

Challenges in the Application of Mathematical Programming Approaches to Enterprise-wide Optimization of Process Industries

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UTC Institute for Advanced Systems Engineering University of Connecticut – School of Engineering May 8, 2017



Motivation for Enterprise-wide Optimization

Global chemical/petrochemical industry

Strong international competition process industry Pressure for reducing costs, inventories and ecological footprint

⇒ **Major goal:** Enterprise-wide Optimization

At interface with Operations Research and Industrial Engineering

A major challenge: optimization models and solution methods

Enterprise-wide Optimization (EWO)



EWO term coined at FOCAPO-2003 (Marco Duran)

EWO involves optimizing the operations of R&D, material supply, manufacturing, distribution of a company to <u>reduce costs</u>, inventories, <u>ecological</u> footprint and to maximize profits, responsiveness.

Key element: Supply Chain

Example: petroleum industry







Trading



Transfer of Crude



Refinery Processing



Products









Pump



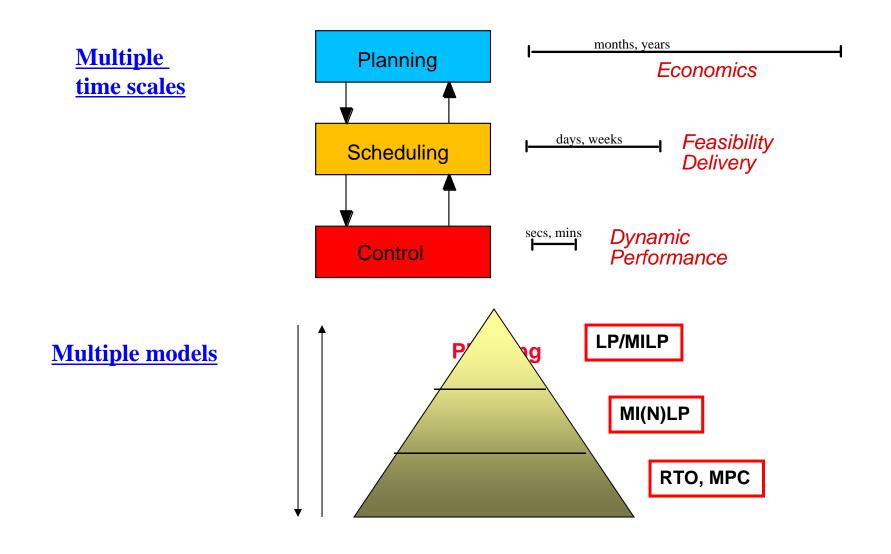
Transfer of Products

Terminal Loading



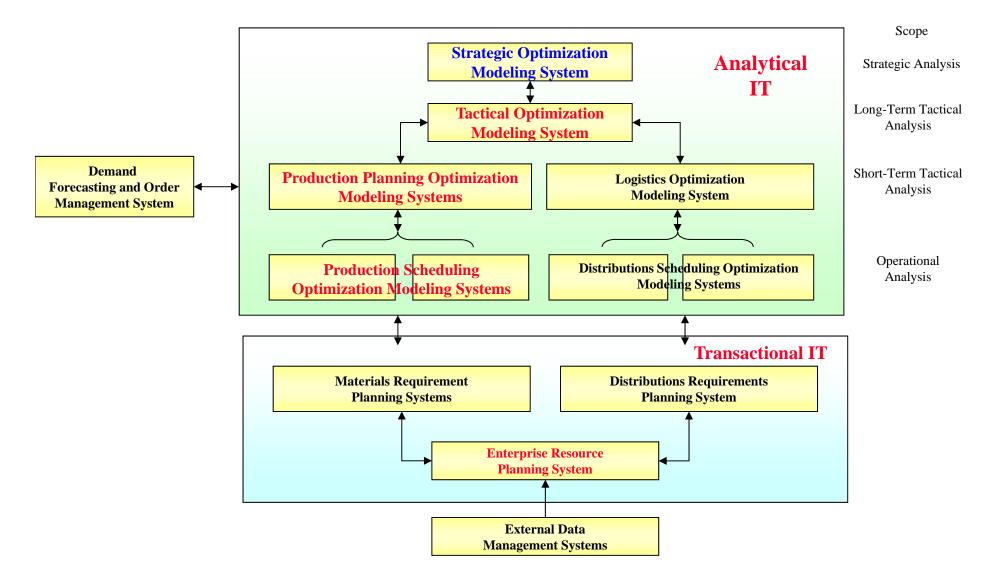
I. Integration of planning, scheduling and control

Key issues:



II. Integration of <u>information and models/solution</u> methods





Source: Tayur, et al. [1999]



Optimization Modeling Framework: Mathematical Programming

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

MINLP: Mixed-integer Nonlinear Programming Problem

Linear/Nonlinear Programming (LP/NLP)

 $\min Z = f(x)$ s.t. h(x) = 0 $g(x) \le 0$

 $x \in \mathbb{R}^n$

LP Codes: CPLEX, XPRESS, GUROBI, XA Very large-scale models Interior-point: solvable polynomial time

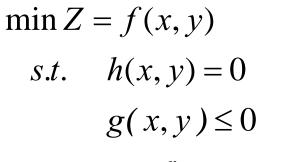
NLP Codes:

CONOPT Drud (1998) IPOPT Waechter & Biegler (2006) Knitro Byrd, Nocedal, Waltz (2006) MINOS Murtagh, Saunders (1995) SNOPT Gill, Murray, Saunders(2006) BARON Sahinidis et al. (1998) Couenne Belotti, Margot (2008) Global Optimization Large-scale models

Issues: Convergence Nonconvexities



Carnegie Mellon Mixed-integer Linear/Nonlinear Programming (MILP/MINLP)



$$x \in R^n, y \in \{0,1\}^m$$

MILP Codes: CPLEX, XPRESS, GUROBI, XA

Great Progress over last decade

MINLP Codes:

DICOPT (GAMS) Duran and Grossmann (1986) a-ECP Westerlund and Petersson (1996) MINOPT Schweiger and Floudas (1998) MINLP-BB (AMPL)Fletcher and Leyffer (1999) SBB (GAMS) Bussieck (2000) Bonmin (COIN-OR) Bonami et al (2006) FilMINT Linderoth and Leyffer (2006) BARON Sahinidis et al. (1998) Couenne Belotti, Margot (2008) Global Optimization New codes over last decade leveraging progress in MILP/NLP

Issues: Convergence Nonconvexities Scalability



Modeling systems

Mathematical Programming

GAMS (Meeraus et al, 1997)

AMPL (Fourer et al., 1995)

AIMSS (Bisschop et al. 2000)

1. Algebraic modeling systems => pure equation models

2. Indexing capability => large-scale problems

3. Automatic differentiation => no derivatives by user

4. Automatic interface with LP/MILP/NLP/MINLP solvers

Have greatly facilitated development and implementation of Math Programming models

Generalized Disjunctive Programming (GDP) $\min Z = \sum_{k} c_{k} + f(x)$



Raman, Grossmann (1994)

Disjunctions

$$\bigvee_{j \in J_{k}} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \leq 0 \\ c_{k} = \gamma_{jk} \end{bmatrix} k \in K$$
$$\Omega(Y) = true$$
$$x \in R^{n}, c_{k} \in R^{1}$$
$$Y_{jk} \in \{ true, false \}$$

s.t. $r(x) \leq 0$

Logic Propositions Continuous Variables Boolean Variables

Codes: LOGMIP (GAMS-Vecchietti, Grossmann, 2005) **EMP** (GAMS-Ferris, Meeraus, 2010)

Other logic-based: Constraint Programming (Hooker, 2000) Codes: CHIP, Eclipse, ILOG-CP

Optimization Under Uncertainty

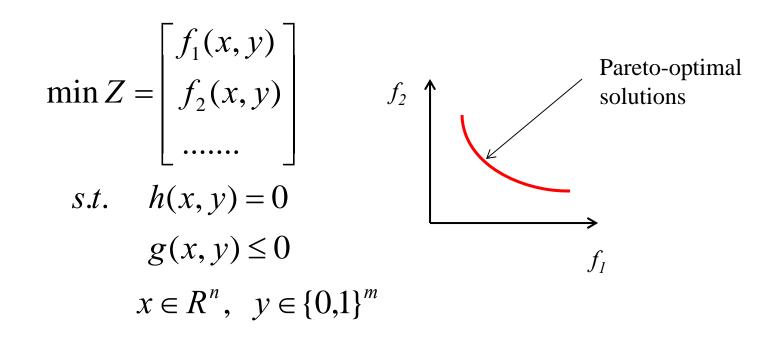


Multistage Stochastic Programming

Birge & Louveaux, 1997; Sahinidis, 2004



Multiobjective Optimization



ε-constraint method: Ehrgott (2000) Parametric programming: Pistikopoulos, Georgiadis and Dua (2007)

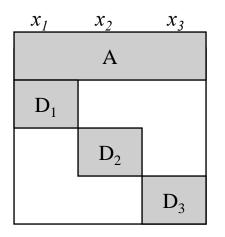
Decomposition Techniques



Lagrangean decomposition

Geoffrion (1972) Guinard (2003)

Complicating Constraints

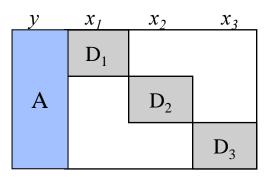


complicating constraints $\begin{array}{c}
\max c^{T}x \\
\hline st Ax = b \\
D_{i}x_{i} = d_{i} \quad i = 1, ..n \\
x \in X = \{x \mid x_{i}, i = 1, ..n, \mid x_{i} \ge 0\} \\
\hline
\end{array}$ Widely used in EWO

Benders decomposition

Benders (1962), Magnanti, Wing (1984)

Complicating Variables



complicating
variables
$$\max a^T y + \sum_{i=1,..n} c_i^T x_i$$
$$y + D_i x_i = d_i \quad i = 1,..n$$
$$y \ge 0, \ x_i \ge 0, \ i = 1,..n$$

Applied in 2-stage Stochastic Programming





http://egon.cheme.cmu.edu/ewocp/

Multidisciplinary team:

Chemical engineers, Operations Research, Industrial Engineering

Researchers:

Carnegie Mellon:

Ignacio Grossmann (ChE) Larry Biegler (ChE) Nick Sahinidis (ChE) John Hooker (OR) Nick Secomandi (Optns Mgmt)

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Overall Goal:

- Novel planning and scheduling models, including consideration of uncertainty
- Effective integration of <u>Production Planning, Scheduling and Real-time Optimization</u>
- Optimization of <u>Entire Supply Chains</u>



EWO Projects and case studies with partner companies

ABB:	Integrating RTN scheduling models with ISA-95 standard				
	Contact: Iiro Harjunkoski	Ignacio Grossmann, Pedro Castro			
Air Liquide:	Optimal Production of Industrial Gases with Uncertain Energy Prices				
_	Contact: Ajit Gopalakrishnan, Irene Lotero, Brian Besancon	Ignacio Grossmann, Carlos Mendez, Natalia Basan			
Aurubis:	Optimal Scheduling for Copper Concentrates Operations				
	Contact: Pablo Garcia-Herreros, Bianca Springub	Ignacio Grossmann, Brenno Menezes, Ynkkai Song			
Braskem:	Dynamic Optimization of Polypropylene Reactors				
	Contact: Rita Majewski, George Ostace	Larry Biegler, Bobby Balsom			
Dow:	Solution Strategies for Dynamic Warehouse Location und	ler Discrete Transportation Costs			
	Contact: John Wassick, Anshul Agrawal, Matt Bassett	Ignacio Grossmann, Braulio Brunaud			
Dow:	Optimization Models for Reliability-based Turnaround Pla	anning Integrated Sites			
	Contact: Satyajith Amaran, Scott Bury, J. Wassick	Nick Sahinidis, Sreekanth Rajagopalan			
Dow:	Parameter Estimation and Model Discrimination of Batch Solid-liquid Reactors				
	Contact: Mukund Patel, John Wassick	Larry Biegler, Yajun Wang			
ExxonMobil:	Optimal Design and Planning of Electric Power Networks				
	Contact: A. Venkatesh, D. Mallapragada, D. Papageorgiou	Ignacio Grossmann, Cristiana Lara			
Mitsubishi E.	Optimization circuitry arrangements for heat exchangers				
	Contact: Christopher Laughman, Arvind U. Raghunathan	Nick Sahinidis, Nick Ploskas			
P&G:	Kinetic Model Parameter Estimation for Product Stability	Contact: Ben Weinstein			
	Larry Biegler, Mark Daichendt				
Praxair:	Mixed-Integer Programming Models for Optimal Design of Reliable Chemical Plants				
	Contact: Jose Pinto, Sivaraman Ramaswam	Ignacio Grossmann, Yixin Ye			
Praxair:	Robust Tactical Planning of Multi-period Vehicle Routing				
	Contact: Jose Pinto, Arul Sundramoorthy	Chrysanthos Gounaris, Anirudh Subramanyam			
SKInnovation: Complex Crude-oil Refinery Scheduling Optimization					
T (1	Contact: Faram Engineer	Ignacio Grossmann, Brenno Menezes			
Total:	Integration of Reservoir Modeling with Oil Field Plannin				
	Contact: Meriam Chebre	Ignacio Grossmann, KinshukVerma			

Major Issues



- The multi-scale optimization challenge

- Linear vs Nonlinear models

- The uncertainty challenge

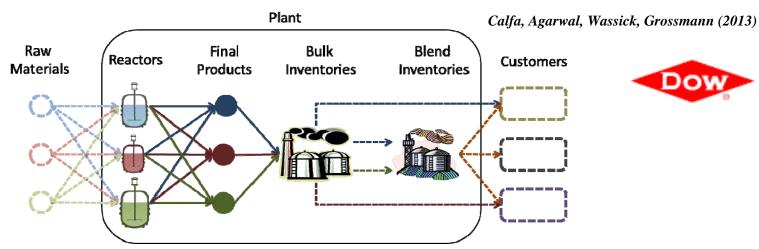
- Economics vs. performance



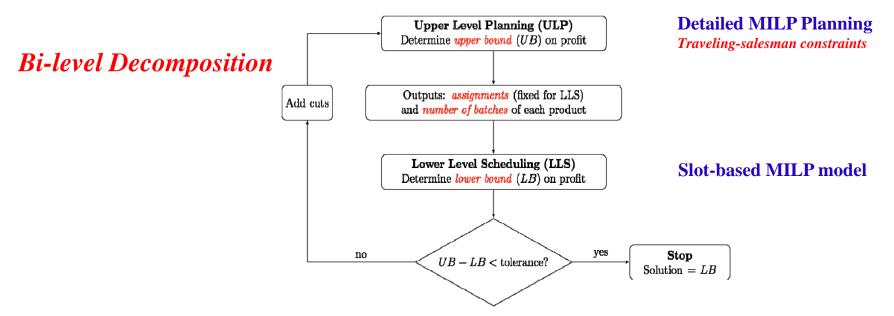
The multi-scale optimization challenge

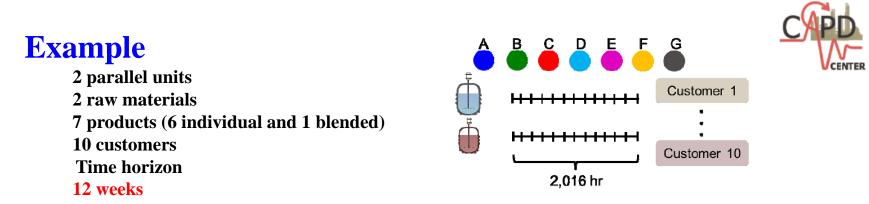
Integrated Planning and Scheduling Batch Plant

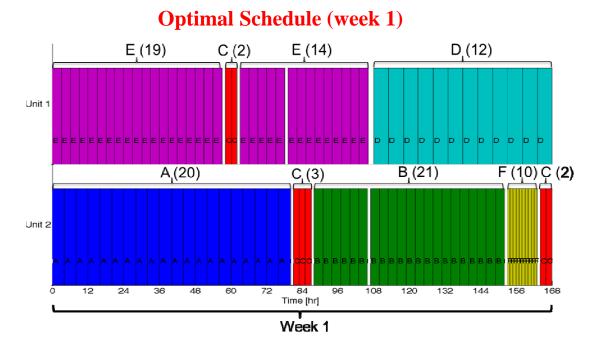




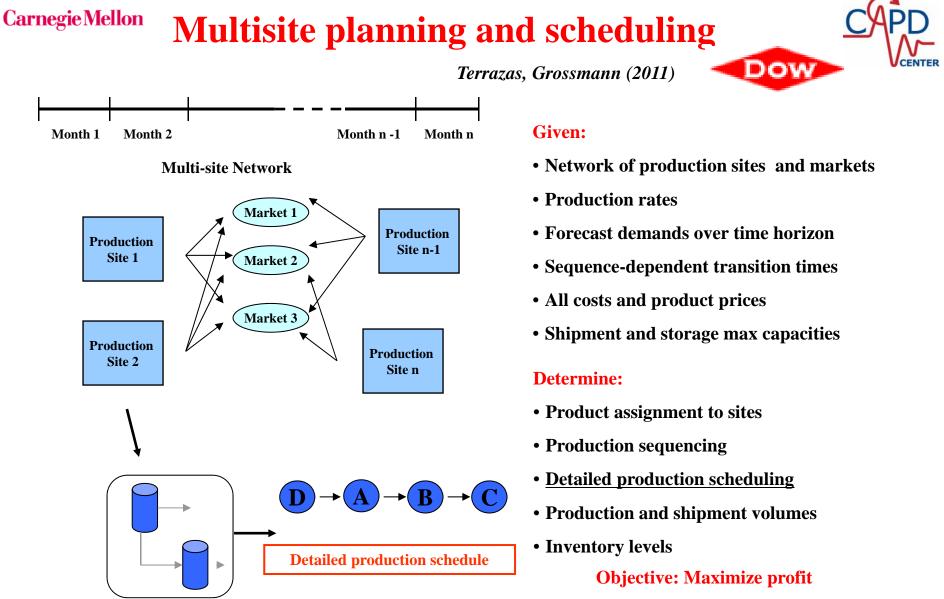
- Batch units operating in parallel
- Sequence-dependent changeovers between products groups
- A subset of products are blended







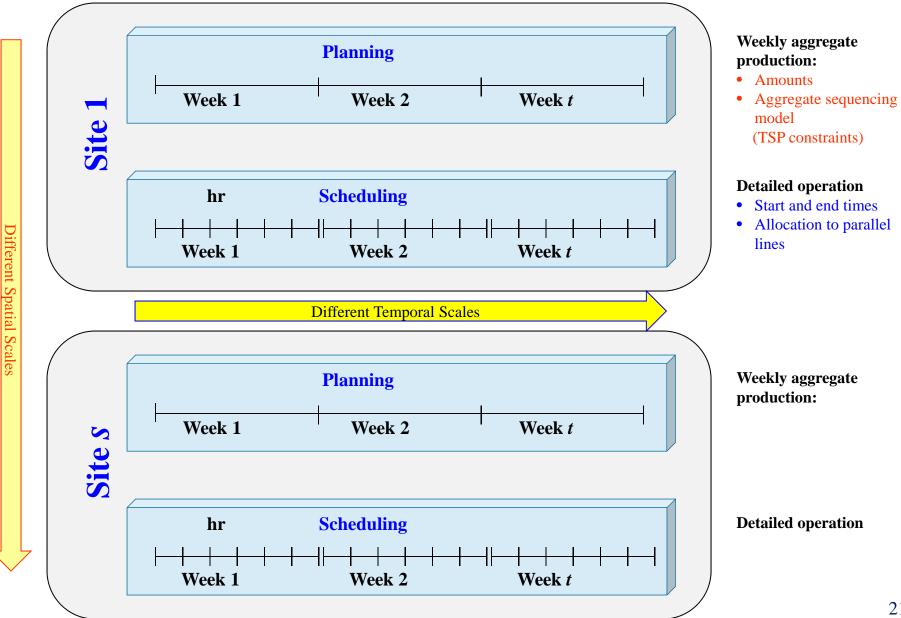
Bilevel decomposition converged in one iteration!Upper level MILP: 1,032 0-11,800 cont.v.3,300 constr.2.5 secLower level MILP: 19,600 0-123,100 cont.v.15,300 constr479 sec



- **Profit** = Sales
- Operating costs Inventory costs
- Distribution costs- Changeover costs

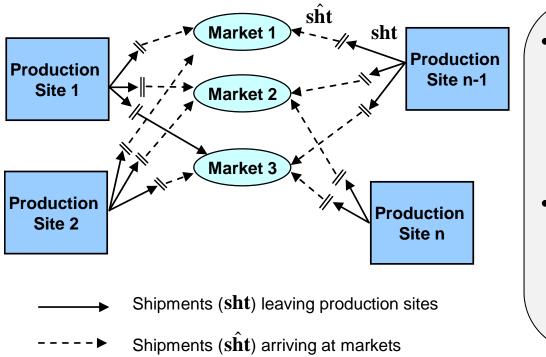
<u>Multi-site</u> planning and scheduling involves different temporal and spatial scales





Bilevel decomposition + Lagrangean decomposition





• Bilevel decomposition

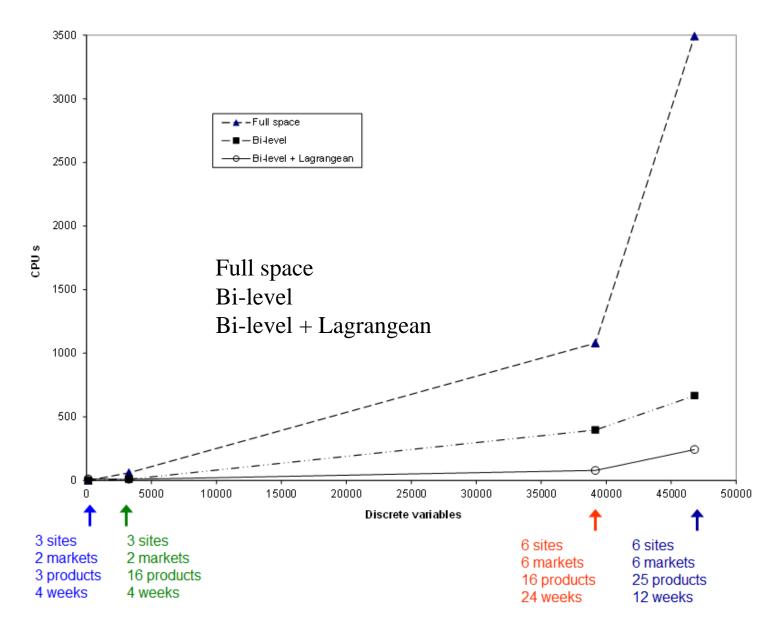
- Decouples planning from scheduling
- Integrates across temporal scale

Lagrangean decomposition

- Decouples the solution of each production site
- Integrates across spatial scale



Large-scale problems

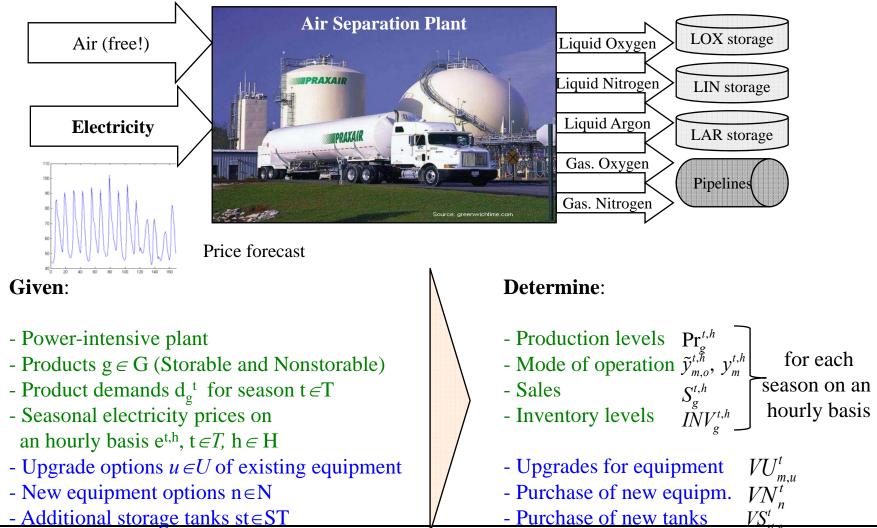




Optimal Multi-scale Capacity Planning under Hourly Varying Electricity Prices

Carnegie Mellon

Mitra, Grossmann, Pinto, Arora (2012)

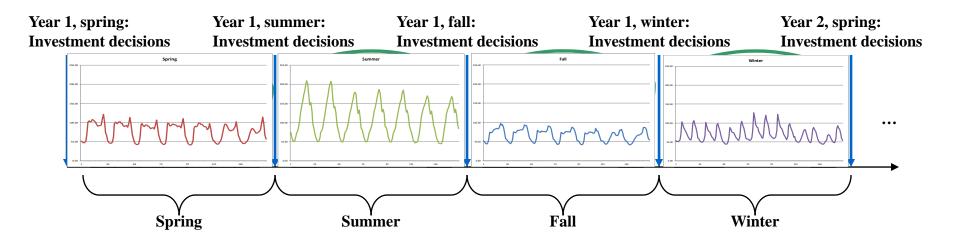


With minimum investment and operating costs



Incorporating design decisions: seasonal variations drive the development of a seasonal model

Carnegie Mellon



- 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

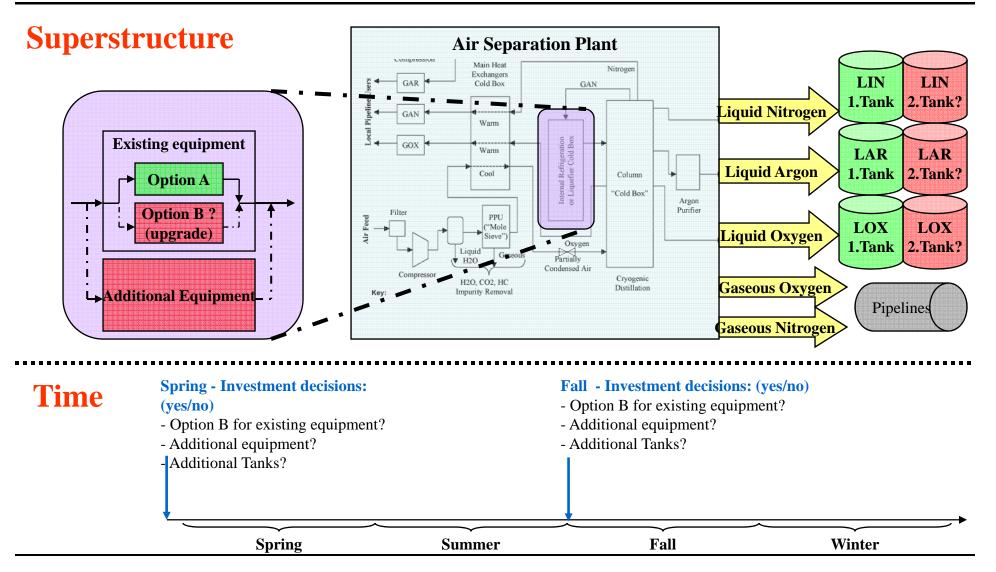
Carnegie Mellon

	$\min OBJ = \sum_{t} (Cost_{ops}^{t} +$	$Cost_{invest}^t$ (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 Additional equipment Idea: additional modes for which variables are controlled by the corresponding binary investment	Strategic Equipment replacement Idea: the corresponding mode has an alternative feasible region	Terms for the objective functi



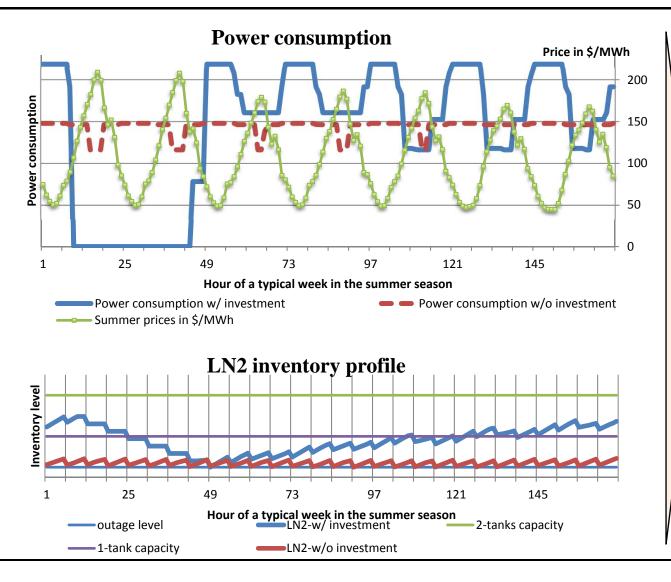
Retrofitting an air separation plant

Carnegie Mellon



- 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. Carnegie Mellon



Remarks on case study

- Annualized costs: \$5,700k/yr
- Annualized savings: \$400k/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%.

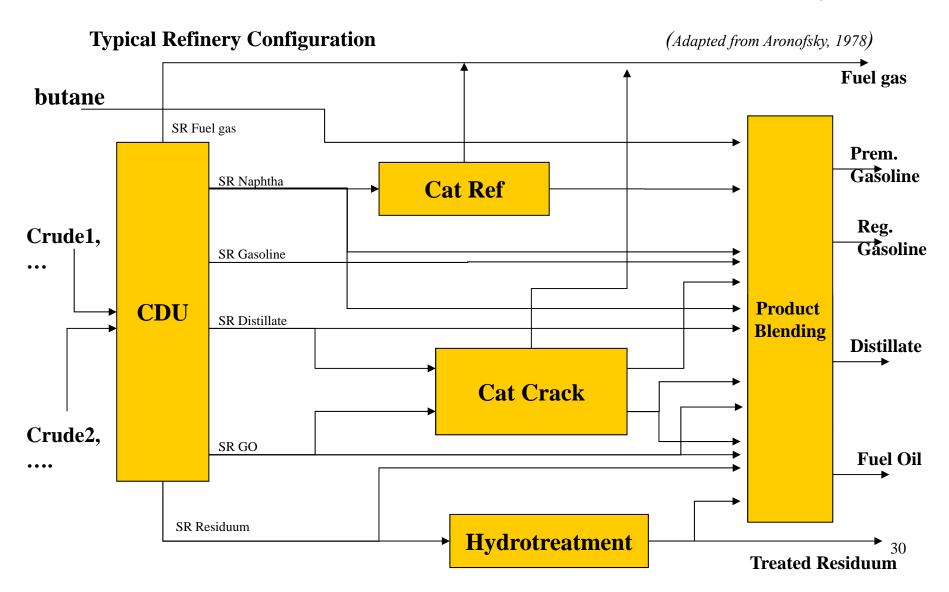
Source: CAPD analysis; Mitra, S., I.E. Grossmann, J.M. Pinto and Nikhil Arora, "Integration of strategic and operational decision- making for continuous power-intensive processes", submitted to ESCAPE, London, Juni 2012



Linear vs. Nonlinear

Nonlinear CDU Models in Refinery Planning Optimization

Alattas, Palou-Rivera, Grossmann (2010)



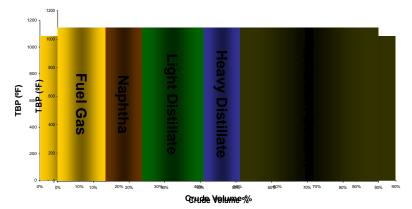


Refinery Planning Models



LP planning models

Fixed yield model Swing cuts model



Nonlinear FI Model (*Fractionating Index*)

- □ FI Model is crude independent
 - FI values are characteristic of the column
 - FI values are readily calculated and updated from refinery data
- □ Avoids more complex, nonlinear modeling equations
- **Generates cut point temperature settings for the CDU**
- □ Adds few additional equations to the planning model



Planning Model Example Results

Crude1	Louisiana	Sweet	Lightest
Crude2	Texas	Sweet	
Crude3	Louisiana	Sour	
Crude4	Texas	Sour	Heaviest

□ Comparison of *nonlinear fractionation index (FI)* with the fixed yield (FY) and swing cut (SC) models

□ Economics: <u>maximum profit</u>

FI yields highest profit

	Model	Case1	Case2	Case3
\longrightarrow	FI	245	249	247
	SC	195	195	191
	FY	51	62	59



Model statistics LP vs NLP

- □ FI model larger number of equations and variables
- □ Impact on solution time
- □ ~30% nonlinear variables

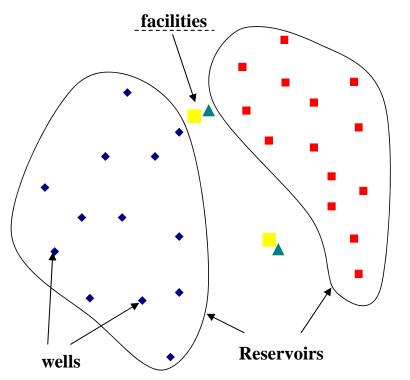
	Model	Variables	Equations	Nonlinear Variables	CPU Time	Solver
	FY	128	143		0.141	
2 Crude	SC	138	163		0.188	CPLEX
Oil Case	FI	1202	1225	348	0.328	CONOPT
3 Crude Oil Case	FY	159	185		0.250	CPLEX
	SC	174	215		0.281	
UII Case	FI	1770	1808	522	0.439	CONOPT
4 Crude Oil Case	FY	192	231		0.218	CPLEX
	SC	212	271		0.241	UPLEA
	FI	2340	2395	696	0.860	CONOPT



Optimal Development of Oil Fields (deepwater)

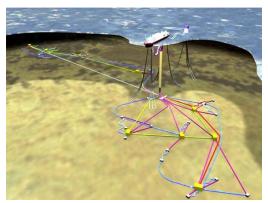


Offshore field having several reservoirs (oil, gas, water)



FPSO (Floating Production Storage Offloading)





Gupta, Grossmann (2011)

ExonMobil

Decisions:

>Number and capacity of FPSO facilities

>Installation schedule for facilities

>Number of sub-seawells to drill

>Oil/gas production profile over time

Objective:

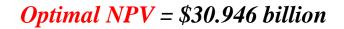
Maximize the Net Present Value (NPV) of the project

MINLP model

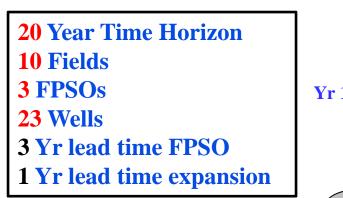
- Nonlinear reservoir behavior
- Three components (oil, water, gas)
- Lead times for FPSO construction
- FPSO Capacity expansion
- Well Drilling Schedule

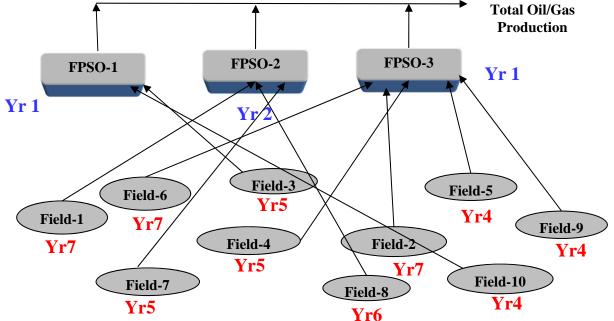


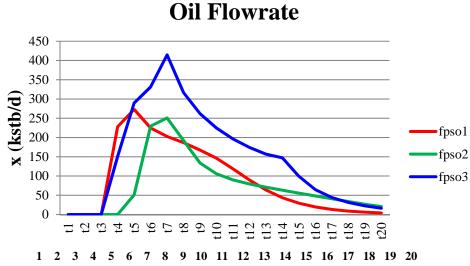
Example











	MINLP	Reformulated MILP
Discrete Var.	483	863
SOS1 Var.	0	800
Continuous Var.	5,684	12,007
Constraints	9,877	17,140
Solver	DICOPT 2x-C	CPLEX 12.2
NPV (billion dollars)	30.946	30.986 (<10% gap)
CPU time(s)	67	16,295



The uncertainty challenge

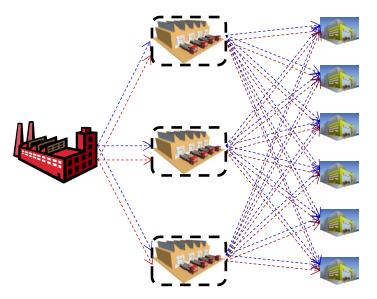
Carnegie Mellon Resilient Supply Chain Design

Garcia-Herreros, Grossmann, Wassick (2014)

Given:

cost by:

- Reliable plant
- Candidate locations for DCs with *risk of disruption*
- Set of customer with deterministic demands for multiple commodities
- Set of *scenarios and their associated probabilities*

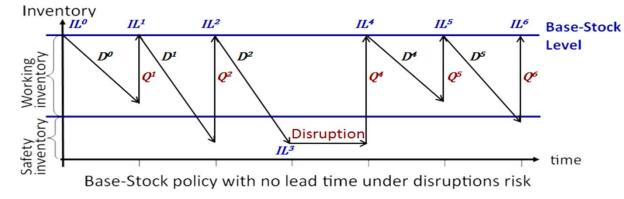


Dow

- Minimize Selecting DCs locations
 - Determining storage capacity for each commodity in selected DCs
 - Allocating demands in every scenario

Carnegie Mellon Distribution Strategy Disruptions give rise to scenarios dh. and the second s Cires-(State DCs serve different customers in different scenarios

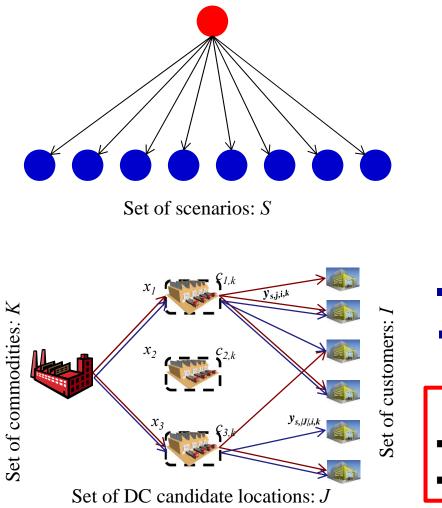
Rerouting produces a stochastic demand on DCs



1. Snyder L. V.; Shen, Z-J. M. Fundamentals of Supply Chain Theory; John Wiley & Sons: Hoboken (NJ), 2011. pp. 63-116.

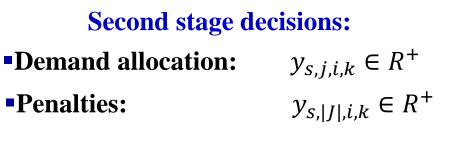
Carnegie Mellon Two-Stage Stochastic Programming





First stage decisions:

DC selection: $x_j \in \{0,1\}$ **DC capacities:** $c_{j,k} \in R^+$



Objective:

- Investment cost
- Expected cost of distribution

1. Birge, J.; Louveaux, F. V. Introduction to stochastic programming (2nd Ed.); Springer: New York (NY), 2011.



Industrial Instance



Supply chain network optimization:

- 1 Production plant
- 29 candidate DCs with disruption probabilities between 0.5% and 3%
- 110 customers
- 61 commodities

Total number of scenarios: $2^{29} \approx 537$ million

		Deterministic	Reduced problem	Reduced problem
		problem	1	2
Dolovont oot of	Number of scenarios	1	30	436
Relevant set of	Max. number of simultaneous disruptions	0	1	2
scenarios	Probability of scenarios	50.3%	85.4%	98.5%
Expected costs	Investment (MM \$)	18.47	18.78	21.56
for scenario set	Total (MM \$):	34.09	48.68	53.85
	Optimality gap for scenario set	0%	0.44%	0.87%
Solution	Full problem upper bound	57.40	56.32	55.89
	Full problem lower bound	48.15	52.43	53.81
	No. of constraints	11,849	304,256	4,397,984
Computational	No. of continuous variables	10,080	251,186	3,626,670
statistics	No. of binary variables	29	29	29
	Solution time	0.1 min	289 min ^a	7,453 min ^a

^a: Strengthened Benders multi-cut

Carnegie Mellon

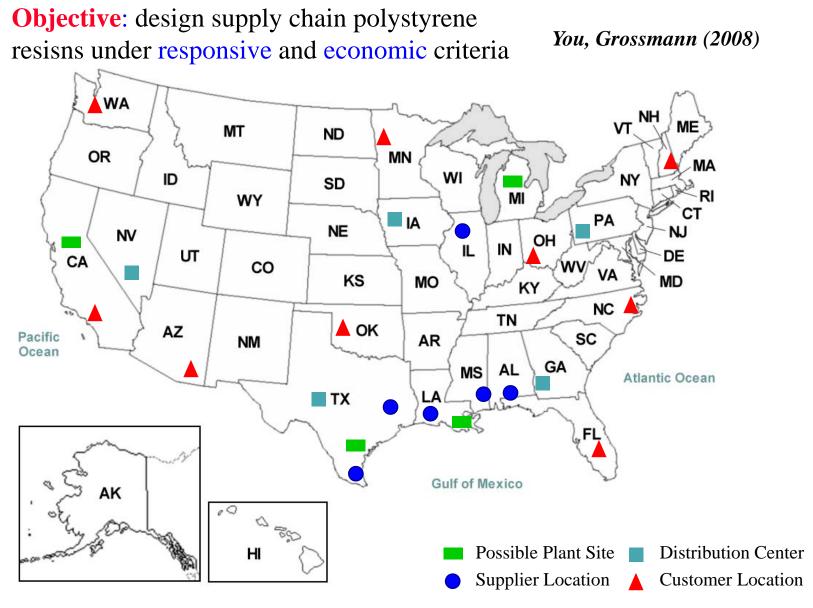


Economics vs. performance?

Multiobjective Optimization Approach

Bi-level optimization

Carnegie Mellon Optimal Design of Responsive Process Supply Chains



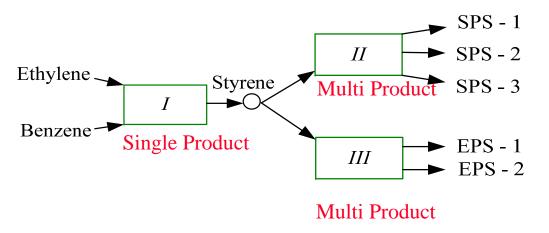


Production Network of Polystyrene Resins

Three types of plants:

- Plant *I*: *Ethylene* + *Benzene* \longrightarrow *Styrene* (1 products)
- Plant *II*: *Styrene* \longrightarrow *Solid Polystyrene (SPS)* (3 products)
- Plant *III*: *Styrene Expandable Polystyrene (EPS)* (2 products)

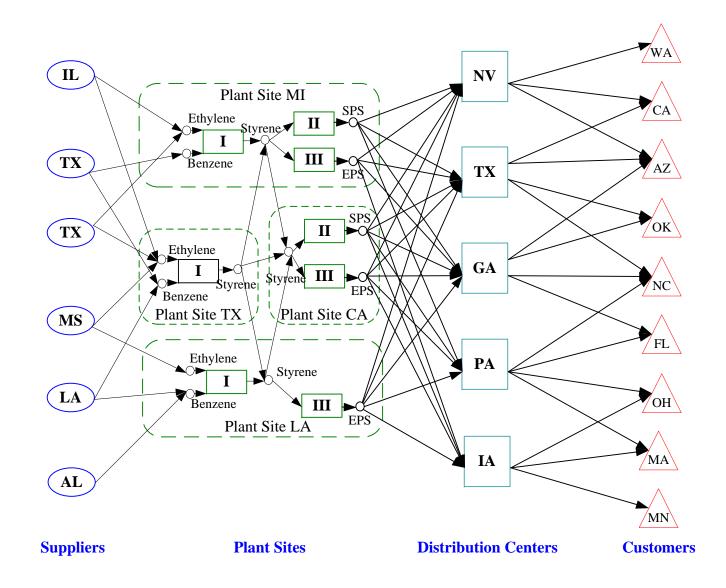
Basic Production Network



Carnegie Mellon

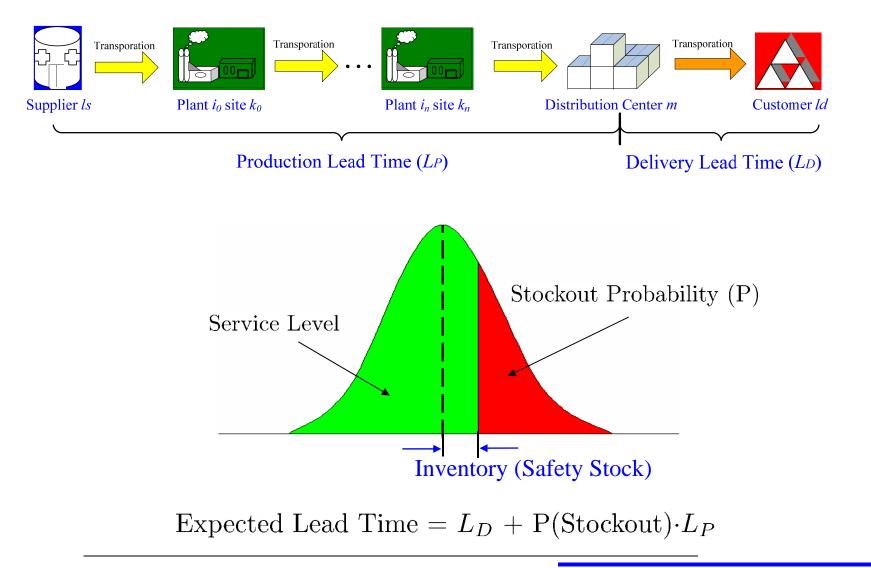
Potential Network Superstructure







Lead Time under Demand Uncertainty





Bi-criterion Multiperiod MINLP Formulation

Bi-criterion

Choose Discrete (0-1), continuous variables

- Objective Function:
 - Max: Net Present Value
 - Min: Expected Lead time
- Constraints:
 - Network structure constraints



Suppliers – plant sites Relationship Plant sites – Distribution Center Input and output relationship of a plant Distribution Center – Customers Cost constraint

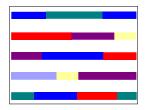
Operation planning constraints



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



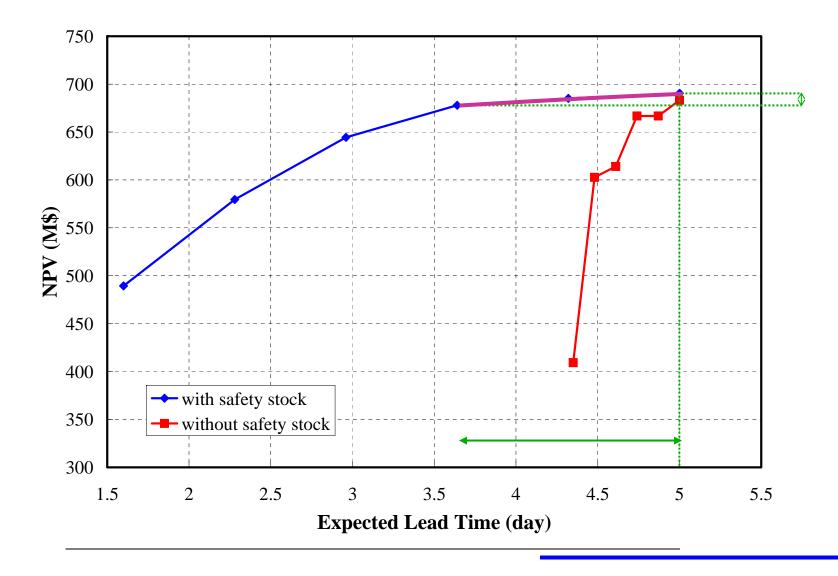
Probabilistic constraints

Chance constraint for stock out (reformulations)



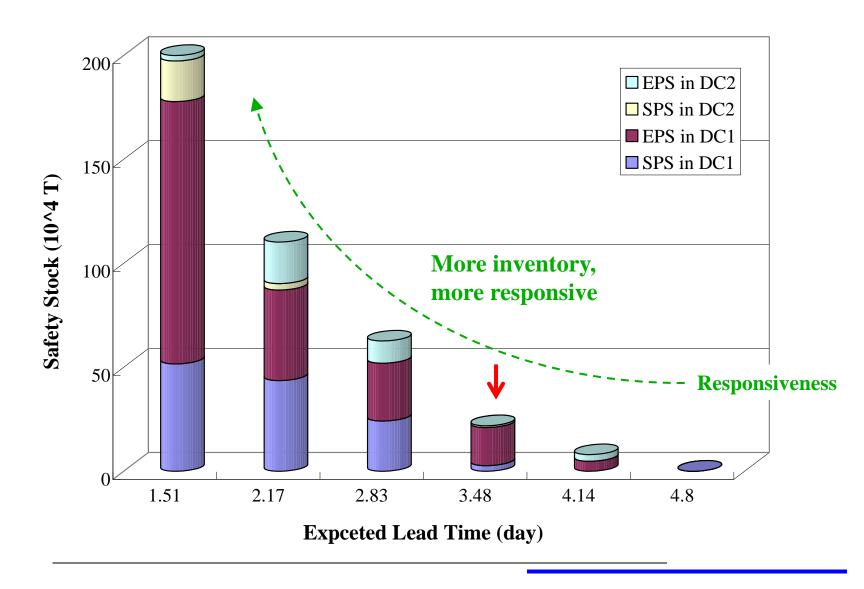


Pareto Curves – with and without safety stock





Safety Stock Levels - Expected Lead Time





Bi-level Optimization for Capacity Planning in Industrial Gas Markets

Motivation

Industrial gas markets are dynamic:

- Suppliers must anticipate demand growth
- Most markets are served locally

Capacity expansion is a major strategic decision:

- Requires large investment cost
- Benefits are obtained over a long horizon

Benefits are sensitive to market behavior:

- Market preferences
- Economic environment

Sensitivity can be reduced by assuming rational behavior:

- Producers try to maximize their profit
- Markets try to minimize their cost

Need to model the conflicting interests of producer and markets





Bilevel optimization







Problem Statement



Given:

- Set of capacitated plants and candidate locations for new plants from leading supplier
- Set of plants from independent suppliers with limited capacity
- Rational markets that select their suppliers according to their own objective function
- Deterministic demands over the time horizon

Maximize net present value (NPV):

- Determine expansion plan
- Considering optimal distribution strategy in each time-period





Bilevel Approach (MILP)



Capacity expansion planning with rational market:

Plants are divided in two: plants from leading supplier (I^1) and plants from independent suppliers (I^2)

max	$NPV = \sum_{t \in T} \frac{1}{(1+R)^{t}} \left\{ \sum_{i \in I^{1}} \sum_{j \in J} P_{t,i,j} y_{t,i,j} - \sum_{i \in I^{1}} \right\}$	$\left[A_{t,i}v_{t,i} + B_{t,i}w_{t,i} + E_{t,i}x_{t,i}\right]$	$x_{t,i} + \sum_{j \in J} \left(E_{t,i} y_{t,i,j} + G_{t,i,j,k} y_{t,i,j} \right) \right\}$
s.t.	$w_{t,i} = V_{t,i}^o + \sum_{t'=1}^t v_{t,i}$	(∀t ∈ T, i ∈ I ¹)	Invest in new plants
	$x_{t,i} \le w_{t,i}$	(∀t ∈ T, i ∈ I ¹)	Expand only open plants
	$c_{t,i} = C_{t,i}^{o} + \sum_{t'=1}^{t} H x_{t-1,i}$	(∀t ∈ T, i ∈ I¹)	Capacity expansion
	$\min \sum_{t \in T} \frac{1}{(1+r)^t} \left[\sum_{j \in J} \sum_{i \in I} P_{t,i,j} y_{t,i,j} \right]$		
	s.t. $\sum_{j \in J} y_{t,i,j} \le c_{t,i}$	(∀t ∈ T, i ∈ I ¹)	Markets minimize cost paid
	$\sum_{j\in J} y_{t,i,j} \le C_{t,i}$	(∀t ∈ T, i ∈ I ²)	Capacity of plants from leader
	$\sum_{i \in I} y_{t,i,j} = D_{t,j}$	(∀t ∈ T, j ∈ J)	Capacity of independent plants
	$c_{j,k}, y_{s,j,i,k} \ge 0; v_{t,i}, w_{t,i}, x_j \in \{0,1\}$	(∀t∈T,i∈I,j∈J)	All markets are satisfied



Illustrative Example



Problem structure:

- 3 existing plants which can be expanded
- 1 new candidate plant
- 3 existing plants which can not be expanded
- 15 markets with deterministic demand for 1 commodity
- 20 time-periods (quarters)

Formulations:

- Single-level (SL): leader selects the markets to satisfy
- Single-level evaluation (*SL-eval*): evaluation of single-level investment decisions in a market driven environment
- Bilevel KKT (*KKT*): KKT reformulation of the bilevel problem
- Bilevel Primal-Dual (*P-D*): Primal-dual reformulation of the bilevel problem









Computational statistics:

Statistics	SL	SL-eval	KKT	P-D
No. of constraints:	680	520	8,460	4,380
No. of continuous variables:	2,240	2,240	6,060	4,220
No. of binary variables:	240	0	3,080	240
Solution time (CPLEX):	0.10 s	0.02 s	193 s	5.72 s
Optimality gap:	0.1%	0.1%	0.1%	0.1%
Results:				
Items of objective function	SL	SL-eval	KKT	P-D
Income from sales [MM\$]:	1,171	805	794	794
Investment in new plants [MM\$]:	0	0	0	0
Capacity expansion cost [MM\$]:	199	199	58	58
Maintenance cost[MM\$]:	94	94	94	94
Production cost[MM\$]:	424	292	279	279
Transportation cost[MM\$]:	14	8	9	9
Total NPV [MM\$]:	440	212	354	354
Market cost[MM\$]:	1,239	1,234	1,234	1,234

Bilevel optimization yields **67% higher NPV (354** *vs* **212 million)** when compared to single-level expansion strategy



- **1. Enterprise-wide Optimization (EWO) of great industrial interest** *Great economic impact for effectively managing complex supply chains*
- **2. Mathematical Programming: major modeling framework**
- **3. Key components in EWO: Planning and Scheduling Modeling challenge:** *Multi-scale modeling (temporal and spatial integration) Linear vs. Nonlinear*

4. Computational challenges lie in:

a) Large-scale optimization models (decomposition, advanced computing)
b) Handling uncertainty (stochastic programming)