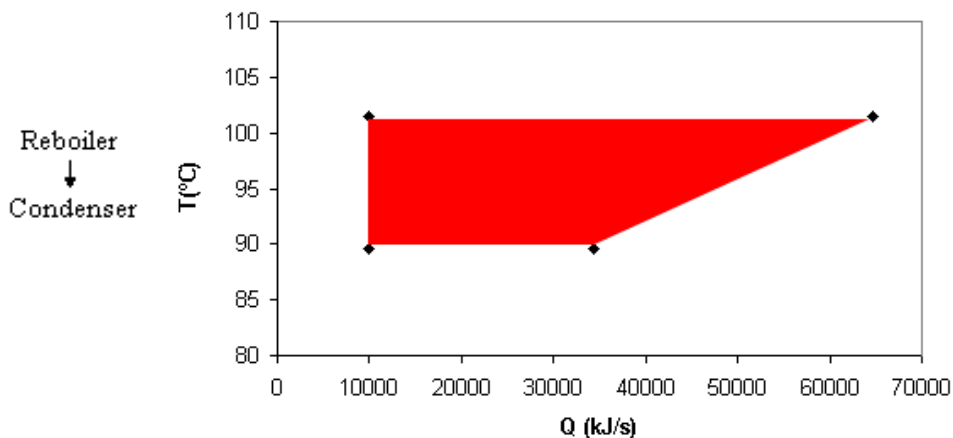
Prod. cost = 1.28 \$/gal

Reduction from \$1.50/gal (base case) to \$1.28/gal !

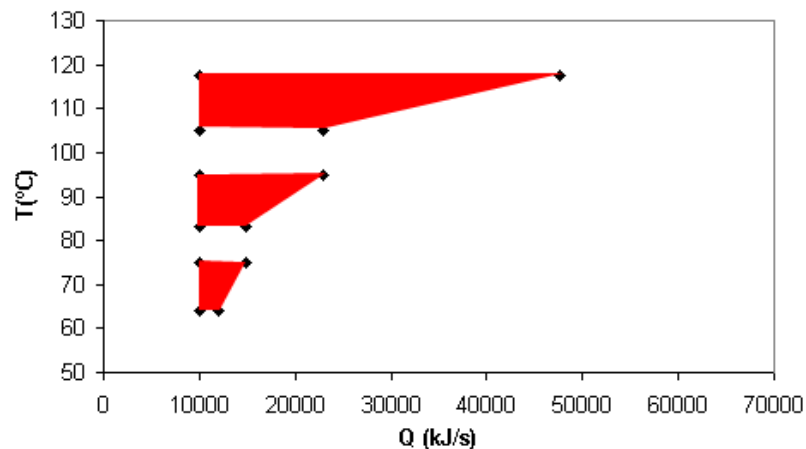
Energy Profiles in Multieffect Columns

Beer Column

Single column

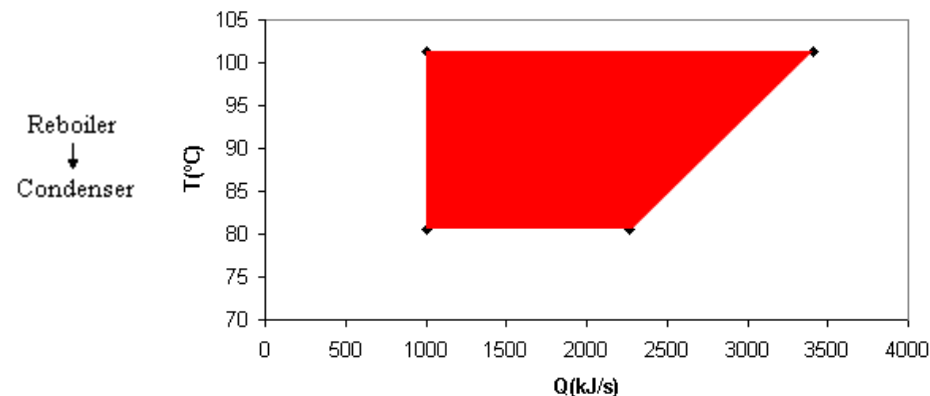


Triple effect column

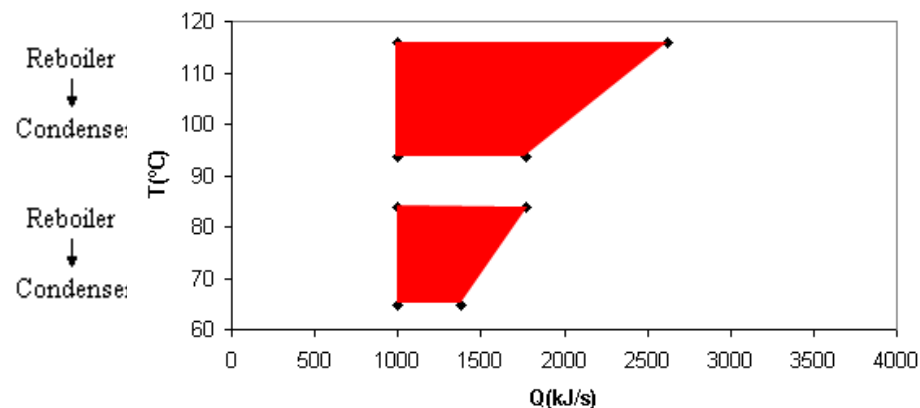


Rectification Column

Single column



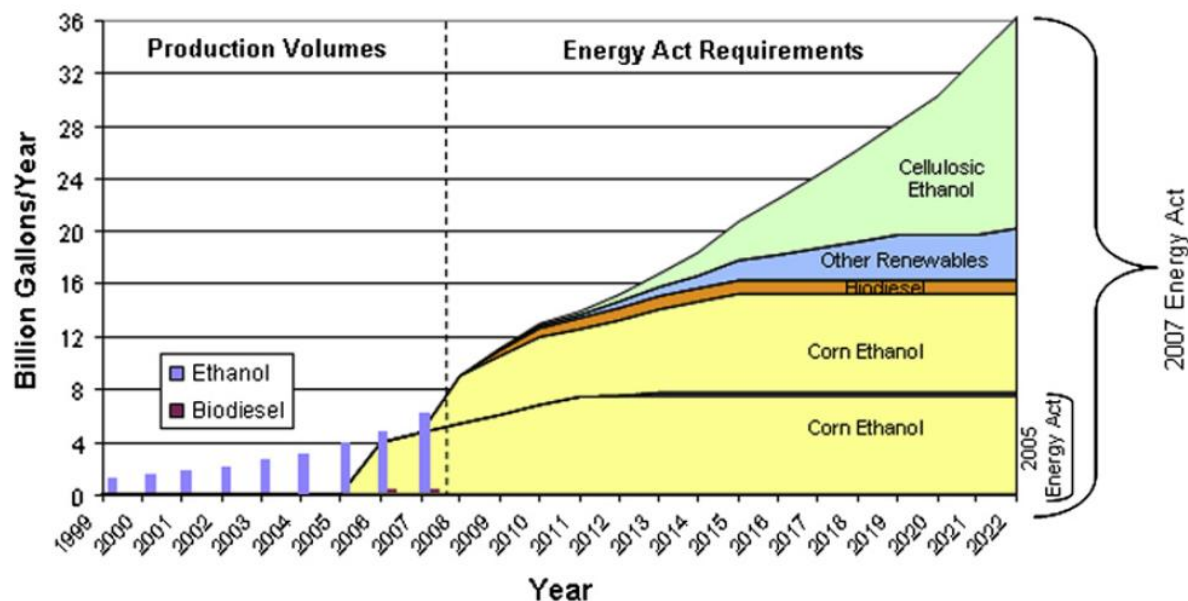
Double effect column



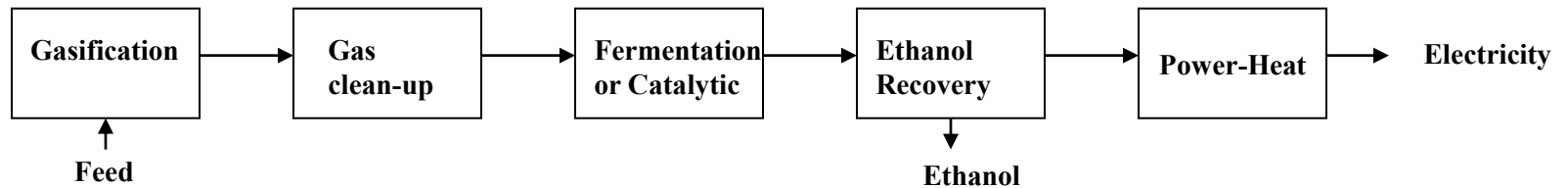
24,918 Btu/gal vs 38,323 Btu/gal

Current ethanol from corn and sugar cane and biodiesel from vegetable oils compete with the **food chain**.

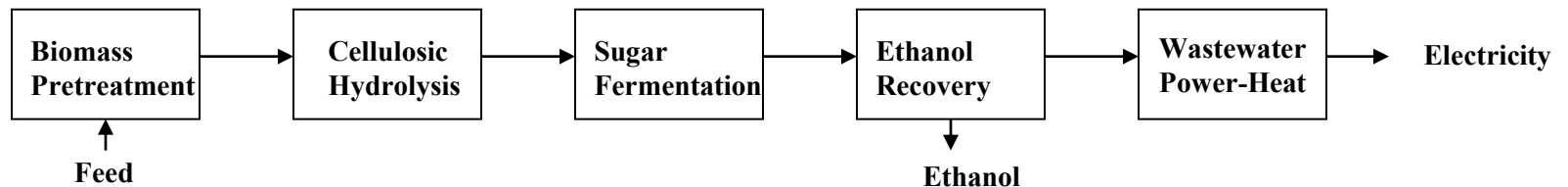
U.S. Government policies support the production of **lignocellulosic based biofuels** and the reuse of wastes and new sources (algae)



a) Thermochemical Process (*gasification*)



b) Hydrolysis Process (*fermentation*)

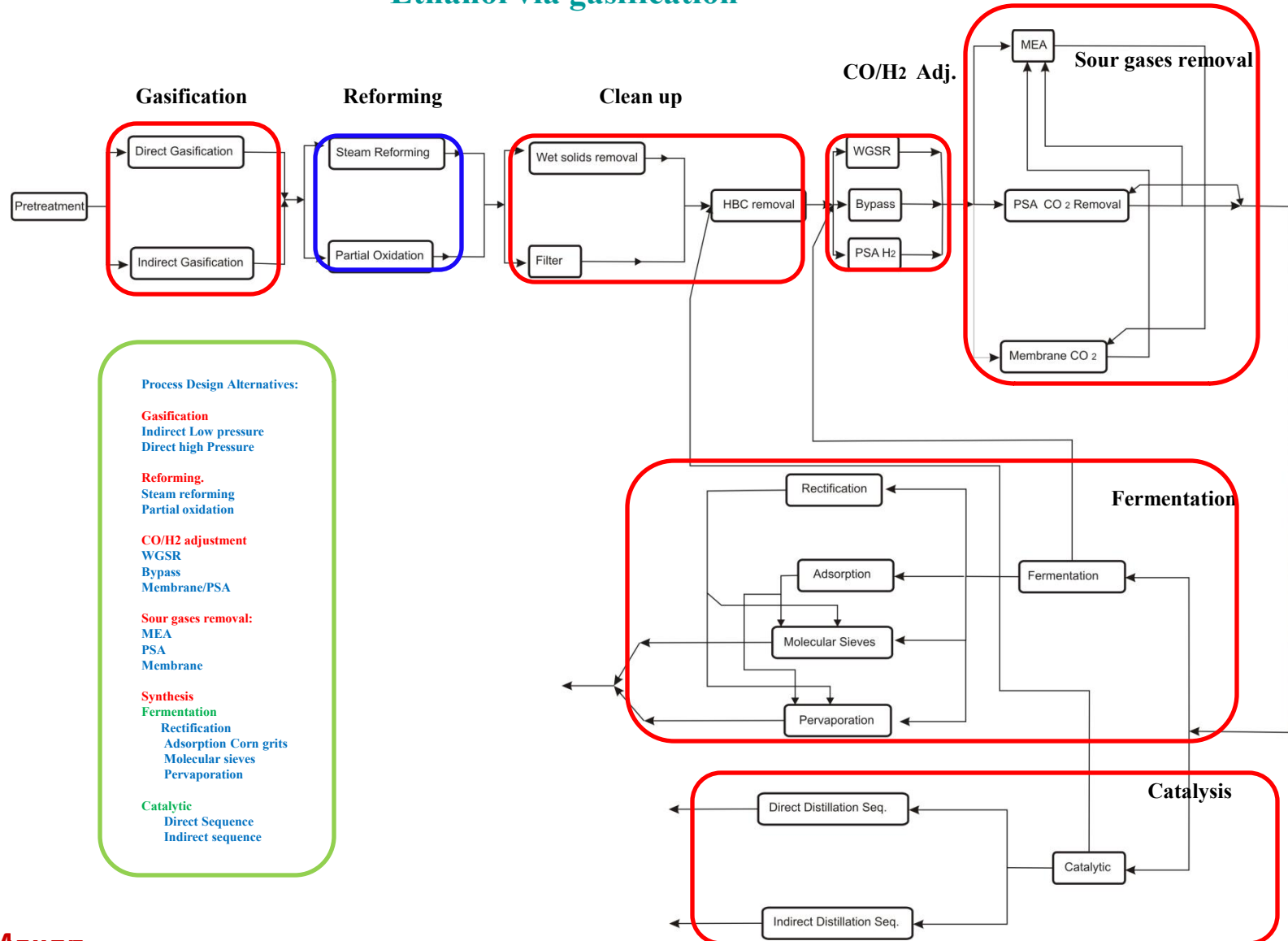


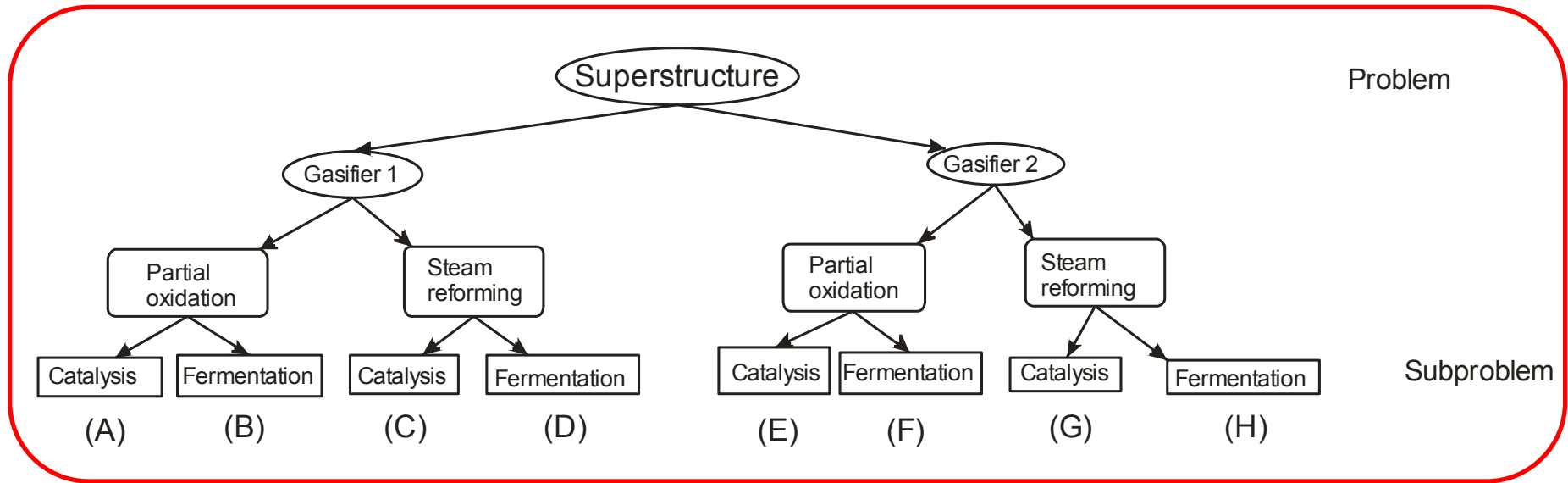
Challenge:

Many alternative flowsheets

Martin, Grossmann (2010)

Ethanol via gasification





Decomposition of GDP in 8 subproblems

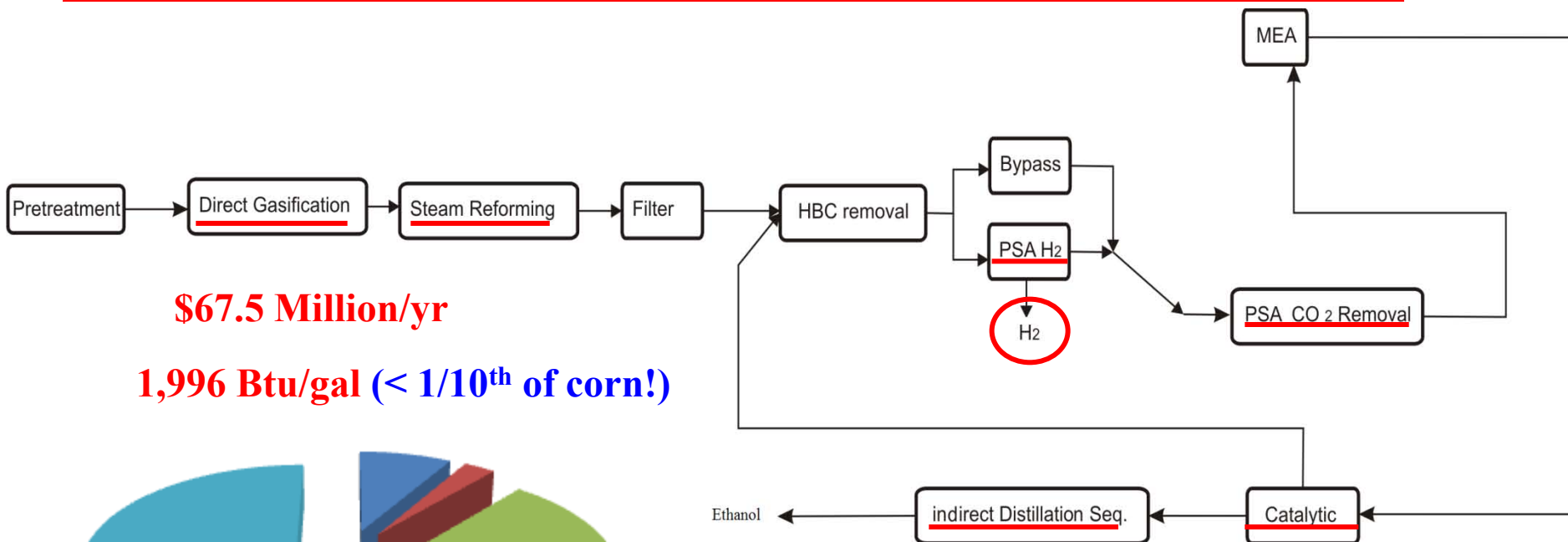
Decision levels: Gasifier

Removal HCs

Reaction of Syn Gas

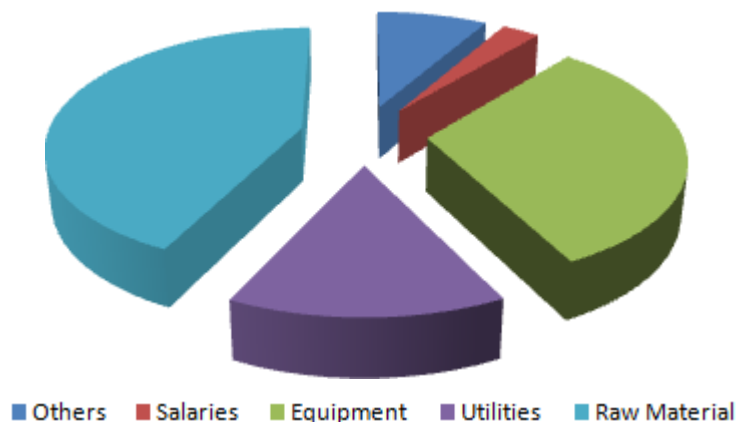


Heat integration and economic evaluation



\$67.5 Million/yr

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



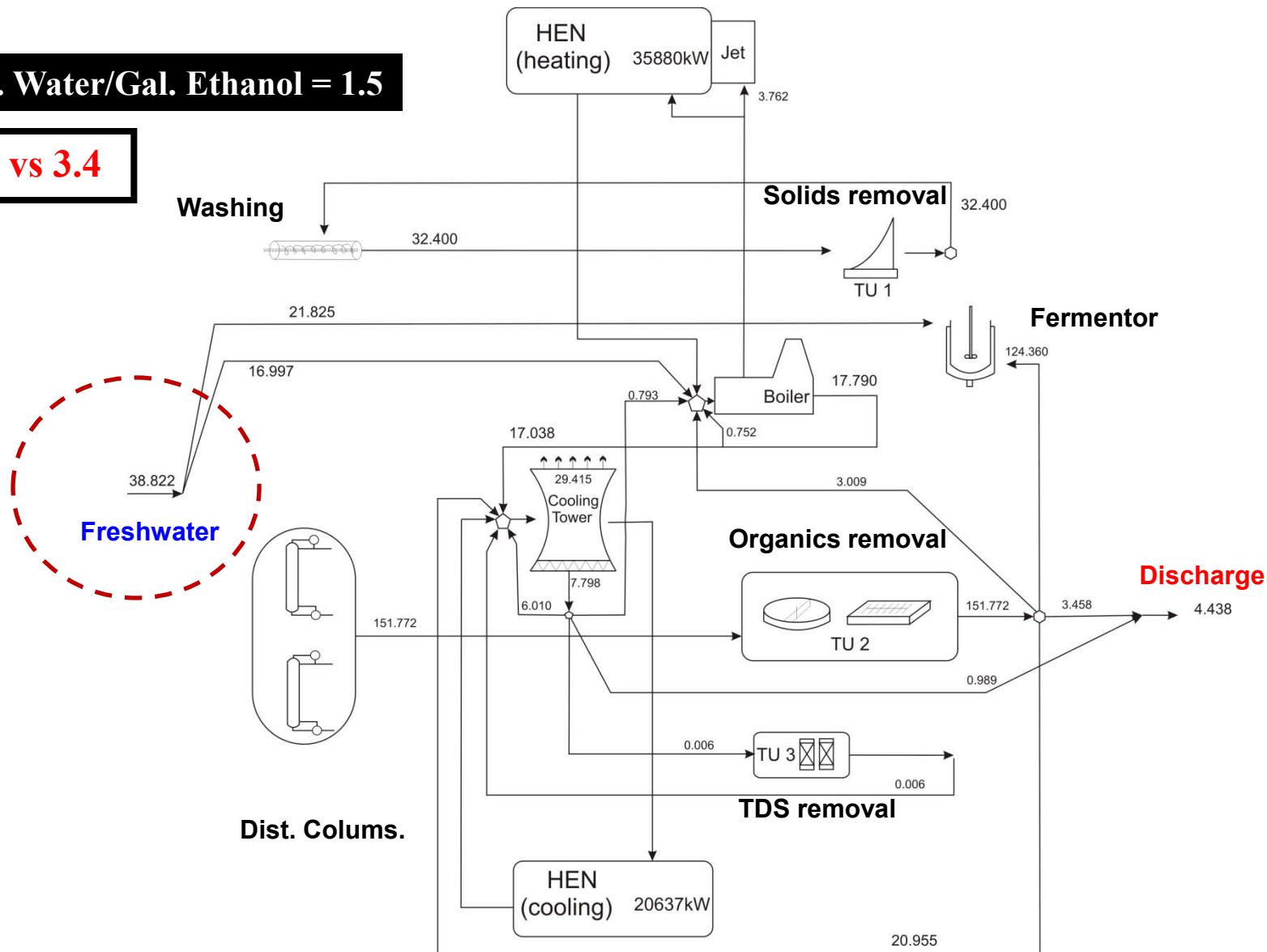
Each NLP subproblem: 7000 eqs., 8000 var
~25 min to solve

Ethanol: \$0.81 /gal (no H₂ credits)
\$ 0.42/gal (H₂ credits)

Low cost is due to H₂ production

Gal. Water/Gal. Ethanol = 1.5

1.5 vs 3.4



Gal. Water/Gal. Ethanol = 4.2

Cellulosic Bioethanol via Gasification

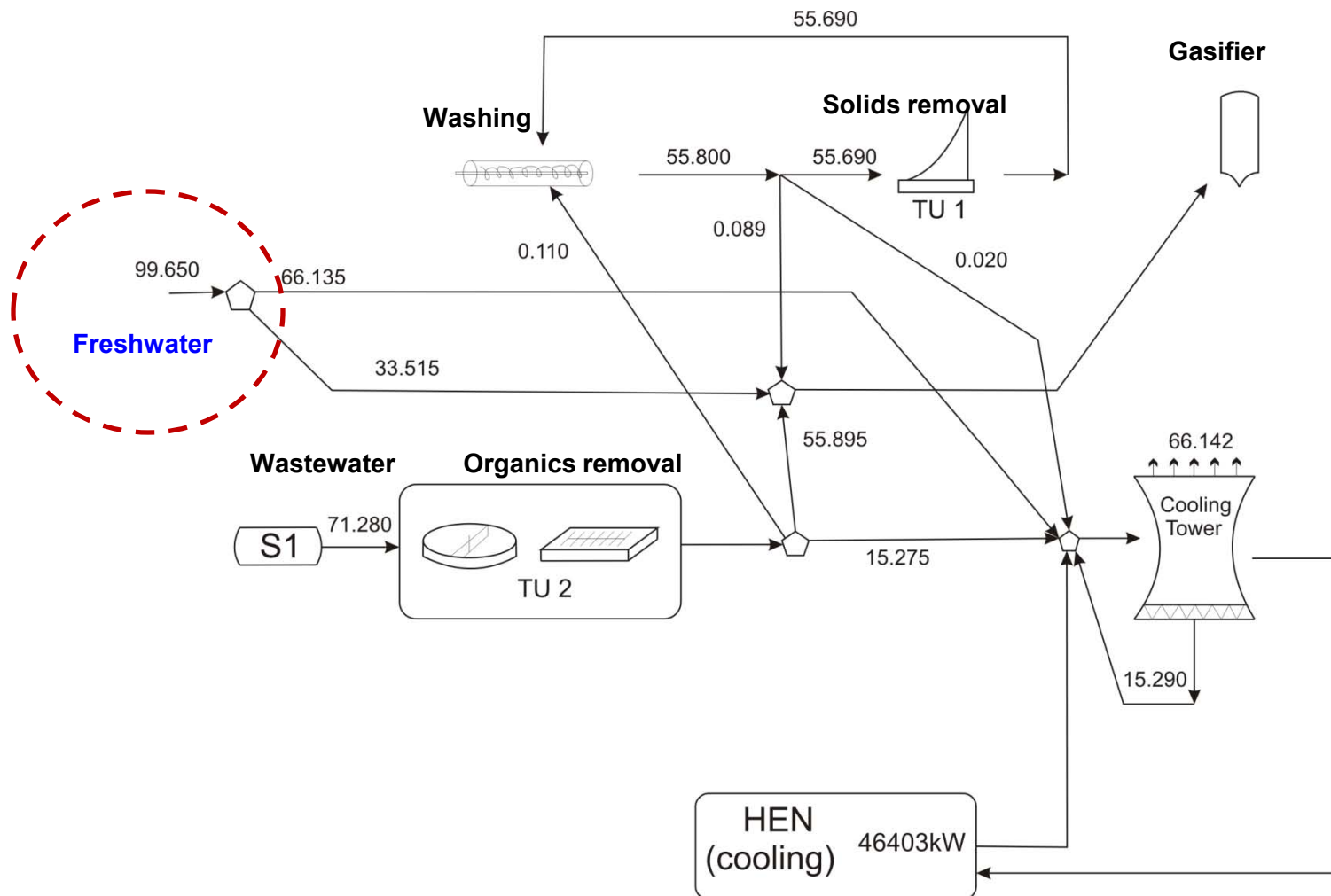


Table Summary of results [6-10]

	Ethanol (Hydrolysis)	Ethanol (Gasification & Catalysis)	Ethanol (Gasification & Fermentation)	FT-Diesel	Hydrogen	Biodiesel (Cooking)	Biodiesel (Algae)
	A	C		D	B	F	E
Total investment (\$MM)	161	335	260	212	148	17	102
Capacity(MMgal/yr)	60	60	60	60	60*	72	72
Biofuel yield (kg/kg _{wet})	0.28	0.20	0.33	0.24	0.11	0.96	0.48
Production cost (\$/gal)	0.80	0.41	0.81	0.72	0.68*	0.70	0.47
Water consumption(gal/gal)	1.66	0.36	1.59	--	--	0.33	0.60
Energy consump. (MJ/gal)	-10.2	-9.5	27.2	-60.0	-3.84*	1.94	1.94
Byproduct	Energy CO ₂	Hydrogen Energy CO ₂	Hydrogen CO ₂	Green Gasoline Energy CO ₂	Energy CO ₂	Glycerol	Glycerol Fertilizer
(*) kg instead of gal							

[6] Martín, M., Grossmann, I.E. (2011) AIChE J. DOI: 10.1002/aic.12544

[7] Martín, M., Grossmann, I.E. Energy optimization of Hydrogen production from biomass. Rev. Submitted to Comp. Chem. Eng.

[8] Martín, M., Grossmann, I.E. Energy optimization of lignocellulosic bioethanol production via Hydrolysis to be submitted AIChE J.

[9] Martín, M., Grossmann, I.E. Process optimization of FT- Diesel production from biomass. To be submitted

[10] Martín, M., Grossmann, I.E. Process optimization bioDiesel production from cooking oil and Algae. To be submitted

Design and Planning under Uncertainty

Goal: robustness in decisions

Design of Responsive Supply Chains

Uncertain demands

Maximize NPV/Minimize responsiveness

Chance constrained MINLP

Design and Planning of Offshore Oilfields

ExxonMobil

Uncertain fields size, deliverability, water

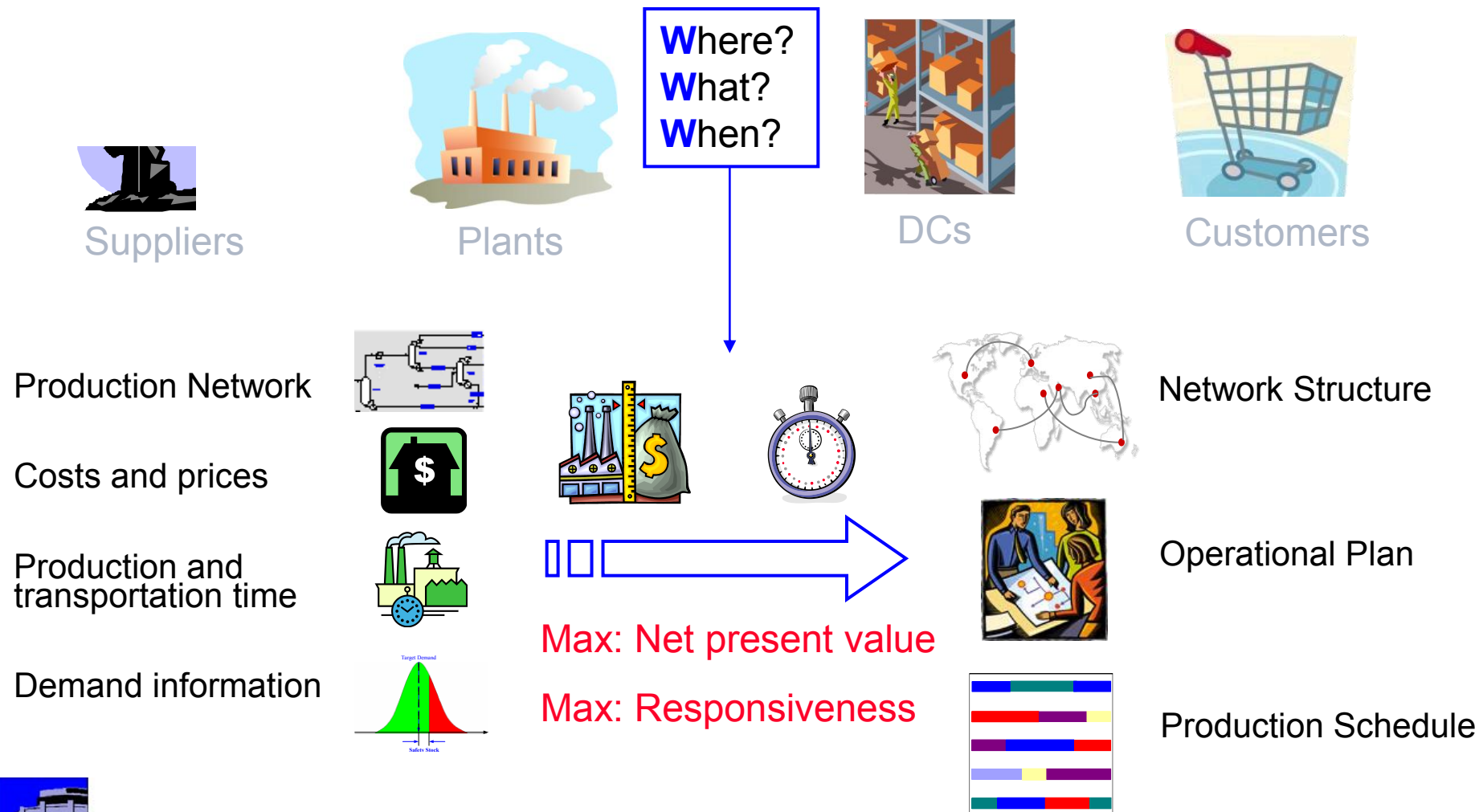
Maximize expected flexibility/Minimize Cost

Multi-stage programming MINLP

A world map with green arrows showing a circular flow of goods and services between various icons representing different sectors: a skyscraper, an airplane, a truck, a warehouse, an oil rig, storage tanks, a semi-truck, a factory, a train, a power plant, offshore oil rigs, a cargo ship, a grain elevator, and a warehouse.

Objective: design supply chains under responsive and economic criteria with consideration of inventory management and demand uncertainty

Problem Statement



Production Network of Polystyrene Resins

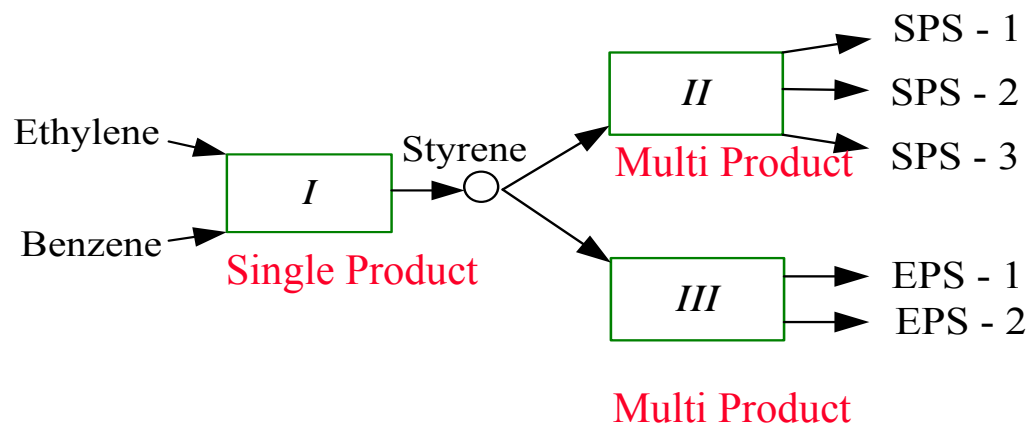
Three types of plants:

Plant I: *Ethylene + Benzene* \longrightarrow *Styrene* (1 products)

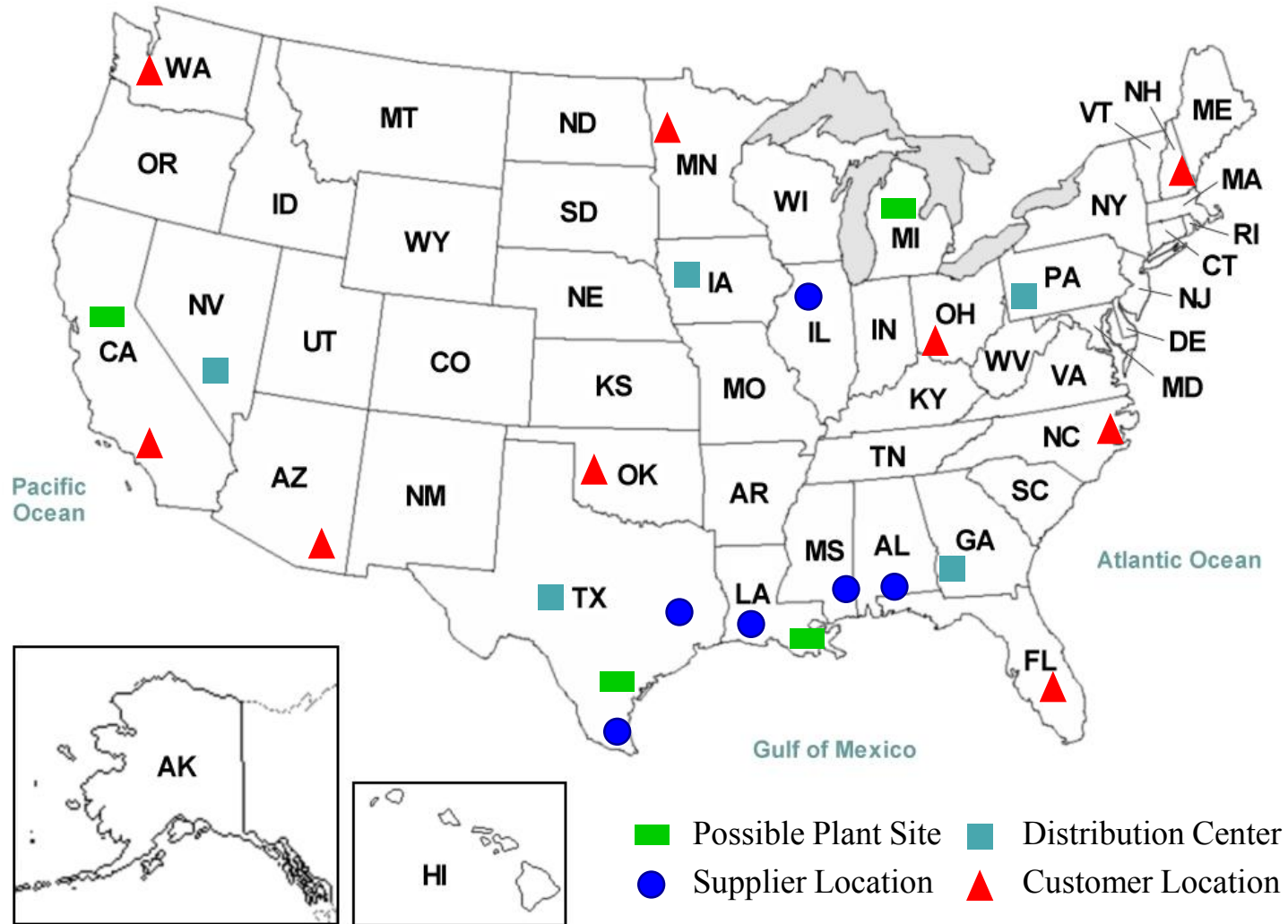
Plant II: *Styrene* \longrightarrow *Solid Polystyrene (SPS)* (3 products)

Plant III: *Styrene* \longrightarrow *Expandable Polystyrene (EPS)* (2 products)

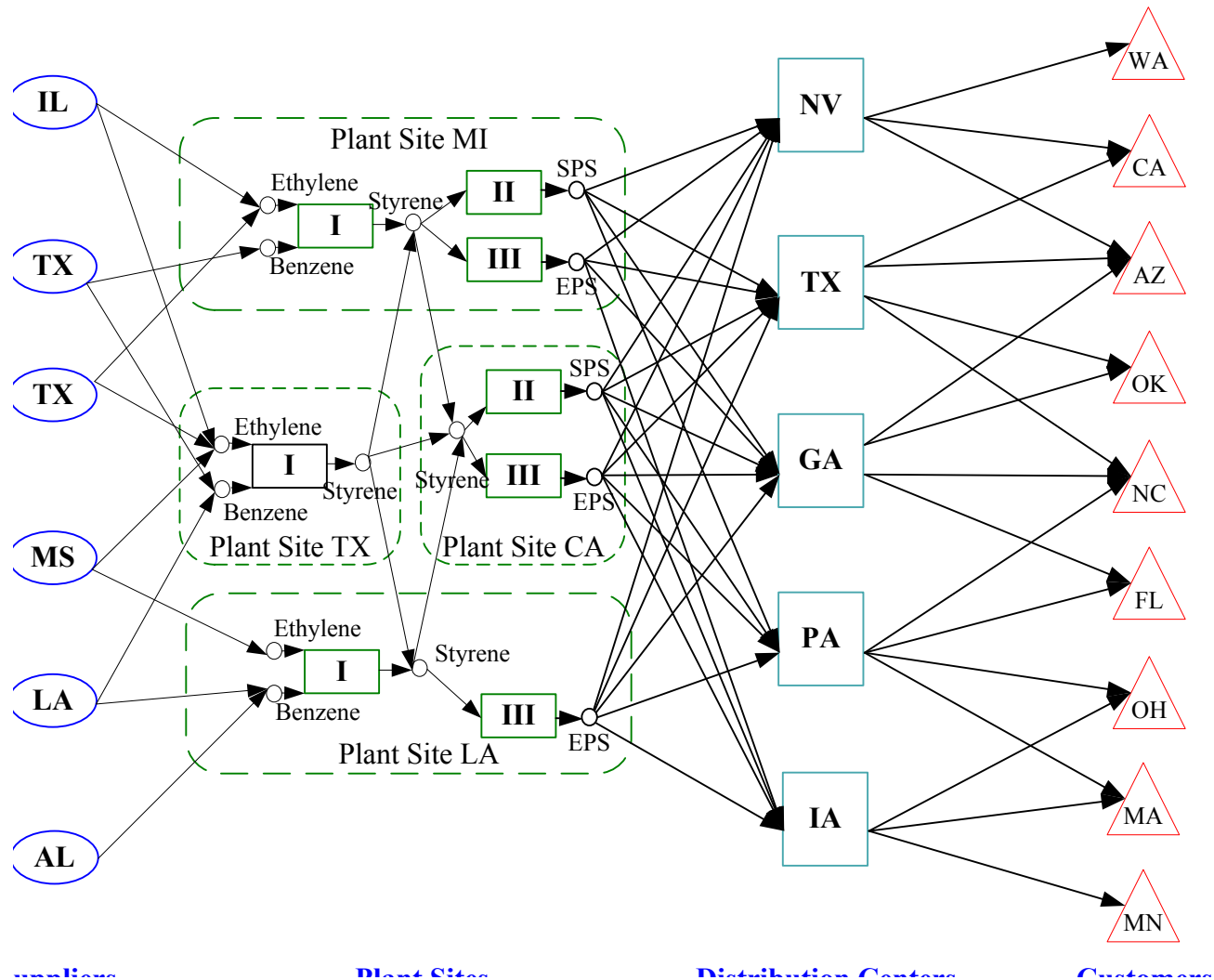
Basic Production Network



Location Map

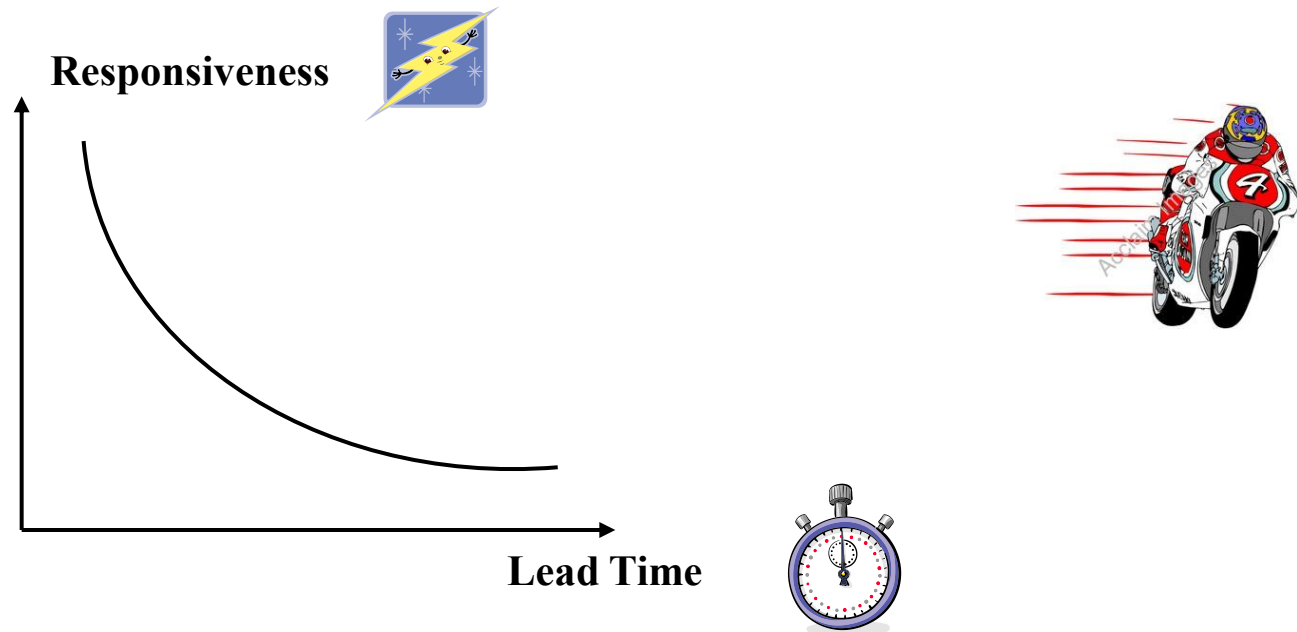


Potential Network Superstructure



Responsiveness - Lead Time

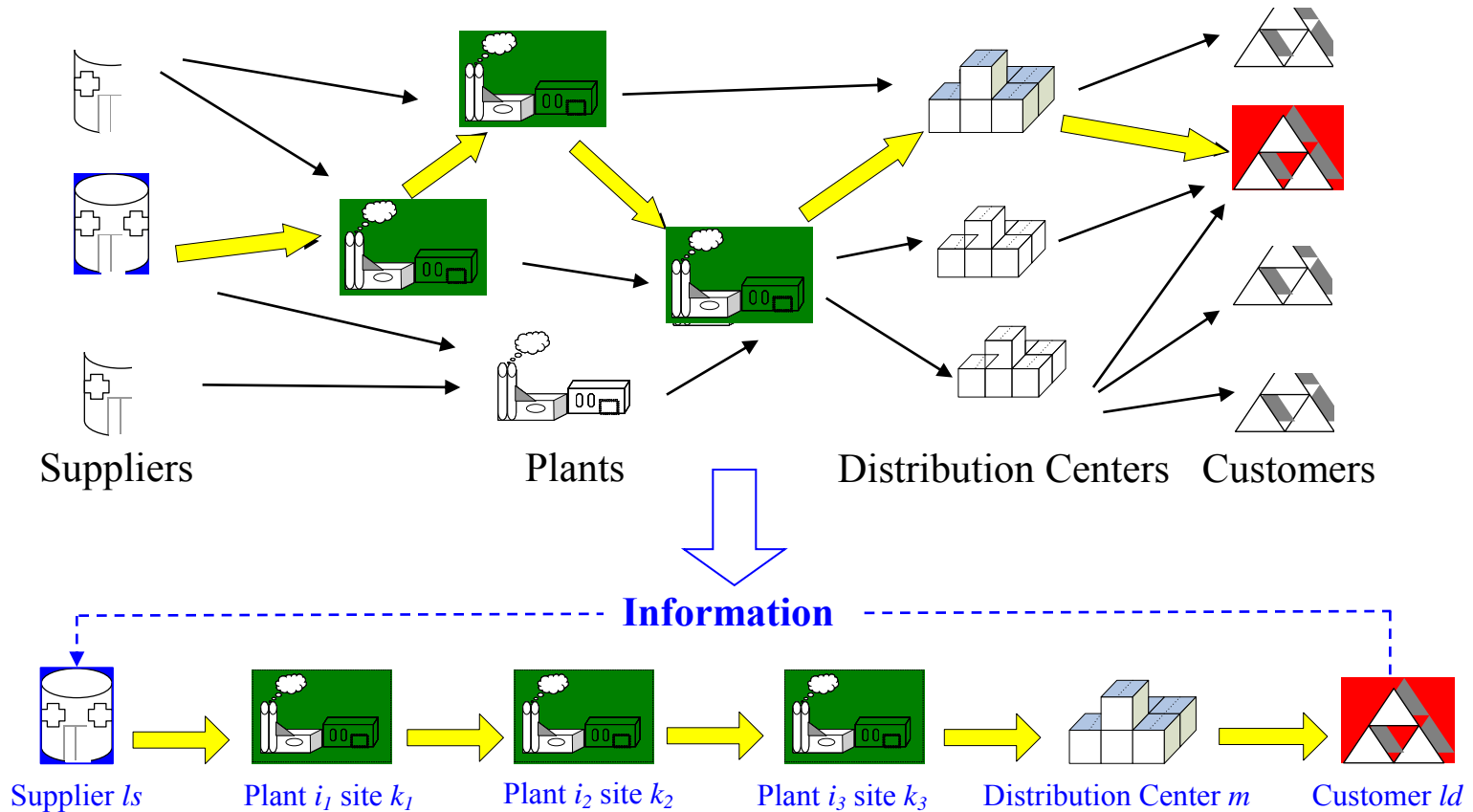
- ♦ **Lead Time:** The **time** of a supply chain network to respond to customer demands and preferences in the **worst case**



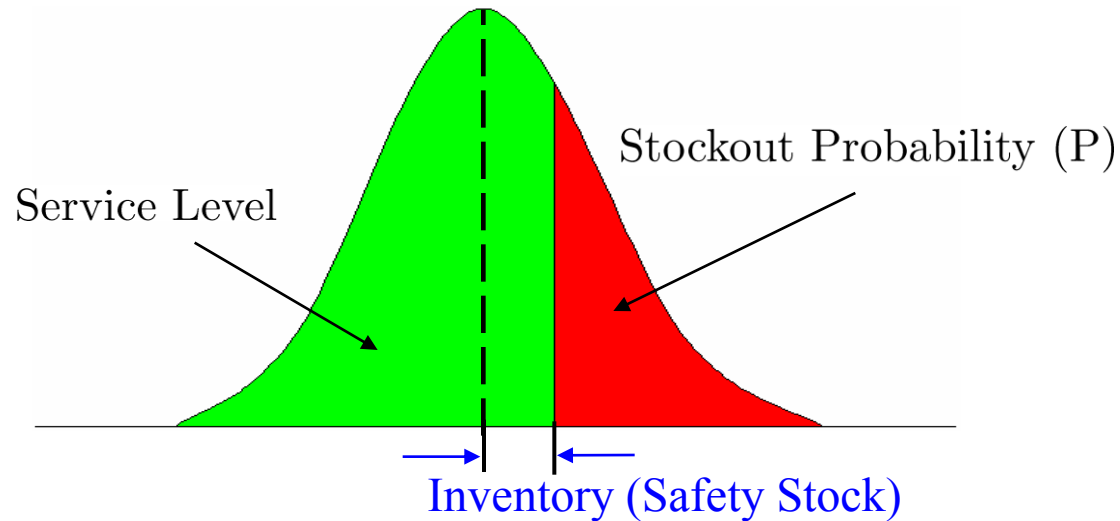
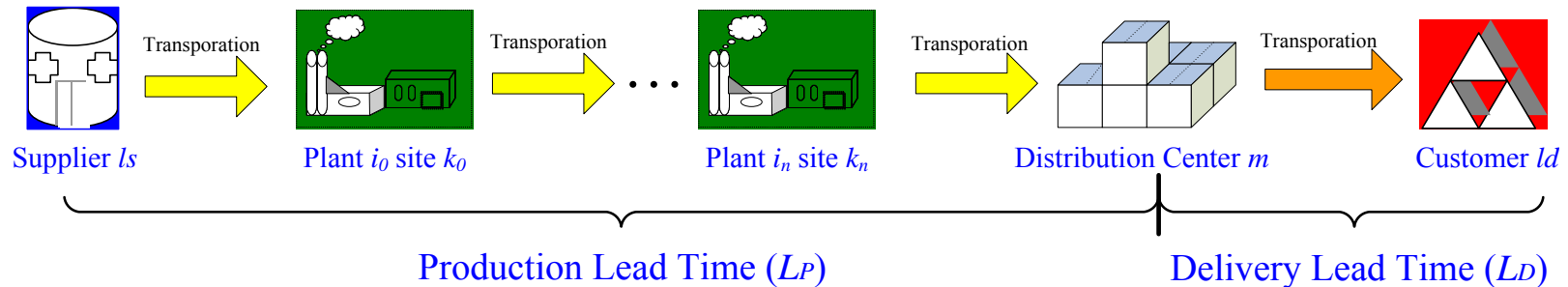
Lead Time is a **measure of responsiveness in SCs**

Lead Time for A Linear Supply Chain

- A supply chain network = \sum Linear supply chains
 - ◆ Assume information transfer instantaneously



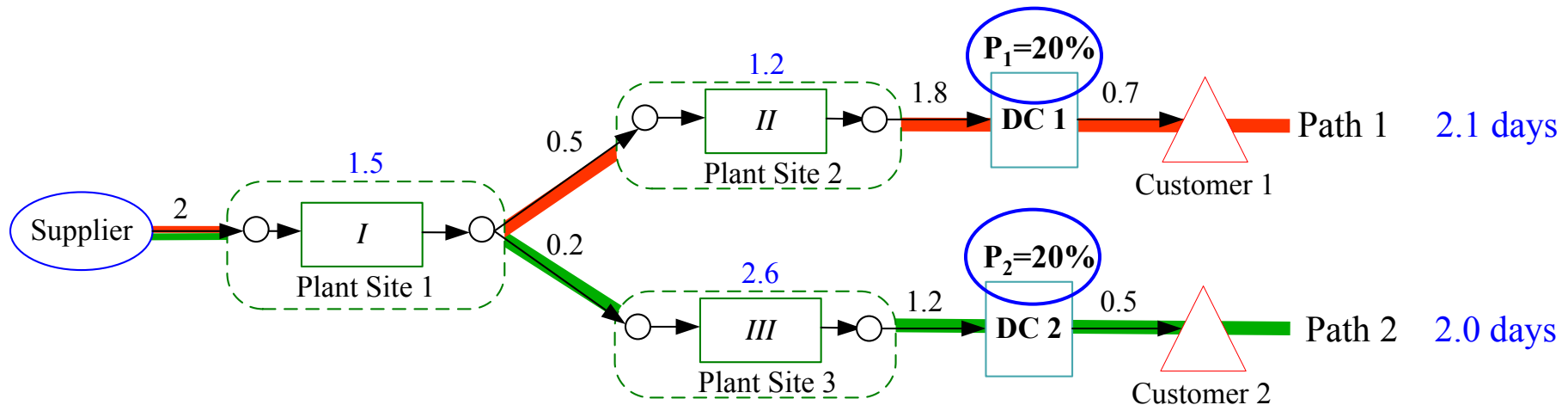
Lead Time under Demand Uncertainty



$$\text{Expected Lead Time} = L_D + P(\text{Stockout}) \cdot L_P$$

Expected Lead Time of SCN

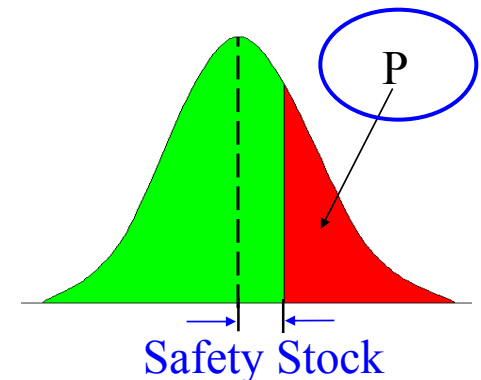
- Expected Lead time of a supply chain network (**uncertain demand**)
 - The **longest** expected lead time for all the paths in the network (**worst case**)
 - Example: A simple SC with all process are **dedicated**



For Path 1: $(2 + 1.5 + 0.5 + 1.2 + 1.8) \times 20\% + 0.7 = 2.1$ days

For Path 2: $(2 + 1.5 + 0.2 + 2.6 + 1.2) \times 20\% + 0.5 = 2.0$ days

Expected Lead Time = $\max \{2.1, 2.0\} = 2.1$ days



Bi-criterion Multiperiod MINLP Formulation

Choose Discrete (0-1), continuous variables

- Objective Function:

- ♦ Max: Net Present Value
 - ♦ Min: Expected Lead time
- } Bi-criterion

- Constraints:

- ♦ Network structure constraints

Suppliers – plant sites Relationship

Plant sites – Distribution Center

Input and output relationship of a plant

Distribution Center – Customers

Cost constraint

- ♦ Operation planning constraints

Production constraint

Capacity constraint

Mass balance constraint

Demand constraint

Upper bound constraint

- ♦ Cyclic scheduling constraints

Assignment constraint

Sequence constraint

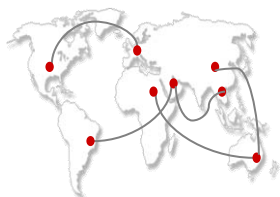
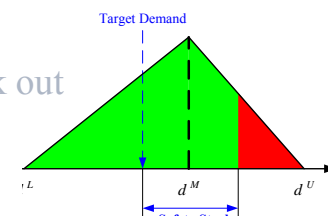
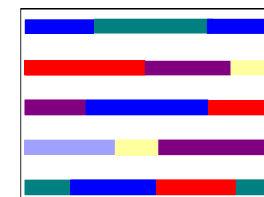
Demand constraint

Production constraint

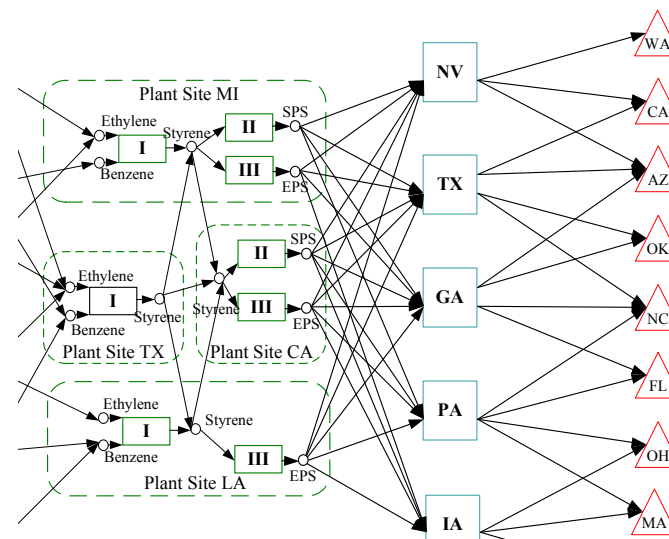
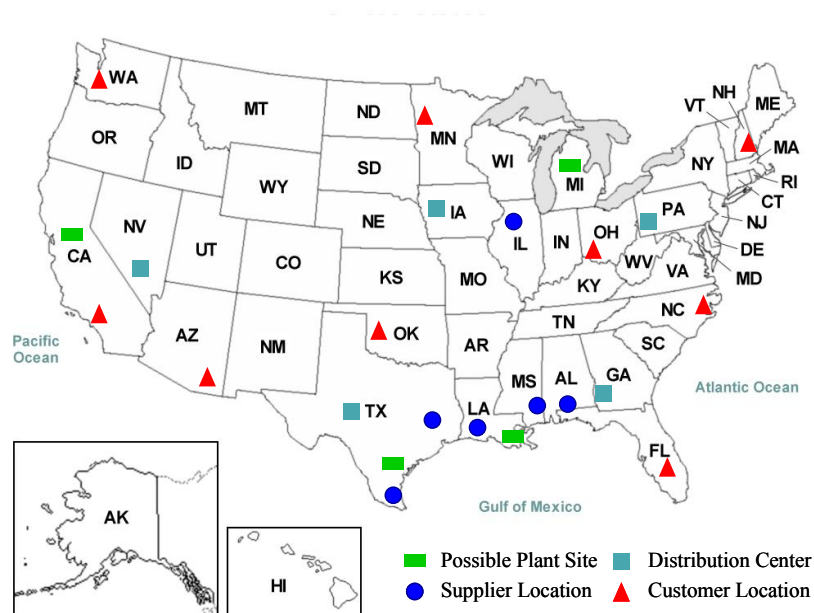
Cost constraint

- ♦ Probabilistic constraints

Chance constraint for stock out
(reformulations)



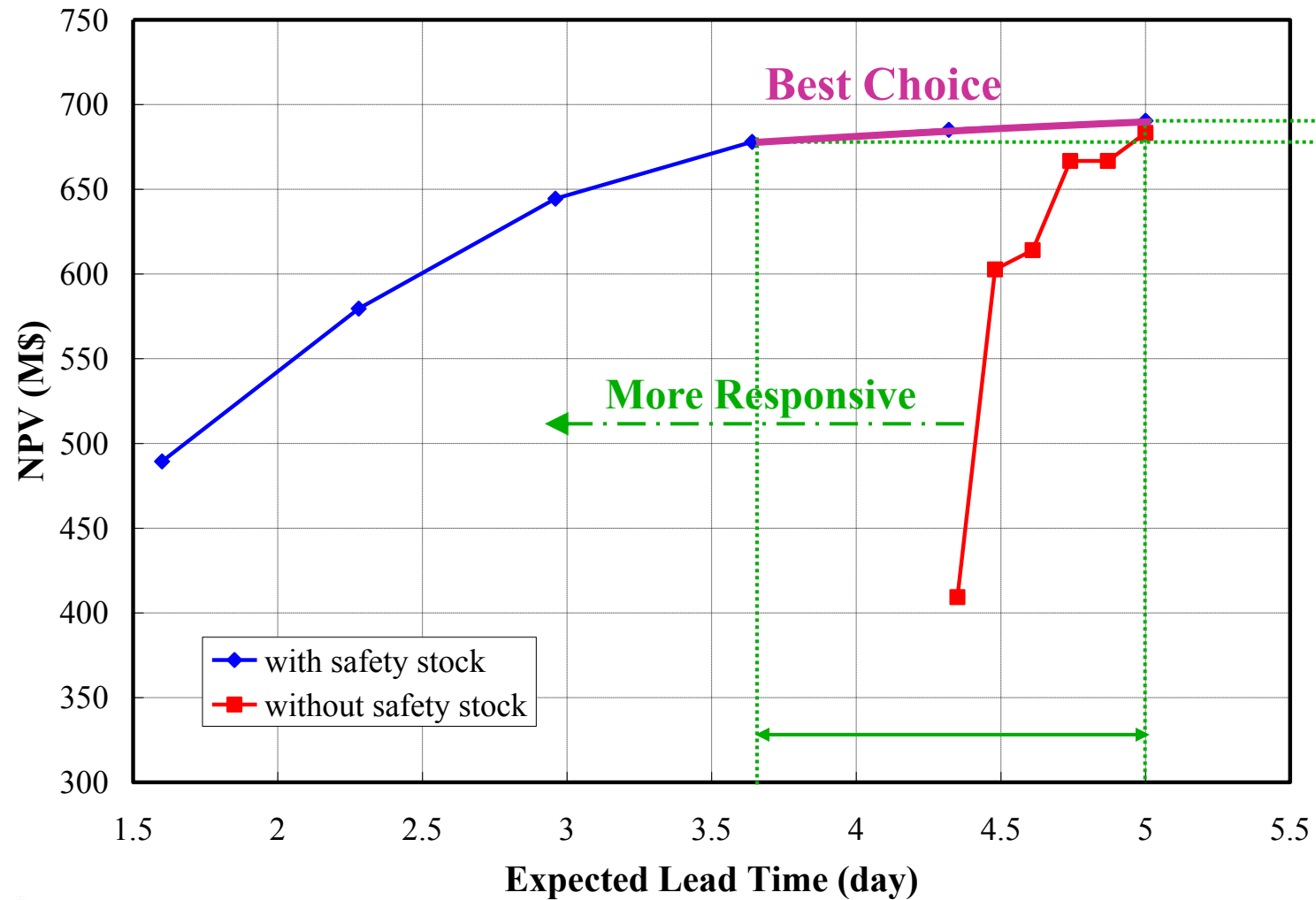
Case Study



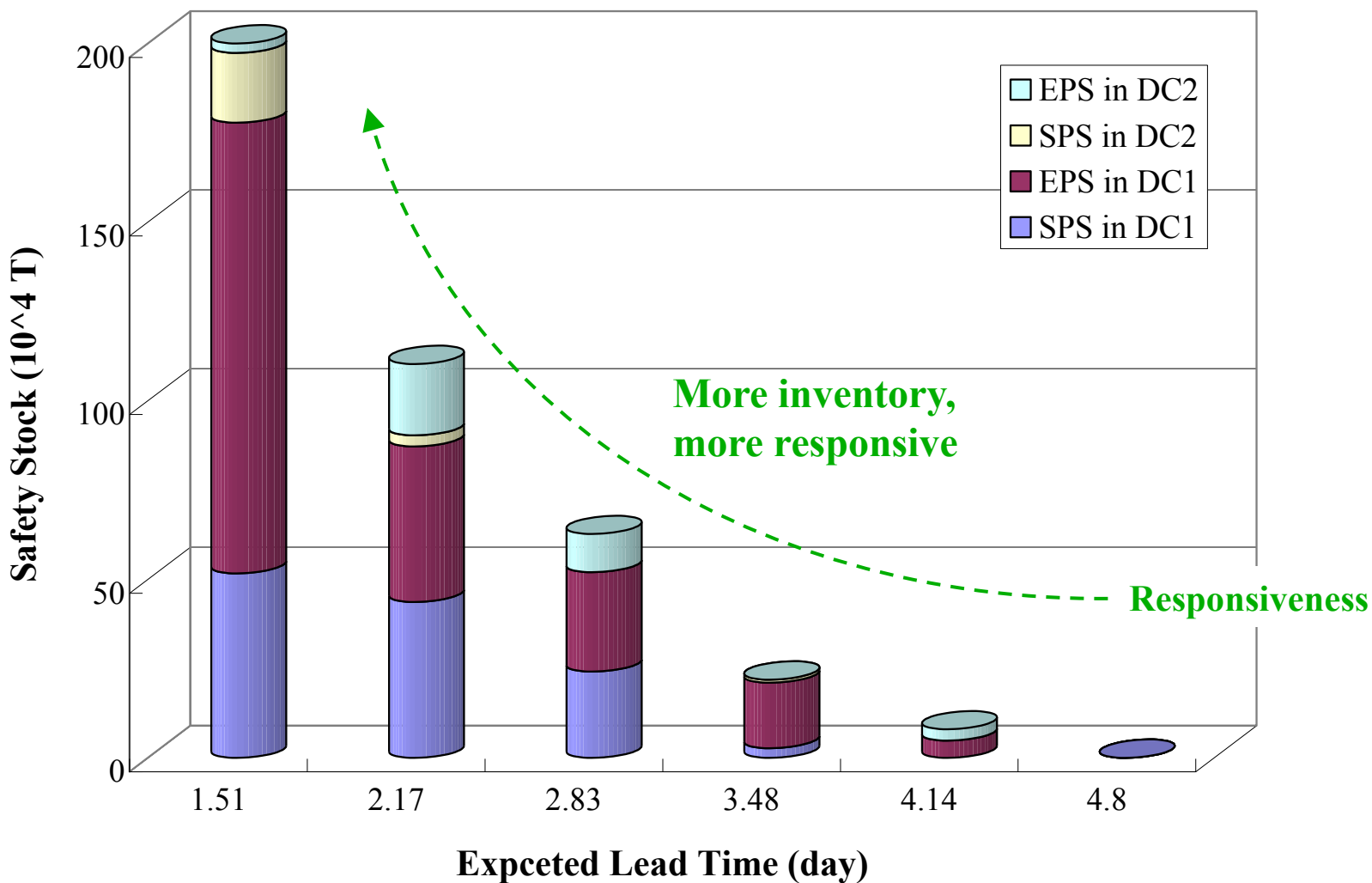
- Problem Size:
 - ◆ # of Discrete Variables: 215
 - ◆ # of Continuous Variables: 8126
 - ◆ # of Constraints: 14617

- Solution Time:
 - ◆ Solver: GAMS/BARON
 - ◆ Direct Solution: > 2 weeks
 - ◆ Proposed Algorithm: ~ 4 hours

Pareto Curves – with and without safety stock

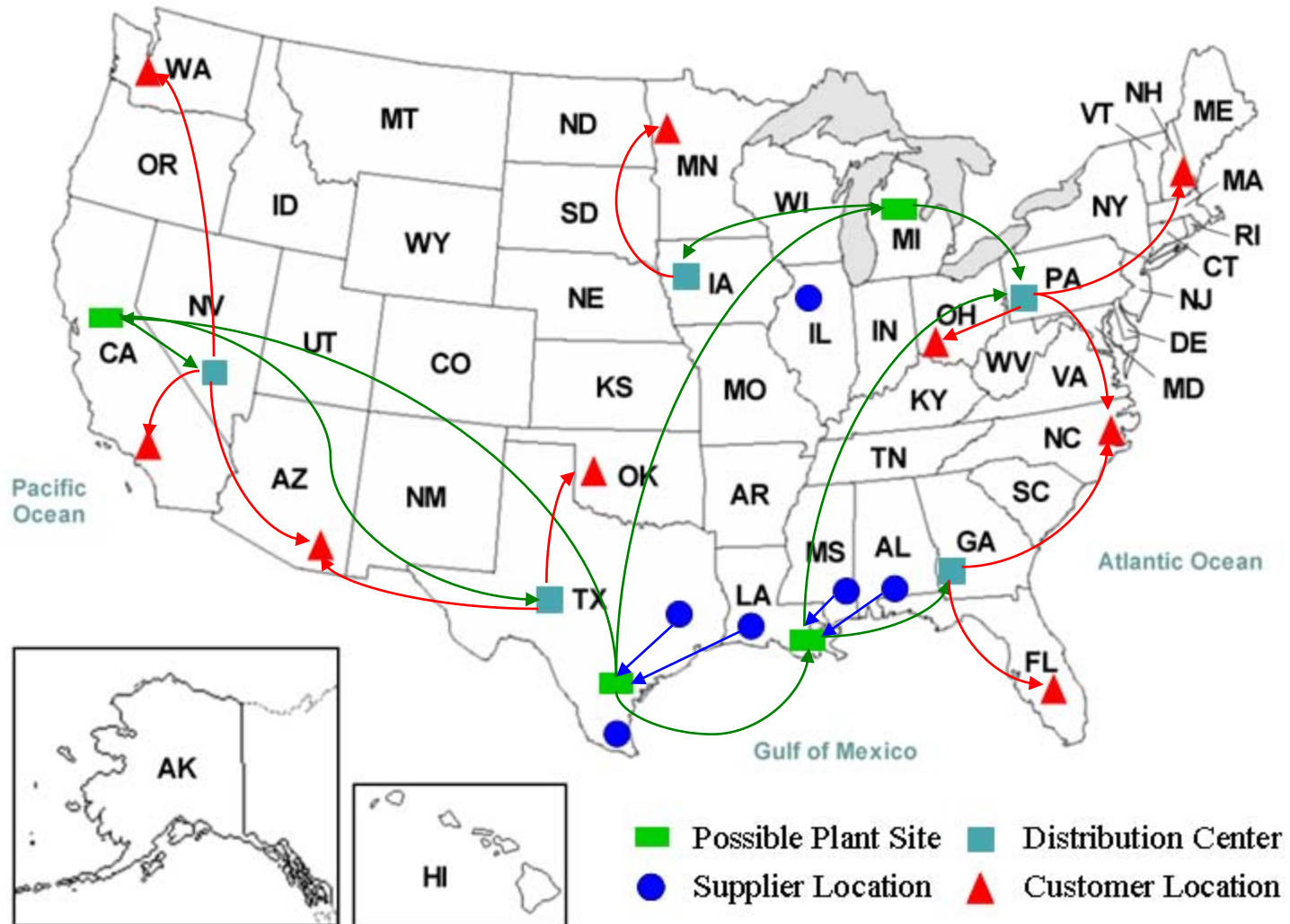


Safety Stock Levels - Expected Lead Time





Network Structure at Location Map



Tarhan, Grossmann (2009)

- Offshore oilfield having several reservoirs **under uncertainty**
- **Maximize the expected net present value (ENPV)** of the project

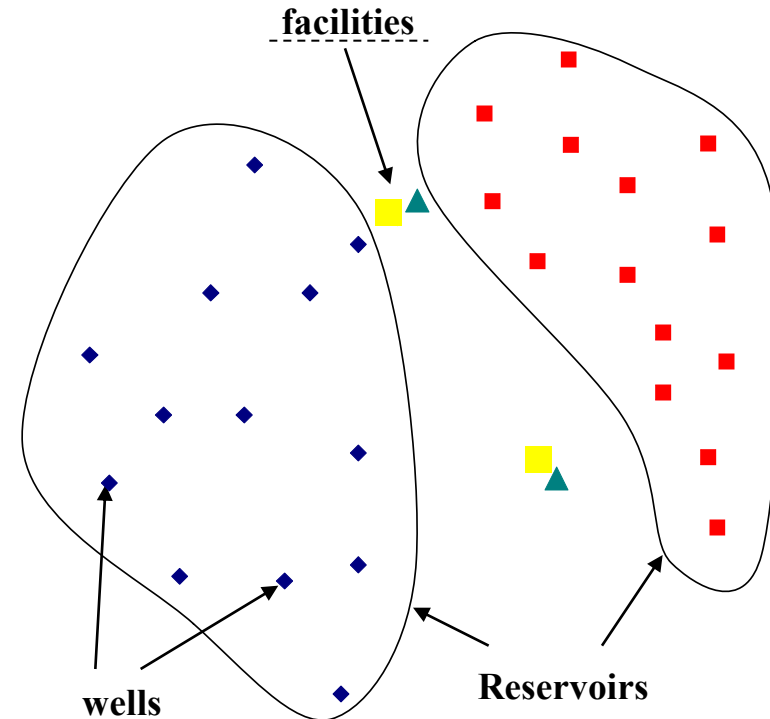
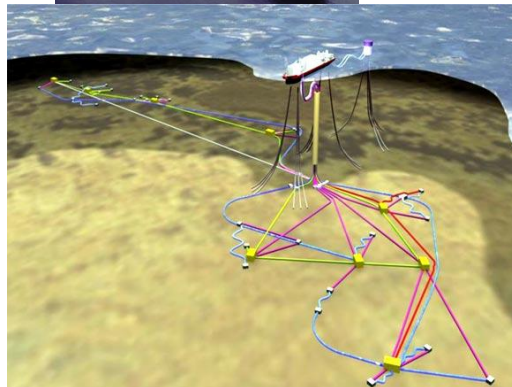
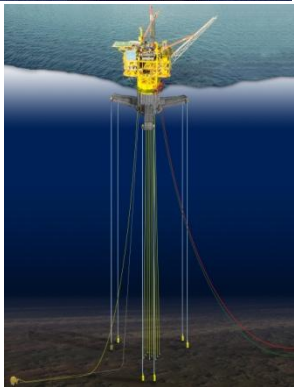
Decisions:

- Number and capacity of TLP/FPSO facilities
- Installation schedule for facilities
- Number of sub-sea/TLP wells to drill
- Oil production profile over time

TLP



FPSO



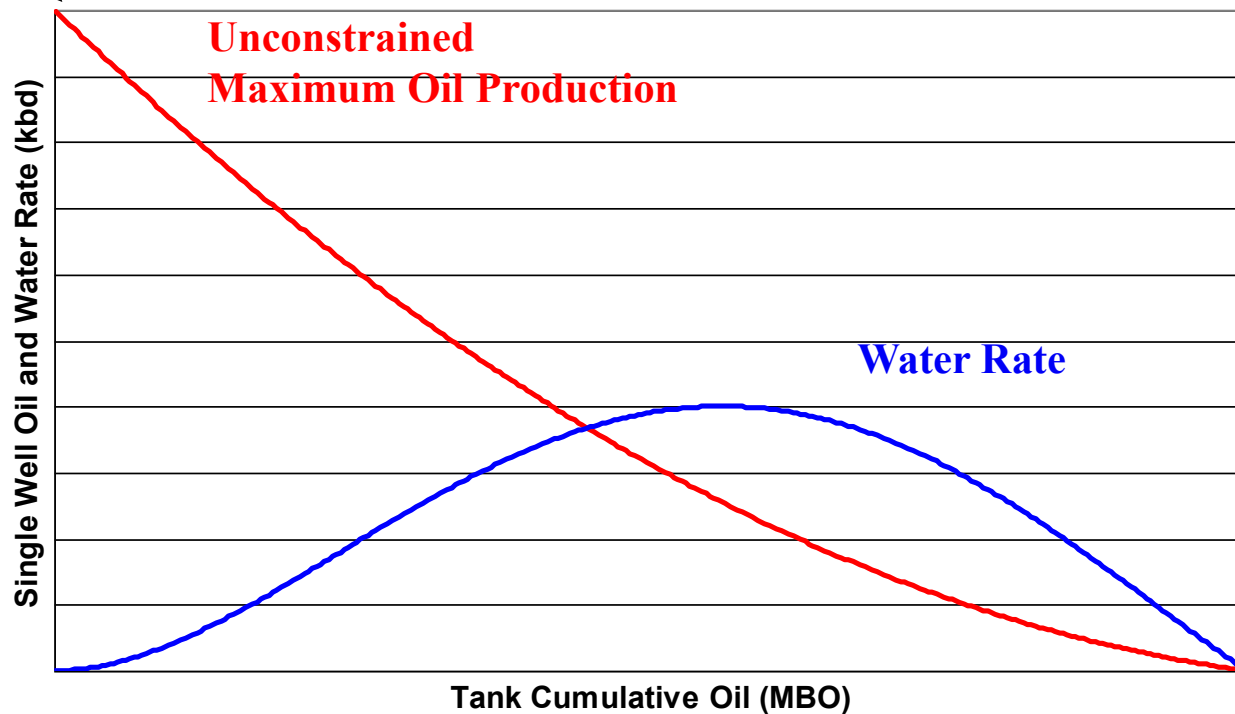
Uncertainty:

- **Initial productivity per well**
- **Size of reservoirs**
- **Water breakthrough time for reservoirs**

Non-linear Reservoir Model

Initial oil
production

Assumption: All wells in the same reservoir are identical.



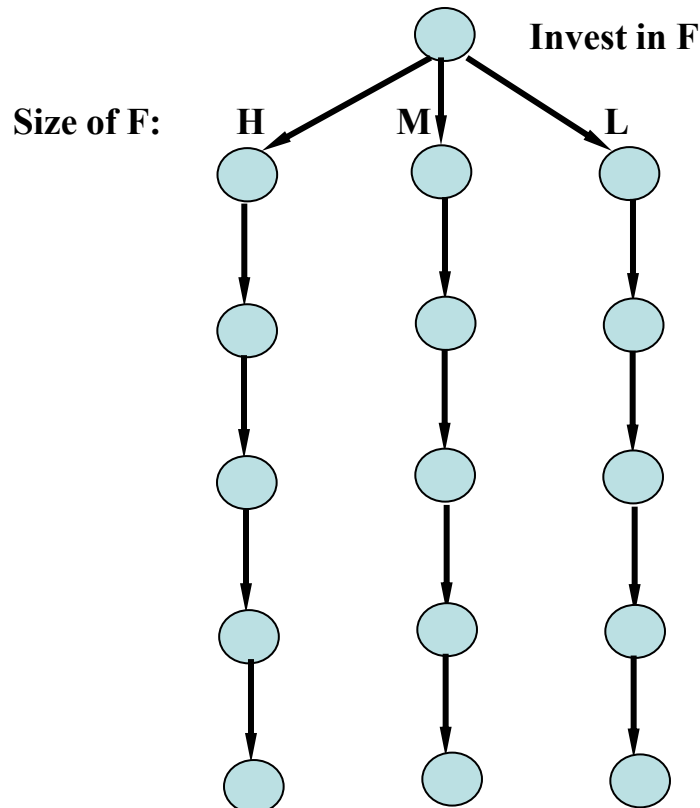
Size of the reservoir

Uncertainty is represented by discrete distributions functions

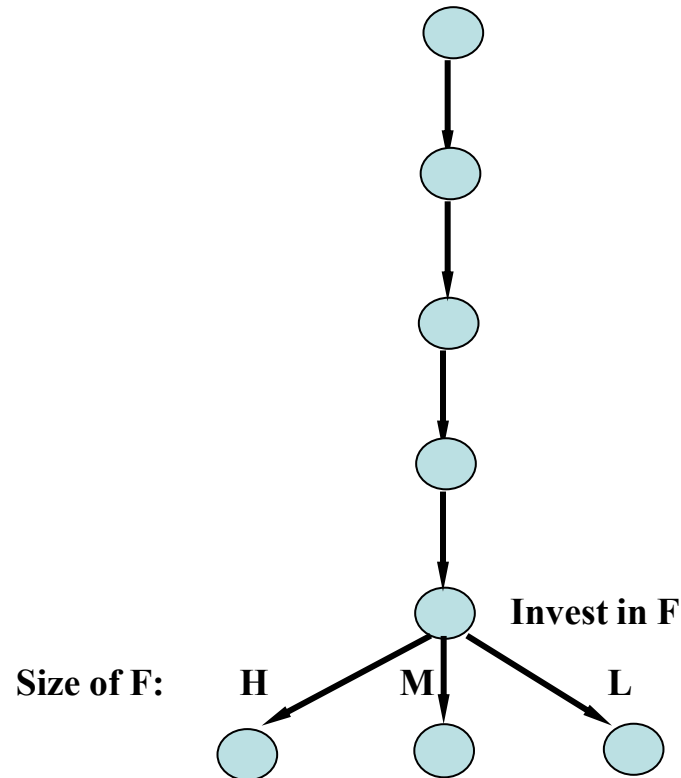
Decision Dependent Scenario Trees

Assumption: Uncertainty in a field resolved as soon as WP installed at field

Invest in F in year 1



Invest in F in year 5



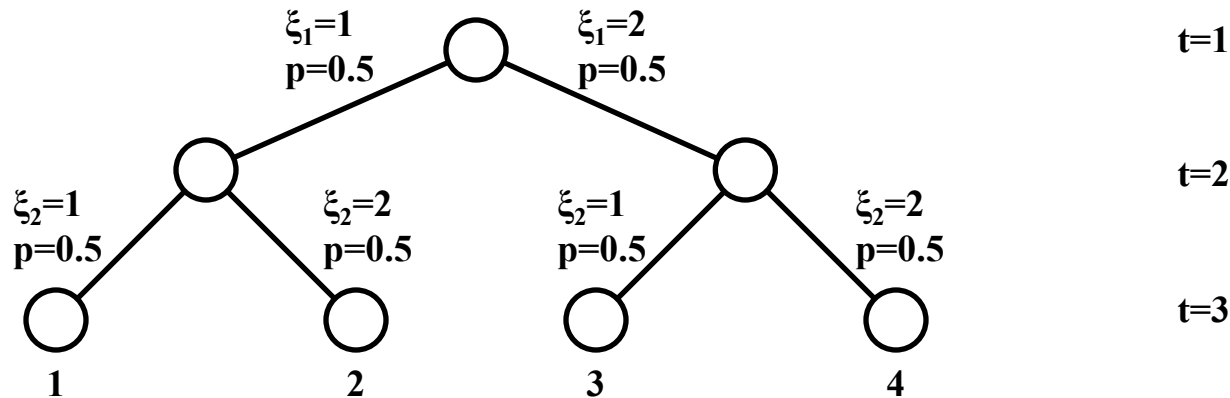
Scenario tree

Not unique: Depends on timing of investment at uncertain fields

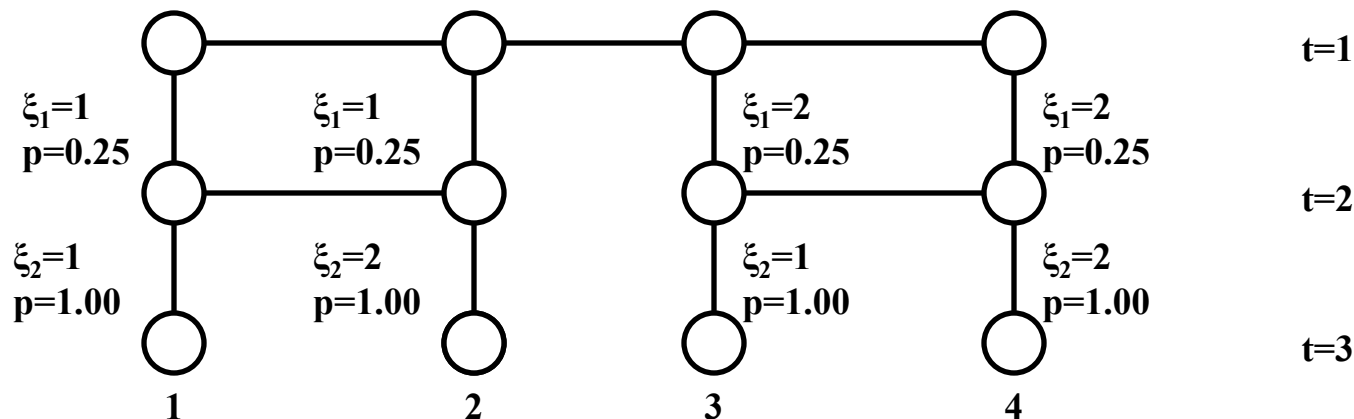
Central to defining a Stochastic Programming Model

Stochastic Programming

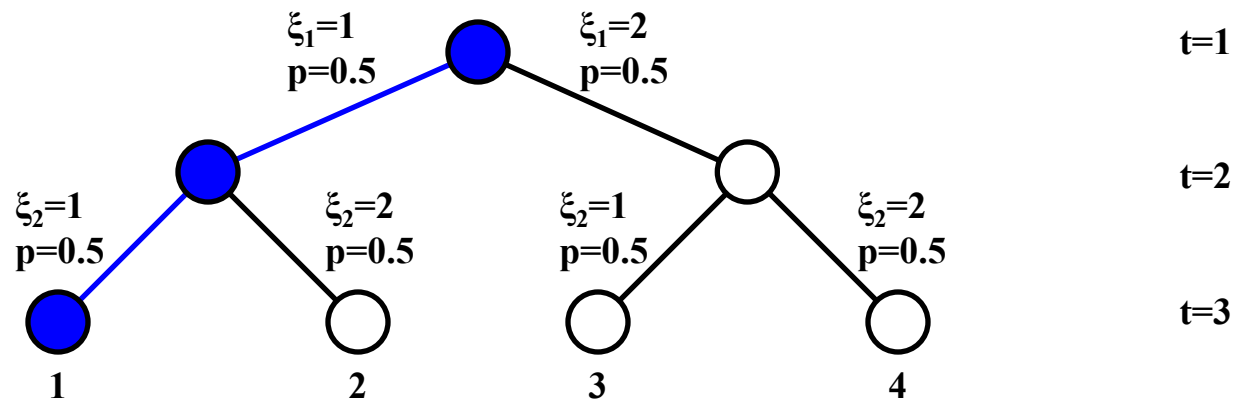
scenario
tree



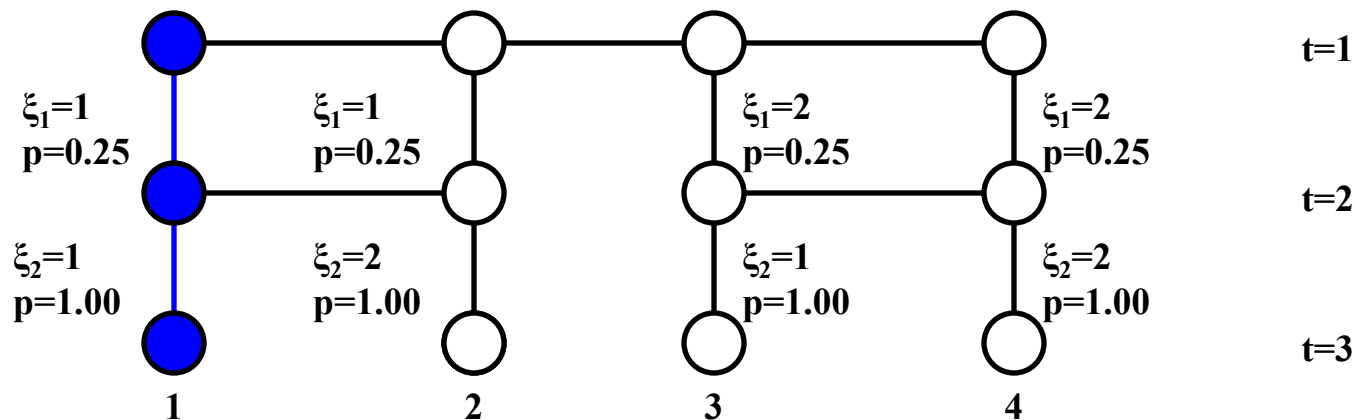
Alternative and equivalent scenario tree structure (Ruszczynski, 1997):



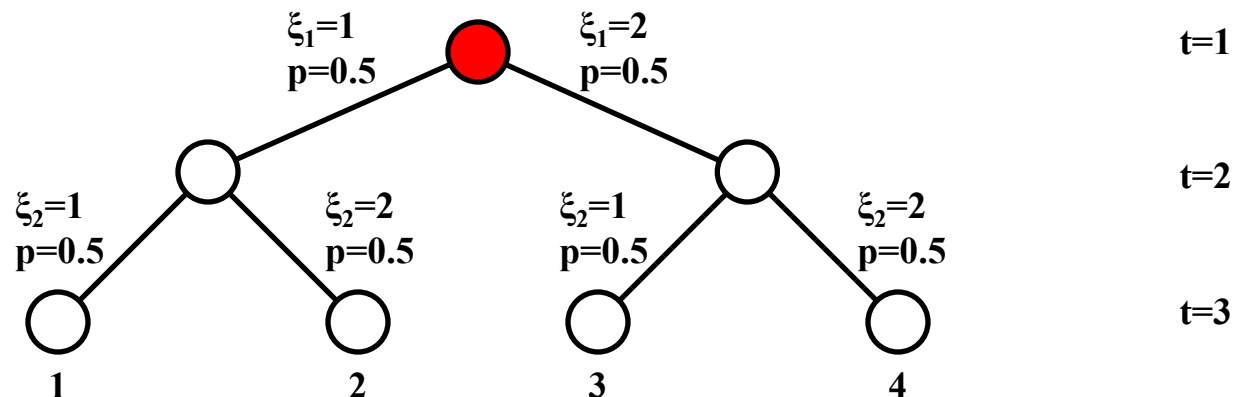
Stochastic Programming



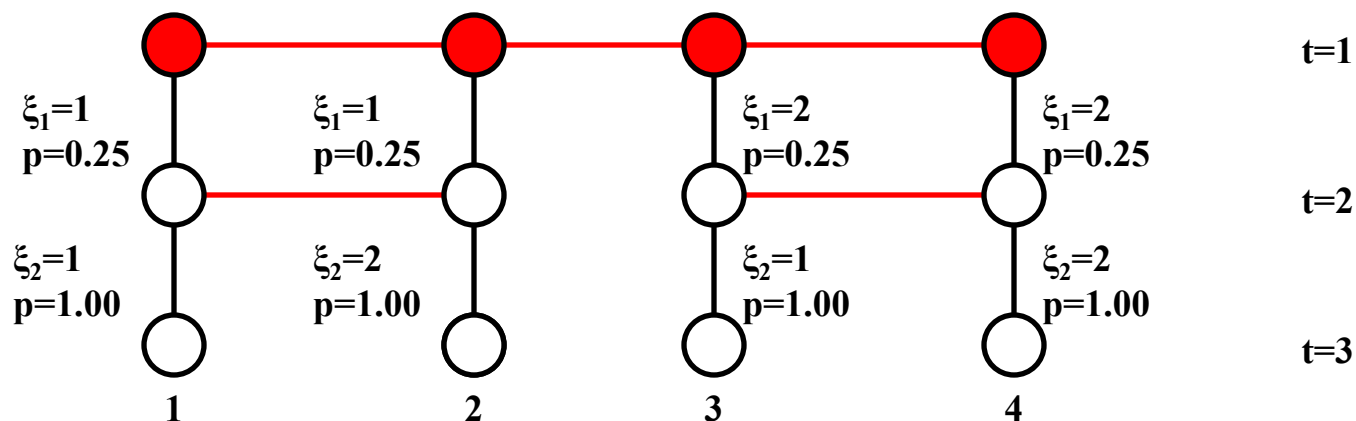
Each **scenario** is represented by a set of unique nodes



Stochastic Programming

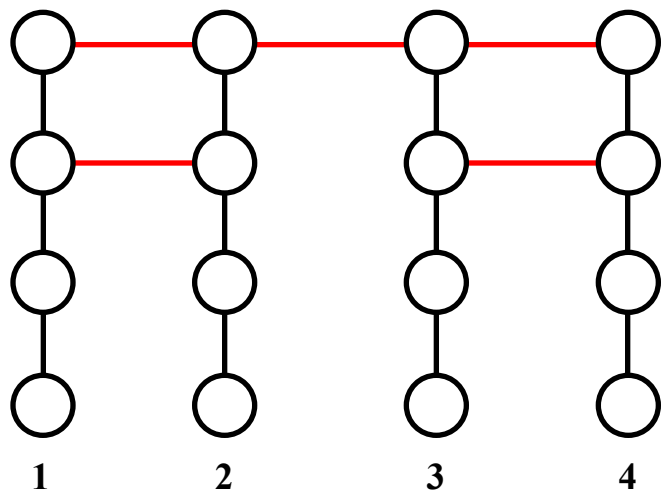
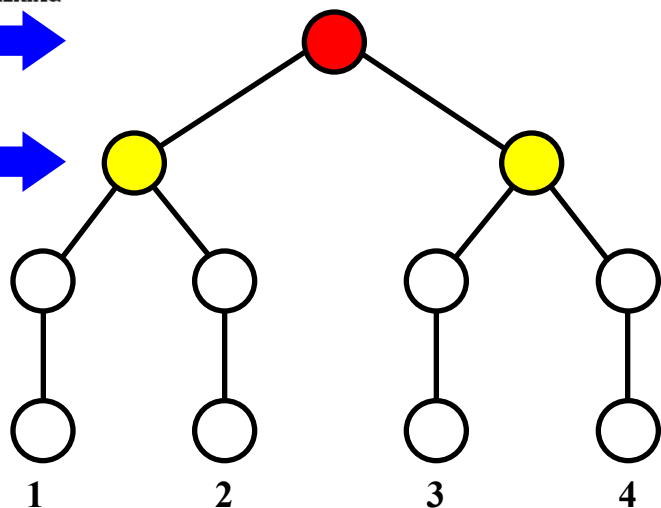


Nodes have **same amount of information** \equiv Nodes are **indistinguishable**



Non-anticipativity constraints

Representation of Decision-Dependence Using Scenario Tree

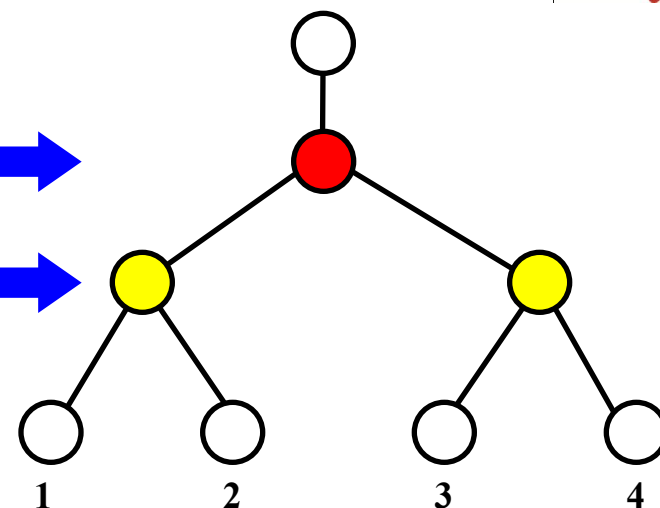


$t=1$

$t=2$

$t=3$

$t=4$

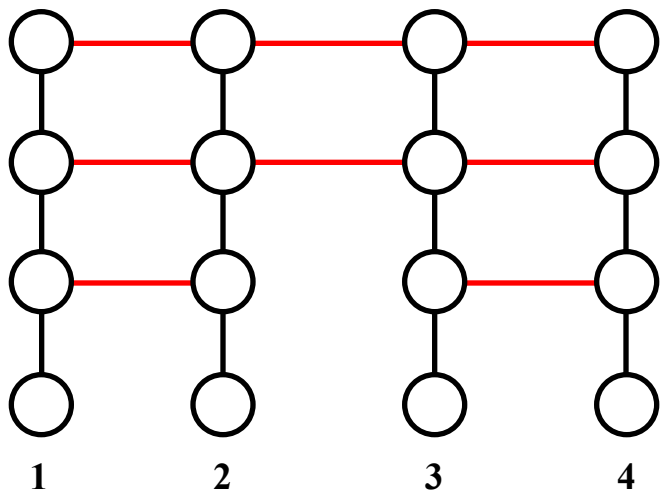


$t=1$

$t=2$

$t=3$

$t=4$



Multi-stage Stochastic Nonconvex MINLP

Maximize.. Probability weighted average of NPV over uncertainty scenarios
subject to

- Equations about economics of the model
 - Surface constraints
 - **Non-linear equations related to reservoir performance**
 - Logic constraints relating decisions
- if there is a TLP available, a TLP well can be drilled

**Every
scenario,
time period**

- **Non-anticipativity constraints**

*Non-anticipativity prevents a decision being taken now from
using information that will only become available in the future*

**Every pair
scenarios,
time period**

Disjunctions (conditional constraints)

**Problem size MINLP increases
exponentially with number of time periods
and scenarios**



**Decomposition algorithm:
*Lagrangean relaxation &
Branch and Bound***

MILP Branch and cut: Colvin, Maravelias (2008)

Formulation of Lagrangean dual

Relaxation

- Relax disjunctions, logic constraints
- Penalty for equality constraints

$b_{\lambda_{uf}^{s,s'}}, y_{\lambda^{s,s'}}, d_{\lambda^{s,s'}} :$

Lagrange Multipliers

$$\begin{aligned} \text{Max } \sum_s p^s & \left[\sum_t \left(c_{1t} q_t^s + c_{2t} d_t^s + c_{3t} y_t^s + \sum_{uf} c_{4t,uf} b_{uf,t}^s \right) \right] \\ & + \sum_{(s,s')} \left[\sum_{uf} b_{\lambda_{uf}^{s,s'}} (b_{uf,1}^s - b_{uf,1}^{s'}) + y_{\lambda^{s,s'}} (y_1^s - y_1^{s'}) + d_{\lambda^{s,s'}} (d_1^s - d_1^{s'}) \right] \\ & \sum_{\tau=1}^t (A_{\tau}^s q_{\tau}^s + B_{\tau}^s d_{\tau}^s + C_{\tau}^s y_{\tau}^s + \sum_{uf} D_{uf,\tau}^s b_{uf,\tau}^s) \leq a_t^s \quad \forall(t, s) \end{aligned}$$

$$\begin{aligned} & \left[\begin{array}{ccc} & Z_t^{s,s'} & \\ q_t^s & = & q_t^{s'} \\ d_{t+1}^s & = & d_{t+1}^{s'} \\ y_{t+1}^s & = & y_{t+1}^{s'} \\ b_{uf,t+1}^s & = & b_{uf,t+1}^{s'} \quad \forall uf \end{array} \right] \vee \left[\neg Z_t^{s,s'} \right] \quad \forall(t, s, s') \\ & Z_t^{s,s'} \Leftrightarrow \bigwedge_{uf \in \mathcal{D}(s,s')} \left[\bigwedge_{\tau=1}^t (\neg b_{uf,\tau}^s) \right] \quad \forall(t, s, s') \\ & b_{uf,1}^s = b_{uf,1}^{s'} \quad \forall(uf, s, s') \\ & d_1^s = d_1^{s'} \quad \forall(s, s') \\ & y_1^s = y_1^{s'} \quad \forall(s, s') \end{aligned}$$

One Reservoir Example

Optimize the planning decisions for an oilfield having **single reservoir** for **10 years**.

Decisions:

Number, capacity and installation schedule of FPSO/TLP facilities

Number and drilling schedule of sub-sea/TLP wells

Oil production profile over time

Uncertain Parameters (Discrete Values)	Scenarios							
	1	2	3	4	5	6	7	8
Initial Productivity <u>per</u> well (kbd)	10	10	20	20	10	10	20	20
Reservoir Size (Mbbbl)	300	300	300	300	1500	1500	1500	1500
Water Breakthrough Time Parameter	5	2	5	2	5	2	5	2

Wells are drilled in groups of 3.

Maximum number of 12 sub-sea wells per year can be drilled.

Maximum of 6 TLP wells per year per TLP facility can be drilled.

Maximum of 30 TLP wells can be connected to a TLP facility.

Construction Lead Time (years)	Wells		Facilities		
	TLP	Sub-sea	TLP	Small FPSO	Large FPSO
	1	1	1	2	4

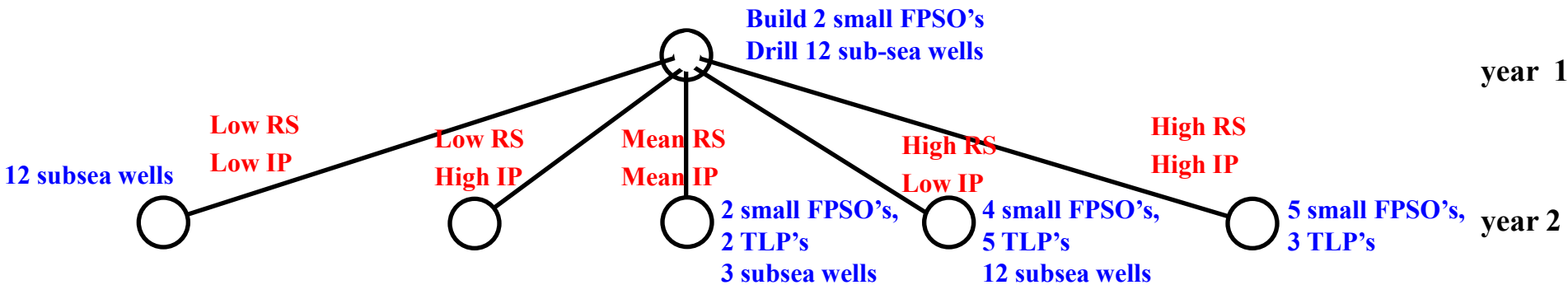
Multistage Stochastic Programming Approach

RS: Reservoir size

IP: Initial Productivity

BP: Breakthrough Parameter

$$E[NPV] = \$4.92 \times 10^9$$



Solution proposes building **2** small FPSO's in the first year and then add new facilities / drill wells (**recourse action**) depending on the positive or negative outcomes.

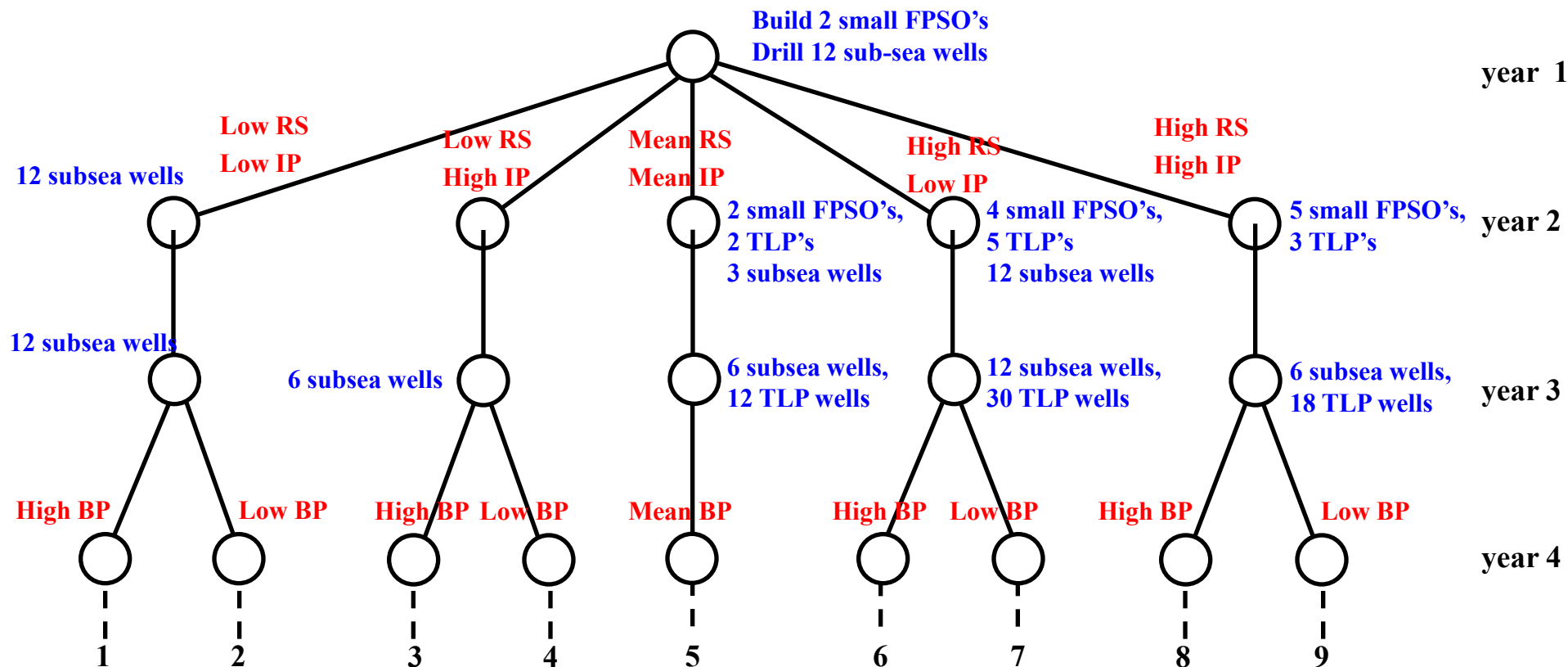
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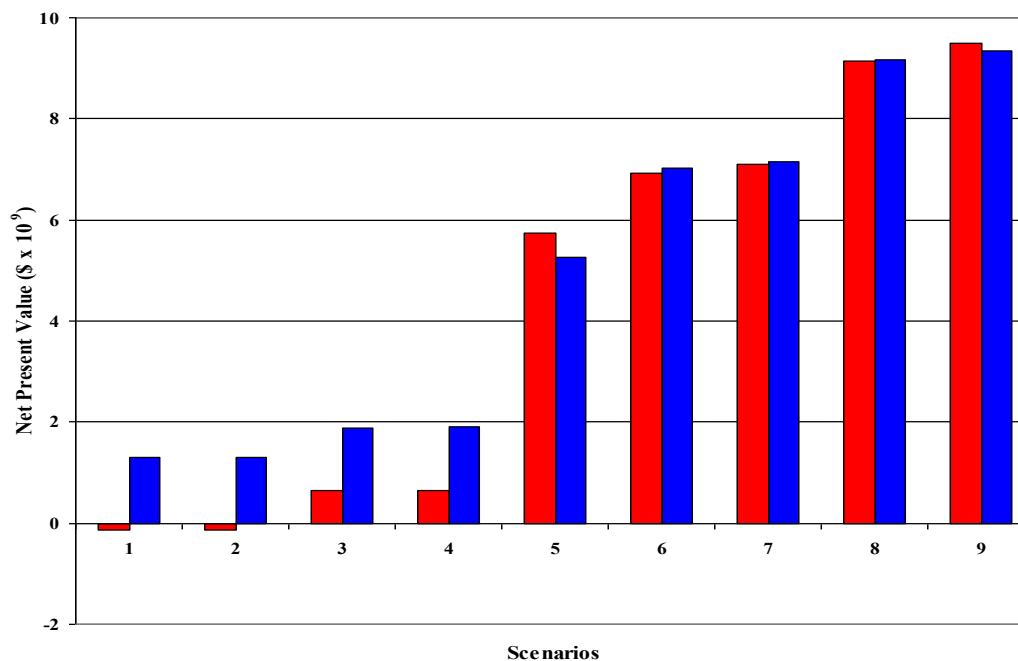
BP: Breakthrough Parameter

$$E[NPV] = \$4.92 \times 10^9$$



Solution proposes building **2** small FPSO's in the first year and then add new facilities / drill wells (**recourse action**) depending on the positive or negative outcomes.

Distribution of Net Present Value



Deterministic Mean Value = \$4.38 x 10⁹



Multistage Stoch Progr = \$4.92 x 10⁹ => 12% higher and more robust

Computation: Algorithm 1: 120 hrs; Algorithm 2: 5.2 hrs

Nonconvex MINLP: 1400 discrete vars, 970 cont vars, 8090 Constraints

Conclusions

1. Effective solution of **nonconvex MINLP and GDP** requires tight lower bounds

Global optimization optimal water networks

2. **Energy and water optimization** yields sustainable designs of biofuel plants

Optimization predicts lower energy and water targets

3. **Robustness** can be effectively introduced with stochastic programming

Design of responsive supply chains, Multistage stochastic in oilfields